Topological Levinson's theorem via index pairings and spectral flow

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Declaration

I, Angus Stuart Alexander, declare that this thesis submitted in partial fulfilment of the requirements for the conferral of the degree Doctor of Philosophy (Mathematics), from the University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. This document has not been submitted for qualifications at any other academic institution.

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Abstract

Using techniques from noncommutative geometry, we explore how Levinson's theorem from scattering theory can be interpreted in a topological manner. We use low-energy resolvent expansions to deduce that the wave operator for short range scattering has a particular universal form. The wave operator does not have this form when certain obstructions occur in the resolvent expansions in even dimensions. Using the form of the wave operator, we apply index theoretic techniques to interpret Levinson's theorem as an index pairing between the K-theory class of the unitary scattering operator and the K-homology class of the generator of dilations on the half-line. A careful analysis of the trace class properties of the scattering operator allows us to provide new proofs of Levinson's theorem in all dimensions. We also compute the spectral flow for Euclidean Schrödinger operators, giving another new proof of Levinson's theorem in all dimensions.

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Contents

Chapter 1

Introduction

1.1 Motivation and history

The overall aim of this thesis is to investigate the topological nature of various aspects of scattering theory for Euclidean Schrödinger operators using techniques from noncommutative geometry and operator algebras. The results of this thesis build in particular on those of Kellendonk, Richard and Tiedra de Aldecoa [96, 97, 98, 140, 141, 142] who initiated the topological study of scattering systems with the observation that the wave operator is a Fredholm operator belonging to a particular C^*-algebra from which its index can be computed directly as a topological invariant.

Mathematical scattering theory has its origins in the physics experiments of the early 20th century, and is now a branch of operator theory devoted to the study of the spectrum of perturbations of self-adjoint linear operators acting on a Hilbert space. The development of scattering theory began with the introduction of the wave operators by Friedrichs [66, 67] and Møller [117], which sparked intense development of the rigorous theory of scattering in the next decades through the works of Kato, Kuroda, Cook, Jauch, Simon, Enss, Amrein, Birman and Kreĭn, to name a few.

Throughout this thesis, we will consider the pair of operators $H_0 = -\sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}$ and $H = H_0 + V$ acting on (some dense domain in) the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$. Here V is the operator of multiplication by a real function which decays sufficiently fast at infinity (see Assumption 2.2.14) and in some later results is required to be smooth as well. Given our assumptions the operator H_0 has no eigenvalues and the operator H has a finite number of eigenvalues. The absolutely continuous spectrum of H and H_0 given by $\sigma_{ac}(H) = \sigma_{ac}(H_0) = [0, \infty) =: \mathbb{R}^+$. When they exist the wave operators are partial isometries defined by

$$W_\pm = \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{itH}\mathrm{e}^{-itH_0}$$

and the unitary scattering operator is given by $S = W_+^* W_-$. Since the scattering operator commutes with H_0, there exists a family $(S(\lambda))_{\lambda\in\mathbb{R}^+}$ of unitary operators on $L^2(\mathbb{S}^{n-1})$ (here $\mathbb{S}^{n-1}$ is the unit sphere in $\mathbb{R}^n$). For each $\lambda \in \mathbb{R}^+$, $S(\lambda)$ is called the scattering matrix at energy λ.

The story for this thesis begins with the work of Levinson [108], who showed that in one dimension the number of eigenvalues N of H (counted with multiplicity) was related to the 'scattering phase' of the pair (H, H_0) by the formula

$$-N = \frac{1}{\pi}(\delta(\infty) - \delta(0)) + \frac{1}{2}M_R(0),$$

where δ is the scattering phase (given by the argument of the determinant of S) and $M_R(0)$ takes either the value zero or one. There are several interesting features to note here. The result is perhaps initially surprising, since scattering data is related to the continuous spectrum of H and eigenvalues to the discrete spectrum of H. This interplay between the discrete and continuous spectrum of H is indicative of the topological nature of Levinson's theorem. Secondly, there is a correction term $M_R(0)$, which can be shown to correspond to the existence of a 'resonance', namely a solution to the equation $H\psi = 0$ which is not square integrable. Such a correction term is only a feature in low dimensions.

Levinson's theorem was generalised several times in the intervening years. Firstly, Newton [123] showed in dimension $n = 3$ that the same relation holds for a spherically symmetric potential V, essentially by changing to polar coordinates and reducing to a one dimensional problem. For a general non-spherically symmetric potential in dimension $n = 3$, Levinson's theorem was proved by Bollé and Osborn [31], however their analysis excludes the exceptional case of the existence of a 'resonance'. To complete their analysis one needs knowledge of the spectral shift function at zero, as described by Newton [124], which contributes an extra $\frac{1}{2}$ to Levinson's theorem in the exceptional case. The analysis of Bollé and Osborn demonstrated that Levinson's theorem is sensitive to the high energy behaviour of the scattering matrix also, a feature which is present for all $n \geq 2$.

Jensen and Kato [88] initiated a study of the low-energy behaviour of the resolvent $R(z) = (H - z)^{-1}$ and in dimension $n = 3$ demonstrated that 'resonances' occur as obstructions to the invertibility of the operator $T(z) = \mathrm{Id} + R_0(z)V$ near $z = 0$, providing an explicit characterisation of resonances as distributional solutions ψ to the equation $H\psi = 0$ which are not square integrable but live in a weighted Sobolev space. Subsequently, Jensen showed [85] that no such obstructions can occur in dimension $n \geq 5$ and that in dimension $n = 4$ [87] the analysis is more involved and that resonances can occur, with an extra logarithmic singularity.

Bollé, Danneels, Gesztesy and Wilk [27, 26] showed that in two dimensions a form of Levinson's theorem holds, with an extra striking feature. In dimension $n = 2$, two kinds of 'resonances' can occur. In the spherically symmetric case, a resonance which behaves like an s-wave can occur and will not contribute to Levinson's theorem, and a resonance which behaves like a p-wave can also occur and contributes an integer to Levinson's theorem in the same way as an eigenvalue. The p-resonances behave in much the same way as resonances in dimension $n = 4$ due to the nature of the singularity at zero.

Jensen and Nenciu provide in [89] a systematic procedure for inverting an operator related to $T(z)$. The procedure of Jensen and Nenciu allows one to invert $T(z)$ by isolating the obstructions to invertibility into the range of a finite sequence of decreasing projections. The range of these projections can be characterised in terms of zero energy eigenvalues and zero energy resonances. In particular [89] provides a detailed expansion in the case $n = 2$ in a more tractable way than [26]. In Chapter 3 we describe this procedure in extensive detail in all dimensions.

In [96] Kellendonk and Richard observe that for scattering with a point interaction in dimensions $n = 1, 2, 3$, the wave operators are of a particular form which is amenable to index theoretic calculations. Kellendonk, Richard and Tiedra de Aldecoa [97, 98, 141] demonstrate that in dimension $n = 1, 3$ the wave operator is given by

$$W_- = \mathrm{Id} + \varphi(D_n)(S - \mathrm{Id}) + K, \tag{1.1}$$

with K a compact operator. Here $\varphi \in C_0(\mathbb{R}) \cap L^2(\mathbb{R})$ is a universal function (in the sense that it does not depend on the potential). For $x \in \mathbb{R}$, φ is given by

$$\varphi(x) = \frac{1}{2}(1 + \tanh{(\pi x)} - i\cosh{(\pi x)}^{-1})$$

and D_n is the self-adjoint generator of the dilation group on $L^2(\mathbb{R}^n)$. In fact the generator D_n of the dilation group plays a central role in scattering theory: it is used to provide a geometric proof of the existence and completeness of the wave operators in [58, 60, 128] and in proofs of the continuity of the scattering matrix [54]. For the index pairing we prove in Chapter 5, the fact that D_n and $\frac{1}{2}\ln{(H_0)}$ are canonically conjugate variables is essential.

Kellendonk and Richard further show that W_- lives in a C^*-algebra E generated by continuous functions of H_0 and D_n with limits at their endpoints. By considering the quotient of E by the ideal J of functions which vanish at their endpoints, the index of W_- can be computed as

$$\mathrm{Index}(W_-) = \mathrm{Wind}(q(W_-)), \tag{1.2}$$

where $\mathrm{Wind}(q(W_-))$ is the winding number of the image of W_- in the quotient E/J. In dimension $n = 1$ this winding number can be determined explicitly and one recovers the original Levinson's theorem [97]. In dimension $n = 3$, the high energy behaviour of the scattering matrix prevents the map $\mathrm{Det}(S(\cdot))$ from defining a loop. As a consequence, Equation (1.2) is not immediately comparable to the work of Bollé, Osborn and Newton, except that in the presence of a resonance an additional factor of $\frac{1}{2}$ is present in agreement with the work of Newton.

In dimension $n = 2$, Richard and Tiedra de Aldecoa show that a similar formula to Equation (1.1) holds with no resonances and in the presence of s-resonances in [142]. Again due to the high-energy behaviour of the scattering operator one cannot deduce immediately the statement of Levinson's theorem of Bollé et al in [26] from the index theoretic picture.

The original work in the present thesis begins at this point and is described in detail in the next section, where we outline the structure of the thesis and the main results.

1.2 Thesis structure and main results

This thesis is organised in the following way.

Chapter 2: The history of scattering theory is intimately linked with that of spectral and perturbation theory for linear operators and so the literature is extensive. Chapter 2 is thus a guided tour of selected topics from scattering theory necessary for understanding the rest of the thesis. In particular, this chapter contains no original results. We begin with an introduction to abstract scattering theory including the wave and scattering operators in Section 2.1 before specialising to perturbations of the Laplacian for the remainder of the thesis, beginning in Section 2.2. We also introduce the generator D_n of the dilation group on $L^2(\mathbb{R}^n)$, which defines the canonically conjugate variable to $\frac{1}{2}\ln(H_0)$.

After establishing the existence and completeness of the wave operators in Section 2.3, we discuss the limiting absorption principle in Section 2.4 and how it can be used to construct a stationary approach to scattering theory in terms of generalised eigenfunctions and Fourier transforms. Of particular interest is the scattering matrix, the stationary representation of the scattering operator. In Section 2.5 we introduce the time delay operator, the spectral shift function and their relationship to the well-known Levinson's theorem. In particular, we describe using heat kernel methods how the high-energy behaviour of the time delay operator and the spectral shift function give rise to Levinson's theorem.

Chapter 3: We demonstrate, using the methods of Jensen and Nenciu [89], a key technical tool in our later analysis of the wave operator. The results we present in this chapter are not new and can be found in various places throughout the literature which we cite as necessary. Decomposing the potential V into $V = vUv$ with $v(x) = |V(x)|^{\frac{1}{2}}$ and $U = \mathrm{sign}(V)$ we obtain an expansion of the inverse of the operator $M(k) = U + vR_0(-k^2)v$ for small k (with $R_0(-k^2) = (H_0 + k^2)^{-1}$). Such an expansion is highly sensitive to the fine structure of the spectrum of H near zero and is dependent on the dimension also. In dimension $n \leq 4$ there are obstructions to the invertibility of $M(k)$, which lead to a definition of zero energy resonances in each dimension. In dimension $n = 2$ the procedure is most difficult and we find two kinds of resonances. For dimension $n \geq 5$, general bounds on the resolvent show that there are no obstructions to the invertibility of the operator $M(k)$. The analysis is generally more complicated in even dimensions due to a logarithmic singularity of the integral kernel of $R_0(-k^2)$ at $k = 0$.

Chapter 4: We demonstrate under certain short-range decay assumptions on the potential V (see Assumption 4.3.1) that the wave operators W_- in dimension $n \geq 2$ have the same universal form as Equation (1.1). The original results in this chapter have appeared in [5] as joint work with Adam Rennie. In Section 4.1 we begin by determining the behaviour at zero of the scattering matrix in all dimensions. These results are well-known in dimension $n \leq 3$, however for $n \geq 4$ we have not found any statements in the literature. We find in Theorem 4.1.7 the new result that for all dimensions $n \geq 4$ the scattering matrix satisfies $S(0) = \mathrm{Id}$ always, with the case $n = 2$ having been established in [142, Theorem 1.1]. This contrasts the behaviour in dimension $n = 1, 3$ [29, 88], where the behaviour of the scattering matrix at zero is known to be sensitive to the presence of resonances.

In Section 4.2 we use the integral representation of the wave operator of Theorem 2.4.29 in terms of generalised eigenfunctions in Lemma 2.4.31 to provide intuition as to why the wave operators have the form of Equation (1.1). Unfortunately, the intuitive methods are not sensitive to the fine structure of the spectrum near zero demonstrated in Chapter 3 and thus are unable to be used to demonstrate the compactness of the remainder term except in dimension $n = 1$, as was the method of proof in [97].

The remainder of the chapter is devoted to a different approach to obtaining the form of the wave operator in the spectral representation. The approach we present has been used to determine the form of the wave operator in dimension $n = 3$ in [141]. In [140] and [142] in two dimensions in the case of no p-resonances the wave operator has been shown to be of a form similar to Equation (1.1) and we demonstrate in Section 4.3.2 the new result that Equation (1.1) holds in dimension $n = 2$ also, in the absence of p-resonances. In Section 4.3.3 we use the resolvent expansions of Chapter 3 to prove the new result that Equation (1.1) holds in all dimensions $n \geq 4$ also, with the exception of dimension $n = 4$ in the presence of resonances, following the technique outlined in [141].

Chapter 5: We show how the form of the wave operator established in Chapter 4 can be used to prove that Levinson's theorem is the result of an index pairing between the class $[D_+] \in K^1\left(C_0(\mathbb{R}^+) \otimes \mathcal{K}\left(L^2\left(\mathbb{S}^{n-1}\right)\right)\right)$ of the dilation operator and the class $[S] \in K_1\left(C_0(\mathbb{R}^+) \otimes \mathcal{K}\left(L^2\left(\mathbb{S}^{n-1}\right)\right)\right)$ of the unitary scattering operator. The index pairing in the generic case $S(0) = \mathrm{Id}$ has appeared in [5] as joint work with Adam Rennie. That Levinson's theorem is a topological result has been established in dimension $n = 1$ [97], $n = 2$ [140, 142] in the absence of p-resonances and $n = 3$ [98, 141].

The technique used in these references is to use the form of the wave operator to show that W_- is an element of a particular C^*-algebra generated by functions of the free

Hamiltonian H_0 and the generator of dilations D_n and to compute the index of the wave operator in the Calkin algebra obtained by taking the quotient by the functions which vanish at the endpoints of the spectrum of H_0 and D_n. In Section 5.1 we present these constructions in detail, as they play a key role later in Chapter 5.

In Section 5.2 we construct a family of Fredholm operators W_U indexed by a class of unitary operators U on $\mathcal{B}(\mathcal{H})$ which vanishes at 0 and ∞ in the spectral representation. The mapping $U \mapsto W_U$ is a new construction. In Theorem 5.3.2 we show that we can write the pairing

$$\langle [D_+], [U] \rangle = -\text{Index}(W_U). \tag{1.3}$$

In Section 5.3 we show that if $S(0) = \text{Id}$ then the pairing of Equation (1.3) holds for $W_- = W_S$, a result which has appeared in [5] as joint work with Adam Rennie.

In dimension $n = 1$ generically and in the presence of resonances in dimension $n = 3$ the condition $S(0) = \text{Id}$ is not satisfied and we require additional effort to correct this behaviour. In Section 5.3.1 we construct a unitary which corrects the low-energy behaviour of the scattering matrix and as a result obtain in Theorem 5.3.16 a new proof of the well-known Levinson's theorem in one dimension.

Theorem 1.2.1. *Let $n = 1$ and S be the scattering operator for $H = H_0 + V$. Then the number of bound states of H is given by*

$$N = \begin{cases} -\frac{1}{2\pi i}\int_0^\infty \text{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda, & \textit{if there exists a resonance,} \\ -\frac{1}{2\pi i}\int_0^\infty \text{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2} & \textit{otherwise.} \end{cases} \tag{1.4}$$

In Section 5.3.2 we demonstrate in dimension $n = 3$ that in the presence of resonances we can correct the value of $S(0)$ in the same manner to obtain an index pairing in Theorem 5.3.20. We find also that to obtain a formula for $\text{Index}(W_-)$ requires a careful analysis of large λ behaviour of $S(\lambda)$ in trace norm, which leads again to a new proof of Levinson's theorem in dimension $n = 3$ in Theorem 5.3.24. The statement is as follows.

Theorem 1.2.2. *Let $n = 3$ and let S be the scattering operator for $H = H_0 + V$. Then the number of bound states of H is given by*

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\text{Tr}(S(\lambda)^* S'(\lambda)) + \frac{i}{4\pi\lambda^{\frac{1}{2}}}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x \right) \mathrm{d}\lambda + \frac{1}{2} M_R(0), \tag{1.5}$$

where $M_R(0) = 1$ if there is a zero energy-resonance and zero otherwise.

In Section 5.3.3 we show that as in dimension $n = 3$ the high energy behaviour of $S(\cdot)$ in trace norm requires some correcting in dimension $n = 2$. After doing so we obtain, in the absence of p-resonances, Theorem 5.3.29, a new proof of Levinson's theorem in dimension $n = 2$ which confirms [26, Theorem 6.3]. The result is as follows.

Theorem 1.2.3. *Let $n = 2$ and let S be the scattering operator for $H = H_0 + V$. Suppose further that there are no p-resonances. Then the number of bound states of H is given by*

$$-N = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x.$$

We conclude Chapter 5 in Section 5.3.4 by applying similar techniques to correct the high energy behaviour of the scattering matrix and obtain in Theorem 5.3.34 a new proof of Levinson's theorem in higher dimensions.

Chapter 6: We apply the spectral flow formula of [47, Theorem 9] to the path of operators $H_t(\alpha) = H_0 + tV + \alpha$, $t \in [0, 1]$, where $\alpha > 0$ is chosen so that $H_t(\alpha)$ defines a path of Fredholm operators. The stationary scattering theory for the pair $(H_0(\alpha), H_1(\alpha))$ is described in Section 6.2. In Section 6.3 we describe the necessary pseudodifferential operator calculus in order to estimate remainder terms in our spectral flow formula. In Section 6.4 we apply the Birman-Kreĭn trace formula and the pseudodifferential operator calculus of [46] to derive a formula for the spectral flow of the path $H_t(\alpha)$ in Theorem 6.4.22 for n odd and Theorem 6.4.23 for n even. We give a new approach to the relationship between the spectral shift function and spectral flow, extending work of Azamov, Carey, Dodds and Sukochev [13, 14].

The even dimensional case is more complicated than the odd dimensional case due to the non-vanishing of certain remainder terms. We conclude Chapter 6 in Section 6.5 where we show how the spectral flow gives rise to Levinson's theorem in all dimensions. Our proof shows that with knowledge of the spectral shift function at zero, Theorem 1.2.3 is applicable to the case of p-resonances also. This is work in progress.

Appendix A: In this appendix we provide some computations of the high-energy behaviour of the spectral shift function appearing in Levinson's theorem using the spectral flow methods of Chapter 6.

Chapter 2

Scattering theory for Schrödinger operators

This chapter contains a brief introduction to some concepts from mathematical scattering theory which are necessary for the understanding of the rest of the thesis, in particular scattering theory for perturbations of the Laplace operator on Euclidean space. Proofs of most results have been included, since the tools and techniques used are often illuminating for later use. The results in this chapter are not new and we do not claim that this chapter is in any way a complete description of scattering theory, even for the Schrödinger operators we restrict ourselves to. The history of scattering theory is intertwined with the history of spectral theory, and so the literature is vast. For a more complete discussion of mathematical scattering theory we refer to [18, 137, 165, 164] and to the extensive references compiled within. Some more physically motivated discussion can be found in [7, 127, 146].

We begin with the abstract theory of scattering, before specialising to Schrödinger operators acting on $L^2(\mathbb{R}^n)$ for the remainder of the thesis.

2.1 Abstract scattering theory

The abstract scattering theory presented here has its origins in the works of Møller [117] and Friedrichs [66, 67], who constructed wave operators explicitly by studying particular integral equations. The abstract scattering theory was first rigorously developed in the works of Kato [92], Cook [53] and Jauch [80, 81]. In this section we follow the presentation of Reed and Simon [137].

Consider two self-adjoint operators A and B on a Hilbert space $\mathcal{H}$. By Stone's theorem [134, Theorem VII.7] we have strongly-continuous one parameter unitary groups $(\mathrm{e}^{-itA})_{t\in\mathbb{R}}$ and $(\mathrm{e}^{-itB})_{t\in\mathbb{R}}$ of operators on $\mathcal{H}$, which we think of as an interacting dynamics A and a free or comparison dynamics B. For a vector $f \in \mathcal{H}$ we say that e^{-itA} is asymptotically free if there exists $f_\pm \in \mathcal{H}$ (here the subscript '$\pm$' refers to two independent vectors, one for '$+$' and one for '$-$') such that

$$0 = \lim_{t\to\pm\infty} \left|\left|\mathrm{e}^{-itB} f_\pm - \mathrm{e}^{-itA} f\right|\right| = \lim_{t\to\pm\infty} \left|\left|\mathrm{e}^{itA}\mathrm{e}^{-itB} f_\pm - f\right|\right|. \tag{2.1}$$

The motivation here is that in the limit as $t \to \pm\infty$ (long before or long after an interaction has occurred) one expects for physical reasons that for any $f \in \mathcal{H}$ the interacting evolution $\mathrm{e}^{-itA} f$ can be approximated by a freely evolving state $\mathrm{e}^{-itB} f_\pm$ for some $f_\pm \in \mathcal{H}$. In most applications (in particular the Schrödinger operators we specialise to) the operator B has no discrete spectrum. In cases where B does have discrete spectrum, we need to choose $f_\pm \in \mathcal{H}_{ac}(B)$ (the absolutely continuous subspace for B). To see this, we suppose that $f_\pm$ is an eigenvector of B and note that the strong limit in Equation (2.1) would exist only if $f_\pm$ is an eigenvector for A with the same eigenvalue. Taking these considerations into account leads to the following definition.

Definition 2.1.1. Let A and B be self-adjoint operators on the Hilbert space $\mathcal{H}$ and let $P_{ac}(B)$ be the projection onto $\mathcal{H}_{ac}(B)$, the absolutely continuous subspace of $\mathcal{H}$ with respect to B. We define the *wave operators* $W_\pm(A, B)$ by the strong limits

$$W_\pm(A, B) := \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{itA}\mathrm{e}^{-itB} P_{ac}(B),$$

if they exist. When $W_\pm(A, B)$ exist we define $\mathcal{H}_\pm = \mathrm{Range}(W_\pm(A, B))$.

Remark 2.1.2. The strong limit is the right one to take here [137, p. 17]. On the one hand the norm limit exists if and only if $A = B$, whilst on the other hand if $\sigma(A)$ is purely discrete, the weak limit exists (and is 0) even though the operators A and B are not necessarily similar in any way.

Proposition 2.1.3. *Let A and B be self-adjoint operators in a Hilbert space $\mathcal{H}$ and suppose that $W_\pm(A, B)$ exist. Then:*

1. *$W_\pm(A, B)$ are partial isometries with initial subspace $\mathcal{H}_{ac}(B)$ and final subspace $\mathcal{H}_\pm$;*
2. *the subspaces $\mathcal{H}_\pm$ satisfy $A\mathcal{H}_\pm \subseteq \mathcal{H}_\pm$ (that is they are invariant for A), there is an inclusion $W_\pm(A, B)\mathrm{Dom}(B) \subset \mathrm{Dom}(A)$ and we have the intertwining relation $AW_\pm(A, B) = W_\pm(A, B)B$; and*
3. *$\mathcal{H}_\pm \subseteq \mathcal{H}_{ac}(A)$.*

Proof. For $f \in \mathcal{H}_{ac}(B)^\perp$ we have $W_\pm f = 0$ by definition. For $f \in \mathcal{H}_{ac}(B)$ we find that

$$\left|\left|\mathrm{e}^{itA}\mathrm{e}^{-itB} P_{ac}(B) f\right|\right| = ||f||$$

for all $t \in \mathbb{R}$ and thus if the wave operators exist we find $||W_\pm(A,B)f|| = ||f||$ and so $W_\pm(A,B)$ are partial isometries.

For the second claim, we note that for fixed $s \in \mathbb{R}$ we have $[\mathrm{e}^{-isB}, P_{ac}(B)] = 0$. So we compute that

$$W_\pm(A,B) = \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{itA}\mathrm{e}^{-itB}P_{ac}(B) = \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{i(s+t)A}\mathrm{e}^{-i(s+t)B}P_{ac}(B) = \mathrm{e}^{isA}W_\pm(A,B)\mathrm{e}^{-isB},$$

or

$$\mathrm{e}^{-isA}W_\pm(A,B) = W_\pm(A,B)\mathrm{e}^{-isB}. \tag{2.2}$$

Then for $f \in \mathrm{Dom}(B)$ we have

$$\begin{aligned}\lim_{s\to 0} W_\pm(A,B)\left(\frac{\mathrm{e}^{-isB}-\mathrm{Id}}{s}\right)f &= W_\pm(A,B)\left[\lim_{s\to 0}\left(\frac{\mathrm{e}^{-isB}-\mathrm{Id}}{s}\right)f\right] \\ &= -iW_\pm(A,B)Bf.\end{aligned}$$

Applying Equation (2.2) we find

$$\left(\frac{\mathrm{e}^{-isA}-\mathrm{Id}}{s}\right)W_\pm(A,B)f = W_\pm(A,B)\left(\frac{\mathrm{e}^{-isB}-\mathrm{Id}}{s}\right)f.$$

As the limit on the right hand side exists, so does the limit on the left and they are equal. So $W_\pm(A,B)f \in \mathrm{Dom}(A)$ for all $f \in \mathrm{Dom}(B)$ and thus

$$\begin{aligned}-iAW_\pm(A,B)f &= \lim_{s\to 0}\left(\frac{\mathrm{e}^{-isB}-\mathrm{Id}}{s}\right)W_\pm(A,B)f = \lim_{s\to 0} W_\pm(A,B)\left(\frac{\mathrm{e}^{-isB}-\mathrm{Id}}{s}\right)f \\ &= -iW_\pm(A,B)B,\end{aligned}$$

which proves the intertwining relation and that $A\mathcal{H}_\pm \subseteq \mathcal{H}_\pm$. By Equation (2.2) we have that $\mathcal{H}_\pm$ are invariant under e^{-isA} for all $s \in \mathbb{R}$, which is enough to prove the claim.

For the third claim, we note that $A|_{\mathcal{H}_\pm}$ is a self-adjoint operator on the Hilbert space $\mathcal{H}_\pm$ ($\mathcal{H}_\pm$ are closed since $W_\pm$ are partial isometries). Furthermore, we have that $W_\pm(A,B) : \mathcal{H}_{ac}(B) \to \mathcal{H}_\pm$ is a unitary and the intertwining relation shows us that $B|_{\mathcal{H}_{ac}(B)}$ is unitarily equivalent to $A|_{\mathcal{H}_\pm}$ with the unitary equivalence given by $W_\pm(A,B)$. Hence $A|_{\mathcal{H}_\pm}$ is purely absolutely continuous and $\mathcal{H}_\pm \subseteq \mathcal{H}_{ac}(A)$, which completes the proof. □

The following result shows that the wave operators have a partially defined composition rule, often referred to as the chain rule, due to Kato [92].

Proposition 2.1.4. *Let A, B and C be self-adjoint operators on a Hilbert space $\mathcal{H}$. If*

$W_\pm(A,B)$ and $W_\pm(B,C)$ exist, then $W_\pm(A,C)$ exist and

$$W_\pm(A,C) = W_\pm(A,B)W_\pm(B,C).$$

Proof. By part 3 of Proposition 2.1.3 we have $\mathrm{Range}(W_\pm(B,C)) \subseteq \mathcal{H}_{ac}(B)$ and thus

$$\lim_{t\to\pm\infty} \left|\left|(\mathrm{Id} - P_{ac}(B))\mathrm{e}^{itB}\mathrm{e}^{-itC}P_{ac}(C)f\right|\right| = 0$$

for any $f \in \mathcal{H}$. Hence we may write

$$\begin{aligned}\mathrm{e}^{itA}\mathrm{e}^{-itC}P_{ac}(C)f &= \mathrm{e}^{itA}\mathrm{e}^{-itB}P_{ac}(B)\mathrm{e}^{itB}\mathrm{e}^{-itC}P_{ac}(C)f \\ &\quad + \mathrm{e}^{itA}\mathrm{e}^{-itB}(\mathrm{Id} - P_{ac}(B))\mathrm{e}^{itB}\mathrm{e}^{-itC}P_{ac}(C),\end{aligned}$$

which converges as $t \to \pm\infty$ to $W_\pm(A,B)W_\pm(B,C)f$, since a product of strongly convergent families of uniformly bounded operators converges strongly (a consequence of the uniform boundedness principle). □

Definition 2.1.5. Let A and B be self-adjoint operators on a Hilbert space $\mathcal{H}$ such that the wave operators $W_\pm(A,B)$ exist. Let $\mathcal{H}_p(A)$ denote the point spectrum subspace of $\mathcal{H}$ associated to A. We say that the wave operators are *asymptotically complete* if $\mathcal{H}_- = \mathcal{H}_+ = (\mathcal{H}_p(A))^\perp$. We say that the wave operators are *complete* if $\mathcal{H}_- = \mathcal{H}_+ = \mathcal{H}_{ac}(A)$.

Remark 2.1.6. Asymptotic completeness is a stronger statement than completeness. In fact, asymptotic completeness is equivalent to the pair of statements $W_\pm(A,B)$ are complete and $\sigma_{sc}(A) = \emptyset$ [149, Theorem IV.2] (here $\sigma_{sc}(A)$ denotes the singular continuous spectrum of A).

The completeness of $W_\pm(A,B)$ can actually be reduced to an existence problem.

Proposition 2.1.7. *Let A and B be self-adjoint operators on the Hilbert space $\mathcal{H}$ and suppose the wave operators $W_\pm(A,B)$ exist. Then $W_\pm(A,B)$ are complete if and only if $W_\pm(B,A)$ exist.*

Proof. First suppose that both $W_\pm(A,B)$ and $W_\pm(B,A)$ exist. Then by the chain rule for wave operators (Proposition 2.1.4) we have

$$P_{ac}(A) = W_\pm(A,A) = W_\pm(A,B)W_\pm(B,A)$$

and thus $\mathcal{H}_{ac}(A) = \mathrm{Range}(W_\pm(A,A)) \subseteq \mathrm{Range}(W_\pm(A,B))$. By Proposition 2.1.3 we have $\mathrm{Range}(W_\pm(A,B)) \subset \mathcal{H}_{ac}(A)$ and thus we have equality.

Now suppose that $W_\pm(A,B)$ exist and are complete. Let $f \in \mathcal{H}_{ac}(A) = \mathrm{Range}(P_{ac}(A))$. As $W_\pm(A,B)$ are complete there exist $f_\pm \in \mathcal{H}$ such that $f = W_\pm(A,B)f_\pm$. Hence we have

$$\lim_{t\to\pm\infty} \left|\left|f - e^{itA}e^{-itB}P_{ac}(B)f_\pm\right|\right| = 0.$$

Using unitarity we thus obtain

$$\lim_{t\to\pm\infty} \left|\left|e^{itB}e^{-itA}f - P_{ac}(B)f_\pm\right|\right| = 0.$$

So $\lim_{t\to\pm\infty} e^{itB}e^{-itA}f = P_{ac}(B)f_\pm$. □

Proposition 2.1.7 seems to imply that the problem of completeness is no harder than existence, however this is not the case. The following common existence result, known as Cook's criterion [53], uses the observation that the operator B is often much simpler in some way than the operator A. Since this is not symmetric in A and B, completeness is often a much more difficult question.

Theorem 2.1.8 (Cook's criterion). *Let A and B be self-adjoint operators on the Hilbert space $\mathcal{H}$ with $\mathrm{Dom}(A) = \mathrm{Dom}(B)$. Suppose there is a set $\tilde{D} \subset \mathrm{Dom}(B) \cap \mathcal{H}_{ac}(B)$ which is dense in $\mathcal{H}_{ac}(B)$ such that for any $f \in \tilde{D}$ there is a $T_0 \in \mathbb{R}$ satisfying*

$$\int_{T_0}^{\infty} \left|\left|(B - A)e^{\pm itB}f\right|\right| \, dt < \infty. \tag{2.3}$$

Then the wave operators $W_\pm(A, B)$ exist.

Proof. Fix $f \in \tilde{D}$ and let $g(t) = e^{itA}e^{-itB}f$. Then g is differentiable and

$$g'(t) = -ie^{itA}(B - A)e^{-itB}f.$$

By assumption there exists $T_0 > 0$ such that the inequality (2.3) holds. Then for $T_0 < s < t$ we can compute

$$||g(t) - g(s)|| \le \int_s^t ||g'(u)|| \, du = \int_s^t \left|\left|(B - A)e^{-iuB}f\right|\right| \, du.$$

For fixed $\psi \in \mathcal{H}$ the function $h : \mathbb{R} \to \mathbb{C}$ defined by $h(t) = \langle g(t), \psi\rangle$ is differentiable with

$$d_\psi(t) := h'(t) = \left\langle (B - A)e^{-itB}f, ie^{-itA}\psi \right\rangle,$$

which is seen to be continuous in t. The fundamental theorem of calculus then tells us that

$$\langle (g(t) - g(s))f, \psi\rangle = \int_s^t \left\langle (B - A)e^{-iuB}f, ie^{-iuA}\psi \right\rangle \, du.$$

Since $\mathrm{Dom}(A) \subset \mathcal{H}$ is dense we find

$$\begin{aligned}||(g(t)-g(s))f|| &= \sup_{||\psi||\leq 1, \psi\in\mathrm{Dom}(A)} |\langle (g(t)-g(s))f, \psi\rangle| \\ &\leq \sup_{||\psi||\leq 1, \psi\in\mathrm{Dom}(A)} \int_s^t \left|\left\langle (B-A)\mathrm{e}^{-iuB}f, i\mathrm{e}^{-iuA}\psi\right\rangle\right| \,\mathrm{d}u \\ &\leq \int_s^t \left|\left|(B-A)\mathrm{e}^{-iuB}f\right|\right| \,\mathrm{d}u.\end{aligned}$$

So we see that

$$\lim_{s,t\to\infty} ||(g(t)-g(s))f|| = 0$$

and thus for all $f \in \tilde{D}$ we have that the limits

$$\lim_{t\to\infty} \mathrm{e}^{itA}\mathrm{e}^{-itB}P_{ac}(B)f = \lim_{t\to\infty} g(t) \tag{2.4}$$

exist. If $f \in \mathcal{H}_{ac}(B)^{\perp} = \tilde{D}^{\perp}$ then the limit (2.4) exists and is zero. By the density of $\tilde{D} \oplus \tilde{D}^{\perp}$ we have that the wave operator $W_+(A,B)$ exists. □

We can use the wave operators to construct a unitary operator which maps incoming states to outgoing states.

Definition 2.1.9. Let A and B be self-adjoint operators such that the wave operators $W_{\pm}(A,B)$ exist. Then we define the *scattering operator* to be

$$S = S(A,B) = (W_+(A,B))^* W_-(A,B).$$

Lemma 2.1.10. *Let A and B be self-adjoint operators such that the wave operators $W_{\pm}(A,B)$ exist. Then the scattering operator S commutes with A. If in addition the wave operators $W_{\pm}(A,B)$ are complete then the scattering operator is unitary.*

Proof. The relation $SA = AS$ follows immediately from the intertwining relation for the wave operators. To see that S is unitary, we check that for all $f, g \in \mathcal{H}$ we have

$$\langle Sf, Sg\rangle = \langle (W_+(A,B))^* W_-(A,B)f, (W_+(A,B))^* W_-(A,B)g\rangle = \langle f, g\rangle,$$

since by completeness we have $\mathrm{Range}(W_+) = \mathrm{Range}(W_-)$. □

2.1.1 Stationary scattering theory

The descriptions of the wave operator in Section 2.1 have been time-dependent in the sense that we directly use $\mathrm{e}^{\pm itA}\mathrm{e}^{\mp itB}$ to describe the wave operators $W_{\pm}(A,B)$. It is sometimes more useful to consider a time-independent (stationary) approach to scattering theory. In this section we give an alternative stationary description of the wave operators. We will make a refinement of this description specific to Schrödinger operators in Section 2.4.2.

Theorem 2.1.11. *Let A and B be self-adjoint operators on a Hilbert space $\mathcal{H}$ with resolvents, defined for $z \in \rho(A) \cap \rho(B)$, given by $R_A(z) = (A - z)^{-1}$ and $R_B(z) = (B - z)^{-1}$. Then for any $f \in \mathrm{Dom}(B)$ and $g \in \mathrm{Dom}(A)$ the wave operators $W_\pm(A, B)$ satisfy*

$$\langle W_\pm(A, B)f, g\rangle = \lim_{\varepsilon \to 0^+} \frac{\varepsilon}{\pi} \int_{\mathbb{R}} \langle R_B(\lambda \mp i\varepsilon)f, R_A(\lambda \mp i\varepsilon)g\rangle \, \mathrm{d}\lambda. \tag{2.5}$$

Proof. We prove the relation for W_+, the proof for W_- being similar. For $\mathrm{Im}(z) > 0$ we have the identity

$$-iz^{-1} = \int_0^\infty \mathrm{e}^{izt} \, \mathrm{d}t.$$

For $f \in \mathcal{H}$, $\varepsilon > 0$, $\lambda \in \mathbb{R}$ and $z = \lambda + i\varepsilon$ we define $h_{\varepsilon,A}(t) = \mathrm{e}^{-i(A - i\varepsilon)t} f$. Then we find

$$R_A(z)f = -i \int_0^\infty \mathrm{e}^{-i(A-z)t} f \, \mathrm{d}t = -i \int_0^\infty \mathrm{e}^{i\lambda t} \mathrm{e}^{-i(A-i\varepsilon)t} f \, \mathrm{d}t = -i(2\pi)^{\frac{1}{2}} [\mathcal{F}^*(\chi_{[0,\infty)} h_{\varepsilon,A})](\lambda),$$

where we are using the notation χ_I for the characteristic function of the set $I \subset \mathbb{R}$ and $\mathcal{F}$ for the one dimensional Fourier transform, which we describe in greater detail in Section 2.2.1. Similarly, we can define for $g \in \mathcal{H}$ the function $h_{\varepsilon,B}(t) = \mathrm{e}^{-i(B-i\varepsilon)t} g$ and check that

$$R_B(z)g = -i(2\pi)^{\frac{1}{2}} [\mathcal{F}^*(\chi_{[0,\infty)} h_{\varepsilon,B})](\lambda).$$

We can now use the Parseval identity to obtain

$$\begin{aligned}
\int_{\mathbb{R}} \langle R_B(\lambda + i\varepsilon)f, R_A(\lambda + i\varepsilon)g\rangle \, \mathrm{d}\lambda &= (2\pi) \int_{\mathbb{R}} \langle [\mathcal{F}^*(\chi_{[0,\infty)} h_{\varepsilon,B})](\lambda), [\mathcal{F}^*(\chi_{[0,\infty)} h_{\varepsilon,A})](\lambda)\rangle \, \mathrm{d}\lambda \\
&= (2\pi) \int_0^\infty \langle \chi_{[0,\infty)}(t) h_{\varepsilon,B}(t), \chi_{[0,\infty)}(t) h_{\varepsilon,A}(t)\rangle \, \mathrm{d}t \\
&= (2\pi) \int_0^\infty \mathrm{e}^{-2\varepsilon t} \langle \mathrm{e}^{-itB} g, \mathrm{e}^{-itA} f\rangle \, \mathrm{d}t \\
&= (2\pi) \int_0^\infty \mathrm{e}^{-2\varepsilon t} \langle \mathrm{e}^{itA} \mathrm{e}^{-itB} g, f\rangle \, \mathrm{d}t.
\end{aligned} \tag{2.6}$$

So if $g \in \mathrm{Dom}(W_+)$ we have

$$\lim_{\varepsilon \to 0^+} 2\varepsilon \int_0^\infty \mathrm{e}^{-2\varepsilon t} \langle \mathrm{e}^{itA} \mathrm{e}^{-itB} g, f\rangle \, \mathrm{d}t = \langle W_+ g, f\rangle. \tag{2.7}$$

Thus, by combining Equations (2.6) and (2.7) we obtain

$$\begin{aligned}\langle W_+ g, f\rangle &= \lim_{\varepsilon\to 0^+} 2\varepsilon \int_0^\infty \mathrm{e}^{-2\varepsilon t}\langle \mathrm{e}^{itA}\mathrm{e}^{-itB} g, f\rangle \,\mathrm{d}t \\ &= \lim_{\varepsilon\to 0^+} \frac{\varepsilon}{\pi}\int_{\mathbb{R}} \langle R_B(\lambda + i\varepsilon) f, R_A(\lambda+i\varepsilon) g\rangle \,\mathrm{d}\lambda,\end{aligned}$$

which is the statement of the theorem. □

The following statement is known as Stone's formula (see [134, Theorem VII.13] for example) and characterises how the resolvent of a self-adjoint operator can be used to describe its spectral projections.

Lemma 2.1.12. *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and for $z \in \rho(A)$ define $R_A(z) = (A - z)^{-1}$. Then for any $f, g \in \mathcal{H}$ and any open interval $I \subseteq \mathbb{R}$ we have*

$$\lim_{\varepsilon\to 0} \frac{\varepsilon}{\pi}\int_I \langle R_A(\lambda \pm i\varepsilon) f, R_A(\lambda \pm i\varepsilon) g\rangle \,\mathrm{d}\lambda = \langle \chi_I(A) f, g\rangle. \tag{2.8}$$

Proof. Let $f, g \in \mathcal{H}$. Functional calculus shows that

$$\frac{\varepsilon}{\pi}\int_I \langle R_A(\lambda \pm i\varepsilon) f, R_A(\lambda \pm i\varepsilon) g\rangle \,\mathrm{d}\lambda = \int_I \left(\int_{\mathbb{R}} \frac{\varepsilon}{\pi(\varepsilon^2 + (\lambda-\rho)^2)} \,\mathrm{d}\langle P_\lambda f, g\rangle\right) \mathrm{d}\rho.$$

Next we define the function

$$f_\varepsilon(\lambda) = \int_I \frac{\varepsilon}{\pi(\varepsilon^2 + (\lambda-\rho)^2)} \,\mathrm{d}\rho.$$

Noting that $|f_\varepsilon(\lambda)| \le 1$ for all λ we may apply Fubini's theorem to interchange the order of integration and obtain the relation

$$\frac{\varepsilon}{\pi}\int_I \langle R_A(\lambda \pm i\varepsilon) f, R_A(\lambda \pm i\varepsilon) g\rangle \,\mathrm{d}\lambda = \int_{\mathbb{R}} f_\varepsilon(\lambda) \,\mathrm{d}\langle P_\lambda f, g\rangle.$$

We can compute the integral defining f_ε explicitly to obtain

$$\lim_{\varepsilon\to 0} f_\varepsilon(\lambda) = \begin{cases} 1, & \text{if } \lambda \in I, \\ \frac{1}{2} & \text{if } \lambda \in \partial\overline{I}, \\ 0, & \text{otherwise.}\end{cases}$$

The result now follows immediately. □

Corollary 2.1.13. *Let A be a self-adjoint operator on a Hilbert space and for $z \in \rho(A)$*

define $R_A(z) = (A - z)^{-1}$. *Then for any* $f, g \in \mathcal{H}$ *we have*

$$\lim_{\varepsilon \to 0} \frac{\varepsilon}{\pi} \int_{\mathbb{R}} \langle R_A(\lambda \pm i\varepsilon) f, R_A(\lambda \pm i\varepsilon) g \rangle \, \mathrm{d}\lambda = \langle f, g \rangle. \tag{2.9}$$

Proof. Take $I = \mathbb{R}$ in Lemma 2.1.12 □

2.2 Hamiltonians and dilation

We are interested in a particular choice of operators A and B in the previous section. We work on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$ for some $n \geq 1$. We will often have need of the Hilbert space

$$\mathcal{P} = L^2(\mathbb{S}^{n-1}),$$

where $\mathbb{S}^{n-1} = \{x \in \mathbb{R}^n : |x| = 1\}$ and the space $L^2(\mathbb{R}^+)$ where $\mathbb{R}^+ = [0, \infty)$ is the non-negative half-line. We will often make the identification

$$\mathcal{H}_{spec} := L^2(\mathbb{R}^+, \mathcal{P}) = L^2(\mathbb{R}^+) \otimes \mathcal{P}.$$

We will also frequently use the Schwarz space $\mathcal{S}(\mathbb{R}^n)$ defined by

$$\mathcal{S}(\mathbb{R}^n) = \left\{ f \in C^\infty(\mathbb{R}^n) : \sup_{x \in \mathbb{R}^n} |x^\alpha [D_\beta f](x)| < \infty \text{ for all multi-indices } \alpha, \beta \right\}.$$

Since $C_c^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$ we have that $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^p(\mathbb{R}^n)$ for $p \in [1, \infty)$.

2.2.1 The free Hamiltonian

Our reference operator of interest is the Laplacian

$$\Delta = -\sum_{j=0}^{n} \frac{\partial^2}{\partial x_j^2}$$

acting initially on $C_c^\infty(\mathbb{R}^n) \subset \mathcal{H}$. The Laplacian and its spectral theory have been studied extensively in the literature, for a detailed discussion we refer the reader to [154, 149, 135, 55, 95]. To describe the spectral properties of the Laplacian, we recall the Fourier transform $\mathcal{F} : \mathcal{H} \to \mathcal{H}$ defined for $f \in \mathcal{S}(\mathbb{R}^n)$ by

$$[\mathcal{F} f](\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\langle x, \xi \rangle} f(x) \, \mathrm{d}x \tag{2.10}$$

and extended by continuity to all of $\mathcal{H}$. We recall that the Fourier transform is a unitary operator with inverse defined by

$$[\mathcal{F}^* f](x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{i\langle x,\xi\rangle} f(\xi)\,\mathrm{d}\xi. \tag{2.11}$$

The Fourier transform is an isomorphism from $\mathcal{S}(\mathbb{R}^n)$ to itself (in fact a homeomorphism when equipped with the Schwarz topology, see [135, Theorem IX.1]). Using the Fourier transform we are able to characterise the maximal domain of definition of Δ and its spectrum. The following result is well-known (see for example [135, Theorem IX.27]).

Theorem 2.2.1. *The Laplacian Δ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^n)$ and thus has a unique self-adjoint extension with domain* $\mathrm{Dom}(\Delta) = \{f \in \mathcal{H} : (\xi \mapsto |\xi|^2[\mathcal{F}f](\xi)) \in \mathcal{H}\}$.

Definition 2.2.2. We denote by H_0 the unique self-adjoint extension of Δ defined by Theorem 2.2.1 and sometimes refer to H_0 as the *free Hamiltonian.*

We know that the Fourier transform 'diagonalises' the operator H_0 in the sense that

$$[\mathcal{F}H_0\mathcal{F}^* f](\xi) = |\xi|^2 f(x) \tag{2.12}$$

for $f \in \mathrm{Dom}(H_0)$.

Definition 2.2.3. We define $X^2 = \mathcal{F}H_0\mathcal{F}$ to be the multiplication operator, given for $f \in \mathcal{S}(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$ by

$$[X^2 f](x) = |x|^2 f(x).$$

We can use the operator H_0 to define a class of weighted Sobolev spaces which we will use throughout this thesis. For a more detailed discussion of Sobolev spaces we refer the reader to [2, 8].

Definition 2.2.4. For any $s, t \in \mathbb{R}$ the *weighted Sobolev space* $H^{s,t} = H^{s,t}(\mathbb{R}^n)$ is given by

$$H^{s,t} = \left\{ f \in \mathcal{S}'(\mathbb{R}^n) : ||f||_{H^{s,t}} = \left|\left|(1+X^2)^{\frac{t}{2}}(1+H_0)^{\frac{s}{2}} f\right|\right|_{\mathcal{H}} < \infty \right\}. \tag{2.13}$$

The main properties of the Sobolev spaces we rely on are summarised in the following (see [8, Chapter 4]).

Theorem 2.2.5. *Fix $s, t \in \mathbb{R}$.*

(a) The Fourier transform $\mathcal{F}$ gives an isomorphism of $H^{s,t}$ with $H^{t,s}$ and the sesquilinear map $\langle\cdot,\cdot\rangle : H^{s,t} \times H^{-s,-t} \to \mathbb{C}$ defined for $f \in H^{s,t}$ and $g \in H^{-s,-t}$ by

$$\langle f, g\rangle = \int_{\mathbb{R}^n} \overline{f(x)} g(x)\,\mathrm{d}x$$

gives a natural duality between $H^{s,t}$ and $H^{-s,-t}$.

(b) For any $p < s$ and $m < t$ the inclusion $H^{s,t} \hookrightarrow H^{p,m}$ is compact.

(c) For any $m > 0$ and $q : \mathbb{R}^n \to \mathbb{C}$ satisfying $|q(x)| \leq C(1 + |x|)^{-m}$ for almost all $x \in \mathbb{R}^n$ the operator of multiplication by q maps $H^{s,t}$ into $H^{s,t+m}$.

(d) The domain of H_0 is the Sobolev space $H^{2,0}$.

Theorem 2.2.5 (b) is often referred to as Rellich's compactness theorem (see for example [8, Theorem 4.1.5]), which we shall make frequent use of along with the mapping properties of multiplication operators in Theorem 2.2.5 (c).

The diagonalisation of Equation (2.12) allows us to determine directly the spectrum of H_0.

Lemma 2.2.6. *The operator H_0 has spectrum $\sigma(H_0) = \sigma_{ac}(H_0) = [0, \infty)$.*

Proof. This follows from the unitarity of the Fourier transform and the spectrum of multiplication operators. □

Equation (2.12) is not the 'correct' diagonalisation, since it is not multiplication by the spectral variable. To find the correct diagonalisation, we introduce a second unitary to rescale the spectral variable appropriately.

Recall that we have defined the spaces $\mathcal{P} = L^2(\mathbb{S}^{n-1})$ and $\mathcal{H}_{spec} = L^2(\mathbb{R}^+) \otimes \mathcal{P}$.

Definition 2.2.7. For $n \geq 2$, $\lambda \in \mathbb{R}^+$ and $\omega \in \mathbb{S}^{n-1}$ we define the operator $\mathcal{U} : \mathcal{H} \to \mathcal{H}_{spec}$ by

$$[\mathcal{U}f](\lambda, \omega) = 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}} f(\lambda^{\frac{1}{2}}\omega)$$

and $F_0 = \mathcal{U}\mathcal{F}$. For $n = 1$, $\mathcal{P} = \mathbb{C}^2$ and $\lambda \in \mathbb{R}^+$ we define $\mathcal{U} : \mathcal{H} \to L^2(\mathbb{R}^+) \otimes \mathcal{P}$ by

$$[\mathcal{U}f](\lambda) = 2^{-\frac{1}{2}}\lambda^{-\frac{1}{2}} \begin{pmatrix} f(\lambda^{\frac{1}{2}}) \\ f(-\lambda^{\frac{1}{2}}) \end{pmatrix}.$$

We define the operator $F_0 : \mathcal{H} \to L^2(\mathbb{R}^+) \otimes \mathcal{P}$ by $F_0 = \mathcal{U}\mathcal{F}$ for all dimensions $n \geq 1$.

The operators F_0 and $\mathcal{U}$ are well-known throughout the spectral theory literature: see [86] for a good discussion of their properties. In dimension $n = 1$ the unitary $\mathcal{U}$ is not unique, depending on a choice of basis for $\mathbb{C}^2$. The diagonalisation of H_0 provided by F_0 provides a more physical interpretation of the spectrum of H_0 as the energy parameter and we will use F_0 to construct a diagonalisation for a perturbed Hamiltonian operator in Section 2.4.2

Lemma 2.2.8. *For $n \geq 2$ the operators $\mathcal{U}$ and F_0 are unitary and for $f \in F_0(\mathrm{Dom}(H_0))$, $\lambda \in \mathbb{R}^+$ and $\omega \in \mathbb{S}^{n-1}$ we have*

$$[F_0 H_0 F_0^* f](\lambda,\omega) = \lambda f(\lambda,\omega). \tag{2.14}$$

Proof. It suffices to check that $\mathcal{U}$ is unitary, since the Fourier transform $\mathcal{F}$ is unitary. For $f, g \in L^2(\mathbb{R}^n)$ we can check directly that

$$\begin{aligned}\langle \mathcal{U}f, \mathcal{U}g\rangle &= \int_{\mathbb{R}^+}\int_{\mathbb{S}^{n-1}} \overline{[\mathcal{U}f](\lambda,\omega)}[\mathcal{U}g](\lambda,\omega)\,\mathrm{d}\omega\,\mathrm{d}\lambda = \int_{\mathbb{R}^+}\int_{\mathbb{S}^{n-1}} 2^{-1}\lambda^{\frac{n-2}{2}}\overline{f(\lambda^{\frac{1}{2}}\omega)}g(\lambda^{\frac{1}{2}}\omega)\,\mathrm{d}\omega\,\mathrm{d}\lambda\\ &= \int_{\mathbb{R}^+}\int_{\mathbb{S}^{n-1}} r^{n-1}\overline{f(r\omega)}g(r\omega)\,\mathrm{d}\omega\,\mathrm{d}r = \int_{\mathbb{R}^n}\overline{f(x)}g(x)\,\mathrm{d}x = \langle f, g\rangle,\end{aligned}$$

where we have made the substitutions $\lambda = r^2$ and $x = r\omega$. Thus the operator $\mathcal{U}$ is unitary as claimed. For the diagonalisation relation of Equation (2.14) it suffices to show that for $f \in \mathrm{Dom}(H_0)$ we have the relation

$$[F_0 H_0 f](\lambda,\omega) = \lambda[F_0 f](\lambda,\omega). \tag{2.15}$$

Define the operator $M : \mathrm{Dom}(H_0) \to \mathcal{H}$ by $[Mf](\xi) = |\xi|^2 f(\xi)$. Then by conjugating both sides of Equation (2.15) with $\mathcal{F}$ and $\mathcal{F}^*$ it suffices to check for $f \in \mathrm{Dom}(H_0)$ that

$$[\mathcal{U}M\mathcal{U}^* f](\lambda,\omega) = \lambda f(\lambda,\omega).$$

So we compute that

$$\begin{aligned}[\mathcal{U}M\mathcal{U}^* f](\lambda,\omega) &= 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}}[M\mathcal{U}^* f](\lambda^{\frac{1}{2}}\omega) = 2^{-\frac{1}{2}}\lambda^{\frac{n+2}{4}}[\mathcal{U}^* f](\lambda^{\frac{1}{2}}\omega)\\ &= \lambda^{\frac{n+2}{4}}\lambda^{-\frac{n-2}{4}} f(|\lambda^{\frac{1}{2}}\omega|^2,\omega) = \lambda f(\lambda,\omega),\end{aligned}$$

which completes the proof. □

Lemma 2.2.8 shows that the operator F_0 provides a direct integral decomposition of the free Hamiltonian H_0. For a detailed discussion of direct integrals we refer the reader to [23, Section 7.1] and [74, Section 7.3]

Even though we have stated that the Fourier transform is not the ‘correct’ diagonalisation of H_0 for scattering purposes, there are still many applications of use to us. We now turn our attention to developing the functional calculus for H_0 explicitly. Since the Fourier transform provides a diagonalisation of H_0, the spectral theorem tells us exactly how to do this. For a function $f : \mathbb{R}^+ \to \mathbb{C}$ with rapidly decaying Fourier transform, we can define the operator $f(H_0)$ acting on a fixed $\psi \in \mathcal{S}(\mathbb{R}^n)$ by

$$[f(H_0)\psi](x) = [\mathcal{F}^*\mathcal{F}f(H_0)\psi](x) = [\mathcal{F}^* M_{\tilde{f}}\mathcal{F}\psi](x), \quad x \in \mathbb{R}^n, \tag{2.16}$$

where $\tilde{f}(\xi) = f(|\xi|^2)$. By writing out the Fourier transforms explicitly, we can write the operator $f(H_0)$ as an integral operator. For $x \in \mathbb{R}^n$ we have

$$\begin{aligned}[f(H_0)\psi](x) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{i\langle x,\xi\rangle} f(|\xi|^2)[\mathcal{F}\psi](\xi)\,\mathrm{d}\xi \\ &= (2\pi)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \mathrm{e}^{i\langle x,\xi\rangle}\mathrm{e}^{-i\langle \xi,y\rangle} f(|\xi|^2)\psi(y)\,\mathrm{d}y\,\mathrm{d}\xi \\ &= \int_{\mathbb{R}^n} K(x,y)\psi(y)\,\mathrm{d}y,\end{aligned}$$

where the integral kernel $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{C}$ is defined by

$$K(x,y) = (2\pi)^{-n} \int_{\mathbb{R}^n} \mathrm{e}^{-i\langle \xi, y-x\rangle} f(|\xi|^2)\,\mathrm{d}\xi, \quad x,y \in \mathbb{R}^n.$$

Defining the function $g : \mathbb{R}^n \to \mathbb{C}$ by $g(\xi) = f(|\xi|^2)$ we have

$$K(x,y) = (2\pi)^{-\frac{n}{2}}[\mathcal{F}g](y-x). \tag{2.17}$$

Thus we see that to describe a function f of the free Hamiltonian H_0 as an integral operator, we need f to be such that we can take the Fourier transform of $g(\xi) = f(|\xi|^2)$. Some preparatory work is required to compute such integrals.

Lemma 2.2.9. *For any $r \in (0,\infty)$ and $0 \neq y \in \mathbb{R}^n$ we have*

$$\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-ir\langle\omega,y\rangle}\,\mathrm{d}\omega = (2\pi)^{\frac{n}{2}}(r|y|)^{-\frac{n-2}{2}} J_{\frac{n-2}{2}}(r|y|), \tag{2.18}$$

where J_ν denotes the Bessel function of the first kind of order ν.

Proof. First we define the constant C_n via

$$C_n = \frac{\mathrm{Vol}(\mathbb{S}^{n-1})}{\int_0^\pi \sin^{n-2}(\theta_1)\,\mathrm{d}\theta_1}.$$

By using spherical coordinates, the volume of the n-sphere can be computed as

$$\begin{aligned}\mathrm{Vol}(\mathbb{S}^{n-1}) &= \int_0^\pi\int_0^\pi \cdots \int_0^\pi\int_0^{2\pi} \sin^{n-2}(\theta_1)\sin^{n-3}(\theta_2)\cdots\sin(\theta_{n-2})\,\mathrm{d}\theta_{n-1}\,\mathrm{d}\theta_{n-2}\,\cdots\,\mathrm{d}\theta_2\,\mathrm{d}\theta_1 \\ &= \frac{2\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}\right)}.\end{aligned}$$

This can be checked in many ways, for example by reducing each integral to a Beta function. We can evaluate the θ_1 integral, for example, via the substitution $u = \sin(\theta_1)$

to obtain

$$\begin{aligned}\int_0^\pi \sin^{n-2}(\theta_1)\,\mathrm{d}\theta_1 &= 2\int_0^{\frac{\pi}{2}} \sin^{n-2}(\theta_1)\,\mathrm{d}\theta_1 = 2\int_0^1 u^{n-2}(1-u^2)^{-\frac{1}{2}}\,\mathrm{d}u \\ &= \int_0^1 v^{\frac{n-3}{2}}(1-v)^{-\frac{1}{2}}\,\mathrm{d}v = \beta\left(\frac{n-1}{2},\frac{1}{2}\right) = \frac{\Gamma\left(\frac{n-1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)},\end{aligned}$$

where β denotes the Beta function and Γ the Gamma function. Thus we can write

$$C_n = \frac{2\pi^{\frac{n-1}{2}}}{\Gamma\left(\frac{n-1}{2}\right)} = \mathrm{Vol}\left(\mathbb{S}^{n-2}\right).$$

We are now able to evaluate the integral in Equation (2.18). Choose spherical coordinates so that θ_1 is the angle between ω and y. Thus $\langle\omega, y\rangle = |y|\cos(\theta_1)$. Then we find

$$\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-ir\langle\omega,y\rangle}\,\mathrm{d}\omega = C_n\int_0^\pi \mathrm{e}^{-ir|y|\cos(\theta_1)}\sin^{n-2}(\theta_1)\,\mathrm{d}\theta_1 = C_n\int_{-1}^1 \mathrm{e}^{-ir|y|u}(1-u^2)^{\frac{n-3}{2}}\,\mathrm{d}u.$$

We now recall a Poisson integral from [61, Equation 7.12.7] for $z \in \mathbb{C}$ and $\mathrm{Re}(\nu) > -1$

$$\int_{-1}^1 \mathrm{e}^{-izu}(1-u^2)^{\nu-\frac{1}{2}}\,\mathrm{d}u = \Gamma\left(\nu+\frac{1}{2}\right)\pi^{\frac{1}{2}}z^{-\nu}2^\nu J_\nu(z).$$

Thus with $z = r|y|$ and $\nu = \frac{n-2}{2}$ we find

$$\begin{aligned}\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-ir\langle\omega,y\rangle}\,\mathrm{d}\omega &= C_n\Gamma\left(\frac{n-1}{2}\right)\pi^{\frac{1}{2}}(r|y|)^{-\frac{n-2}{2}}2^{\frac{n-2}{2}}J_{\frac{n-2}{2}}(r|y|) \\ &= (2\pi)^{\frac{n}{2}}(r|y|)^{-\frac{n-2}{2}}J_{\frac{n-2}{2}}(r|y|),\end{aligned}$$

as required. □

The right hand side of Equation (2.18) is the integral kernel of the Hankel transform, which when combined with the statement of Lemma 2.2.9 give a description of the Fourier transform of functions which are invariant under rotations.

Definition 2.2.10. Let $\mathcal{S}(\mathbb{R}^+)$ be the restriction of odd Schwarz functions on all of $\mathbb{R}$ to the half-line. We define the *Hankel transform* of order $\nu \in \mathbb{C}$ with $\mathrm{Re}(\nu) > -1$, denoted $H_\nu : \mathcal{S}(\mathbb{R}^+) \to \mathcal{S}(\mathbb{R}^+)$ by

$$[H_\nu\psi](\mu) = \int_{\mathbb{R}^+} \psi(\lambda)(\mu\lambda)^{\frac{1}{2}}J_\nu(\mu\lambda)\,\mathrm{d}\lambda.$$

Remark 2.2.11. The Hankel transform is actually the integral transform diagonalising the differential operator associated to the Bessel differential equation obtained by considering only the radial component of H_0 in polar coordinates. We will make use of this transform in Chapter 4 when developing intuition for the form of the wave operators. Although we have only defined the Hankel transform for $\psi \in \mathcal{S}(\mathbb{R}^+)$, one can check that the Hankel transform extends to a unitary operator from $L^2(\mathbb{R}^+, r^{\frac{1}{2}}\,\mathrm{d}r)$ to itself, see [113]. A comprehensive collection of Hankel transforms can be found in [126].

Lemma 2.2.12. *Suppose $\psi \in \mathcal{S}(\mathbb{R}^n)$ is invariant under rotations. Let $\tilde{\psi}$ be defined by $\tilde{\psi}(r) = r^{\frac{n-1}{2}}\psi(r)$. Then the Fourier transform of ψ is given by*

$$[\mathcal{F}\psi](\xi) = |\xi|^{-\frac{n-1}{2}}[H_{\frac{n-2}{2}}\tilde{\psi}](|\xi|), \quad \xi \in \mathbb{R}^n,$$

where H_ν denotes the Hankel transform of order ν.

Proof. We take the Fourier transform of ψ and change to polar coordinates to obtain

$$[\mathcal{F}\psi](\xi) = (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n} \mathrm{e}^{-i\langle \xi, y\rangle}\psi(y)\,\mathrm{d}y = (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^+} r^{n-1}\psi(r)\left(\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-ir\langle \xi,\omega\rangle}\,\mathrm{d}\omega\right)\mathrm{d}r.$$

Applying Lemma 2.2.9 we then have

$$\begin{aligned}[\mathcal{F}\psi](\xi) &= (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^+} r^{n-1}\psi(r)\left((2\pi)^{\frac{n}{2}}(r|\xi|)^{-\frac{n-2}{2}}J_{\frac{n-2}{2}}(r|\xi|)\right)\mathrm{d}r\\ &= |\xi|^{-\frac{n-1}{2}}\int_{\mathbb{R}^+} r^{\frac{n-1}{2}}\psi(r)(r|\xi|)^{\frac{1}{2}}J_{\frac{n-2}{2}}(r|\xi|)\,\mathrm{d}r\\ &= |\xi|^{-\frac{n-1}{2}}[H_{\frac{n-2}{2}}\tilde{\psi}](|\xi|).\end{aligned}$$

□

An essential operator in our spectral analysis of H_0 is the resolvent operator. For $z \in \rho(H_0)$ with $\mathrm{Arg}(z) \in (0, 2\pi)$, we can define (using the holomorphic functional calculus) the resolvent operator (often called the free resolvent) by

$$R_0(z) = (H_0 - z)^{-1}. \tag{2.19}$$

We can apply the techniques just described to obtain an explicit formula for the free resolvent in any dimension.

Corollary 2.2.13. *For $z \in \rho(H_0)$ with $\mathrm{Arg}(z) \in (0, 2\pi)$ the integral kernel of the resolvent $R_0(z) = (H_0 - z)^{-1}$ is given for $x, y \in \mathbb{R}^n$, $x \neq y$, by*

$$R_0(x, y, z) = \frac{i}{4}(2\pi)^{-\frac{n-2}{2}}z^{\frac{n-2}{4}}|x-y|^{-\frac{n-2}{2}}H^{(1)}_{\frac{n-2}{2}}(z^{\frac{1}{2}}|x-y|), \tag{2.20}$$

where $H^{(1)}_\nu := J_\nu + iY_\nu$ denotes the Hankel function of the first kind of order ν, described in [1, Chapters 9 and 10].

Proof. For $r > 0$ define $\psi(r) = (r - z)^{-1}$, so that $R_0(z) = \psi(H_0)$. By [125, Equation

1.4.13] the Hankel transform of $\tilde{\psi}(r) = r^{\frac{n-1}{2}}(r^2 - z)^{-1}$ is given by

$$\left[H_{\frac{n-2}{2}}\tilde{\psi}\right](\mu) = \frac{i}{4}(2\pi)^{-1} z^{\frac{n-2}{4}} \mu^{\frac{1}{2}} H^{(1)}_{\frac{n-2}{2}}(z^{\frac{1}{2}}\mu). \tag{2.21}$$

Hence using Equation (2.17) the integral kernel of the free resolvent is given explicitly for $x, y \in \mathbb{R}^n$ by

$$R_0(x, y, z) = (2\pi)^{-\frac{n}{2}}[\mathcal{F}\psi](y - x) = \frac{i}{4}(2\pi)^{-\frac{n-2}{2}} z^{\frac{n-2}{4}} |x - y|^{-\frac{n-2}{2}} H^{(1)}_{\frac{n-2}{2}}(z^{\frac{1}{2}}|x - y|), \tag{2.22}$$

as claimed. □

In odd dimensions the formula is particularly nice, for example if $n = 3$ then

$$R_0(x, y, z) = \frac{\mathrm{e}^{iz^{\frac{1}{2}}|x-y|}}{4\pi|x - y|}. \tag{2.23}$$

One can explicitly compute the integral kernel of the resolvent in higher odd dimensions in terms of polynomials in $|x - y|$ also, see for example [56, Theorem 3.3]. The even dimensional cases are complicated by a logarithmic singularity of the Hankel function near the origin, as we shall see in Chapter 3 where we discuss expansions of the resolvent for small z.

2.2.2 The perturbed Hamiltonian

In this section we describe a class of perturbations of our free Hamiltonian H_0 by real valued potentials V satisfying certain decay assumptions. Such operators $H = H_0 + V$ are known as Schrödinger operators and have been studied extensively since the introduction of the Schrödinger equation in [147]. The study of such perturbations motivated much of the development of perturbation theory and thus the literature is vast, we refer the reader to [21, 23, 95, 135, 136, 137] and the references therein for a more comprehensive discussion.

The most basic and minimal assumption we make on our potential V is the following.

Assumption 2.2.14. The function $V : \mathbb{R}^n \to \mathbb{R}$ is real-valued and for almost all $x \in \mathbb{R}^n$ satisfies $|V(x)| \leq C(1 + |x|)^{-\rho}$ for some $\rho > 1$.

Throughout this thesis we will need to strengthen Assumption 2.2.14 in various places by requiring greater decay.

Lemma 2.2.15. *Suppose that V satisfies Assumption 2.2.14. Then the operator $H = H_0 + V$ is essentially self-adjoint with $\sigma_{ess}(H) = [0, \infty)$. Moreover, $C_c^\infty(\mathbb{R}^n)$ is a core for H.*

Proof. We use the Kato-Rellich theorem (see [135, Theorem X.12] for example). It is immediate that $\mathrm{Dom}(H_0) \subset \mathrm{Dom}(V) := \mathcal{H}$. For $z \in \rho(H_0)$ we have that $R_0(z)V$ is compact by [158, Lemma 7.21] and thus V is H_0-relatively compact. The Kato-Rellich theorem [135, Theorem X.12] then tells us that H is self-adjoint on $\mathrm{Dom}(H_0)$, bounded from below, and $\sigma_{ess}(H) = \sigma_{ess}(H_0) = [0, \infty)$. That $C_c^\infty(\mathbb{R}^n)$ is a core for H follows from the fact that it is a core for H_0. □

Definition 2.2.16. For a function V satisfying Assumption 2.2.14 we call the operator $H = H_0 + V$ a (short-range) *perturbed Hamiltonian.*

The following fact, due to Kato [93], guarantees that there are no eigenvalues of H embedded in the continuous spectrum. A simple proof in the case that V is compactly supported can be found as [164, Theorem 6.1.1].

Theorem 2.2.17 (Kato's theorem)**.** *Suppose that V satisfies Assumption 2.2.14. Then the operator $H = H_0 + V$ has no positive eigenvalues.*

The number of eigenvalues is known to be finite for $\rho > 2$, although proofs are rather involved so we provide only references. The statement we use here is [164, Section 7.4.2]. Many explicit bounds on the number of eigenvalues are discussed in [151, Chapter 7].

Theorem 2.2.18. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 2$. Then the operator $H = H_0 + V$ has finitely many eigenvalues.*

2.2.3 The dilation operator

We first consider the (one-dimensional) Dirac operator $D = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}$ with $\mathrm{Dom}(D) = C_c^\infty(\mathbb{R}) \subset L^2(\mathbb{R})$. It is well-known that D is essentially self-adjoint and so has a unique self-adjoint extension which we also denote by D. The one-dimensional Fourier transform shows that D is unitarily equivalent to the multiplication operator M defined by $[Mf](\xi) = \xi f(\xi)$ and thus $\sigma(D) = \sigma_{ac}(D) = \mathbb{R}$.

By Stone's theorem the operator D defines a strongly continuous one-parameter unitary group $(V(t))_{t\in\mathbb{R}}$ acting on $L^2(\mathbb{R})$. As is well-known, $V(t)$ acts on $f \in L^2(\mathbb{R})$ by

$$[V(t)f](x) = [\mathrm{e}^{-itD} f](x) = f(x - t) \tag{2.24}$$

so that D is the generator of the translation group on $\mathbb{R}$. Since the operator H_0 has absolutely continuous spectrum $\sigma(H_0) = [0, \infty)$ we are interested in the Hilbert space $L^2(\mathbb{R}^+)$. We can naturally identify $L^2(\mathbb{R}^+)$ with $L^2(\mathbb{R})$ via the following.

Lemma 2.2.19. *The map $L : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+)$ defined for $\lambda \in \mathbb{R}^+$ by $[Lf](\lambda) = \lambda^{-\frac{1}{2}} f(\ln(\lambda))$ is unitary.*

Proof. We check that for $f, g \in L^2(\mathbb{R})$ we have

$$\langle Lf, Lg\rangle = \int_{\mathbb{R}^+} \overline{[Lf](\lambda)}[Lg](\lambda)\,\mathrm{d}\lambda = \int_{\mathbb{R}^+} \lambda^{-1}\overline{f(\ln(\lambda))}g(\ln(\lambda))\,\mathrm{d}\lambda = \int_{\mathbb{R}} \overline{f(y)}g(y)\,\mathrm{d}y = \langle f, g\rangle,$$

where we have made the substitution $y = \ln(\lambda)$. So the map L is an isometry. The inverse map $L^{-1} : L^2(\mathbb{R}^+) \to L^2(\mathbb{R})$ is given for $y \in \mathbb{R}$ by $[L^{-1}g](y) = \mathrm{e}^{\frac{y}{2}}g(\mathrm{e}^y)$. It is readily checked that L^{-1} is an isometry also and thus L is unitary as claimed. □

The following result shows how the translation group of Equation (2.24) and the generator of translations act when mapped to $L^2(\mathbb{R}^+)$ by the unitary L.

Lemma 2.2.20. *The group $(U_+(t))_{t\in\mathbb{R}}$ defined by $U_+(t) = LV(-t)L^*$ is given for $\lambda \in \mathbb{R}^+$ by*

$$[U_+(t)f](\lambda) = \mathrm{e}^{\frac{t}{2}}f(\mathrm{e}^t\lambda)$$

and the action of the self-adjoint generator D_+ of U_+ on $f \in C_c^\infty(\mathbb{R}^+)$ is given, for $\lambda \in \mathbb{R}^+$, by

$$[D_+f](\lambda) = \left(\frac{\lambda}{i}\frac{\mathrm{d}f}{\mathrm{d}\lambda} + \frac{1}{2i}f(\lambda)\right).$$

Proof. Direct computation shows that for $f \in L^2(\mathbb{R}^+)$ and $\lambda \in \mathbb{R}^+$ we have

$$\begin{aligned}[U_+(t)f](\lambda) &= [LV(-t)L^*f](\lambda) = \lambda^{-\frac{1}{2}}[V(-t)L^*f](\ln(\lambda)) \\ &= \lambda^{-\frac{1}{2}}[L^*f](\ln(\lambda) + t) = \lambda^{-\frac{1}{2}}\mathrm{e}^{\frac{\ln(\lambda)+t}{2}}f(\mathrm{e}^{\ln(\lambda)+t}) = \mathrm{e}^{\frac{t}{2}}f(\mathrm{e}^t\lambda),\end{aligned}$$

as claimed. We can then use Stone's theorem to compute the self-adjoint generator D_+ of the unitary group $(U_+(t))$ via the computation

$$\begin{aligned}[D_+f](\lambda) &= -i\left(\frac{\mathrm{d}}{\mathrm{d}t}[U_+(t)f](\lambda)\right)\bigg|_{t=0} = -i\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\frac{t}{2}}f(\mathrm{e}^t\lambda)\right)\bigg|_{t=0} \\ &= -i\left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\mathrm{e}^{\frac{t}{2}}f(\mathrm{e}^t\lambda) + \lambda\mathrm{e}^{\frac{3t}{2}}f'(\mathrm{e}^t\lambda)\right)\bigg|_{t=0} = \left(\frac{1}{2i}f(\lambda) + \frac{\lambda}{i}f'(\lambda)\right),\end{aligned}$$

which shows that D_+ takes the form claimed. □

We call D_+ the generator of dilations on $L^2(\mathbb{R}^+)$ and use the group structure to describe a simple and useful functional calculus for D_+.

Lemma 2.2.21. *Suppose that $\varphi \in \mathcal{S}(\mathbb{R}^+)$ (with $\mathcal{S}(\mathbb{R}^+)$ defined in Definition 2.2.10). Then for $f \in \mathrm{Dom}(D_+)$ we have*

$$[\varphi(D_+)f](\lambda) = (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}} [\mathcal{F}^*\varphi](t)[U_+(t)f](\lambda)\,\mathrm{d}t, \quad \lambda \in \mathbb{R}^+.$$

Proof. We let $\varphi \in \mathcal{S}(\mathbb{R}^+)$ and define for $\xi \in \mathbb{R}$ the multiplication operator $[M_\varphi f](\xi) = \varphi(-\xi)f(\xi)$. Then for $\lambda \in \mathbb{R}^+$ we have

$$\begin{aligned}[\varphi(D_+)f](\lambda) &= [LL^*\varphi(D_+)f](\lambda) = [L\varphi(-D)L^*f](\lambda)\\ &= [L\mathcal{F}\mathcal{F}^*\varphi(-D)L^*f](\lambda) = [L\mathcal{F}M_\varphi\mathcal{F}^*L^*f](\lambda).\end{aligned}$$

For $\xi \in \mathbb{R}$ we can explicitly write

$$\begin{aligned}[\mathcal{F}M_\varphi\mathcal{F}^*g](\xi) &= (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}} \mathrm{e}^{-iy\xi}\varphi(y)[\mathcal{F}^*g](y)\,\mathrm{d}y\\ &= (2\pi)^{-1}\int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{e}^{-iy(\xi-u)}\varphi(-y)g(u)\,\mathrm{d}u\,\mathrm{d}y\\ &= (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}\left((2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}} \mathrm{e}^{-iy(\xi-u)}\varphi(-y)\,\mathrm{d}y\right)\mathrm{d}u\\ &= (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}\varphi](u-\xi)g(u)\,\mathrm{d}u.\end{aligned}$$

So for $\lambda \in \mathbb{R}^+$ we find

$$\begin{aligned}[\varphi(D_+)f](\lambda) &= [L\mathcal{F}M_\varphi\mathcal{F}^*L^*f](\lambda) = \lambda^{-\frac{1}{2}}[\mathcal{F}M_\varphi\mathcal{F}^*L^*f](\ln(\lambda))\\ &= (2\pi)^{-\frac{1}{2}}\lambda^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}\varphi](u-\ln(\lambda))[L^*f](u)\,\mathrm{d}u\\ &= (2\pi)^{-\frac{1}{2}}\lambda^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}\varphi](u-\ln(\lambda))\mathrm{e}^{\frac{u}{2}}f(\mathrm{e}^u)\,\mathrm{d}u.\end{aligned}$$

Now make the substitution $t = \ln(\lambda) - u$ to obtain

$$\begin{aligned}[\varphi(D_+)f](\lambda) &= (2\pi)^{-\frac{1}{2}}\lambda^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}^*\varphi](\ln(\lambda)-u)\mathrm{e}^{\frac{u}{2}}f(\mathrm{e}^u)\,\mathrm{d}u\\ &= (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}^*\varphi](t)\mathrm{e}^{-\frac{t}{2}}f(\mathrm{e}^{-t}\lambda)\,\mathrm{d}t\\ &= (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}^*\varphi](t)[U_+(t)f](\lambda)\,\mathrm{d}t,\end{aligned}$$

which completes the proof. □

We can now construct an operator which diagonalises the generator of dilations by using our unitaries.

Definition 2.2.22. We define the *Mellin transform* $\mathcal{M} : L^2(\mathbb{R}^+) \to L^2(\mathbb{R})$ by $\mathcal{M} = \mathcal{F}L^*$, where L is defined in Lemma 2.2.19 .

Lemma 2.2.23. *The Mellin transform is given explicitly for $f \in C_c^\infty(\mathbb{R}^+)$ and $x \in \mathbb{R}$ by*

$$[\mathcal{M}f](x) = (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}^+} y^{-\frac{1}{2}-ix}f(y)\,\mathrm{d}y \tag{2.25}$$

and satisfies $\mathcal{M}D_+\mathcal{M}^* = M$*, where* M *is the multiplication operator by the variable in* $L^2(\mathbb{R})$*.*

Proof. Equation (2.25) follows from the definitions of $\mathcal{F}$ and L. The diagonalisation relation is a consequence of the relation $D_+ = L^*DL$ and the fact that the Fourier transform diagonalises the differentiation operator D. □

We can easily generalise the group of dilations to $L^2(\mathbb{R}^n)$ also.

Definition 2.2.24. We define the *dilation group* $(U_n(t))_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^n)$ by the formula

$$[U_n(t)f](x) = \mathrm{e}^{\frac{nt}{2}} f(\mathrm{e}^t x), \quad x \in \mathbb{R}^n.$$

Lemma 2.2.25. *We have that* $(U_n(t))$ *is a strongly continuous one-parameter unitary group and the self-adjoint generator* D_n *of* U_n *is given on* $f \in C_c^\infty(\mathbb{R}^n)$ *by*

$$[D_n f](x) = \frac{1}{i}\sum_{j=1}^n x_j \frac{\partial f}{\partial x_j} + \frac{n}{2i} f(x), \quad x \in \mathbb{R}^n.$$

Proof. That $(U_n(t))$ defines a strongly continuous one-parameter unitary group can be readily checked. Fix $f \in C_c^\infty(\mathbb{R}^n)$. To determine the self-adjoint generator D_n, we again use Stone's theorem to find for $x \in \mathbb{R}^n$ that

$$\begin{aligned}
[D_n f](x) &= -i\left(\frac{\mathrm{d}}{\mathrm{d}t}[U_n(t)f](x)\right)\Big|_{t=0} = -i\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\frac{nt}{2}} f(\mathrm{e}^t x)\right)\Big|_{t=0} \\
&= -i\left(\frac{n}{2}\mathrm{e}^{\frac{nt}{2}} f(\mathrm{e}^t x) + \mathrm{e}^{\frac{nt}{2}} \sum_{j=1}^n \frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{e}^t x_j)\frac{\partial f}{\partial x_j}(\mathrm{e}^t x)\right)\Big|_{t=0} \\
&= -i\left(\frac{n}{2} f(x) + \sum_{j=1}^n x_j \frac{\partial f}{\partial x_j}\right),
\end{aligned}$$

so that D_n is given by the claimed formula. □

Lemma 2.2.26. *The operator* D_n *anticommutes with the Fourier transform. The operator* $\mathcal{U}$ *of Definition 2.2.7 satisfies* $\mathcal{U}D_n\mathcal{U}^* = 2D_+ \otimes \mathrm{Id}$*, and* $F_0 D_n F_0^* = -2D_+ \otimes \mathrm{Id}$*.*

Proof. For $f \in C_c^\infty(\mathbb{R}^n)$ define the operators M_j by $[M_j f](x) = x_j \frac{\partial f}{\partial x_j}$. We compute for $\xi \in \mathbb{R}^n$ that

$$[\mathcal{F}M_j f](\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\langle x,\xi\rangle}[M_j f](x)\,\mathrm{d}x = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\langle x,\xi\rangle} x_j \frac{\partial f}{\partial x_j}\,\mathrm{d}x.$$

Integrating by parts in the x_j variable and using the compact support of f to eliminate boundary conditions we obtain for $\xi \in \mathbb{R}^n$ that

$$\begin{aligned}
[\mathcal{F}M_j f](\xi) &= -(2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(x) \frac{\partial}{\partial x_j} \left(x_j \mathrm{e}^{-i\langle x,\xi\rangle} \right) \mathrm{d}x \\
&= -(2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(x) \mathrm{e}^{-i\langle x,\xi\rangle} \,\mathrm{d}x - \xi_j (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(x)(-ix_j) \mathrm{e}^{-i\langle x,\xi\rangle} \,\mathrm{d}x \\
&= -[\mathcal{F}f](\xi) - \xi_j \frac{\partial}{\partial \xi_j} [\mathcal{F}f](\xi) \\
&= -[(\mathrm{Id} + M_j)\mathcal{F}f](\xi).
\end{aligned}$$

Using Lemma 2.2.25 the operator D_n is given by

$$D_n = \frac{n}{2i} \mathrm{Id} + \frac{1}{i} \sum_{j=1}^{n} M_j.$$

So for $f \in C_c^\infty(\mathbb{R}^n)$ and $\xi \in \mathbb{R}^n$ we find

$$\begin{aligned}
[\mathcal{F}D_n f](\xi) &= \frac{n}{2i}[\mathcal{F}f](\xi) + \frac{1}{i} \sum_{j=1}^{n} [\mathcal{F}M_j f](\xi) = \frac{n}{2i}[\mathcal{F}f](\xi) - \frac{1}{i} \sum_{j=1}^{n} [(\mathrm{Id} + M_j)\mathcal{F}f](\xi) \\
&= -\frac{n}{2i}[\mathcal{F}f](\xi) - \frac{1}{i} \sum_{j=1}^{n} [M_j \mathcal{F}f](\xi) = -[D_n \mathcal{F}f](\xi),
\end{aligned}$$

so that D_n anticommutes with $\mathcal{F}$. Fix $\lambda \in \mathbb{R}^+$ and $\omega \in \mathbb{S}^{n-1}$. We next check that for $f \in C_c^\infty(\mathbb{R}^n)$ that

$$[\mathcal{U}M_j f](\lambda, \omega) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} [M_j f](\lambda^{\frac{1}{2}}\omega) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} \lambda^{\frac{1}{2}} \omega_j \frac{\partial f}{\partial x_j}(\lambda^{\frac{1}{2}}\omega).$$

So for $f \in C_c^\infty(\mathbb{R}^n)$ we use the chain rule to see that

$$\begin{aligned}
\sum_{j=1}^{n} [\mathcal{U}M_j f](\lambda, \omega) &= \sum_{j=1}^{n} \left(2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} \lambda^{\frac{1}{2}} \omega_j \frac{\partial f}{\partial x_j}(\lambda^{\frac{1}{2}}\omega) \right) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} 2\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} f(\lambda^{\frac{1}{2}}\omega) \\
&= 2\lambda \left(\frac{\mathrm{d}}{\mathrm{d}\lambda} \otimes \mathrm{Id} \right) ([\mathcal{U}f](\lambda, \omega)) - \frac{n-2}{2} [\mathcal{U}f](\lambda, \omega).
\end{aligned}$$

Thus for $f \in C_c^\infty(\mathbb{R}^n)$ we find

$$\begin{aligned}
[\mathcal{U}D_n f](\lambda, \omega) &= \frac{n}{2i}[\mathcal{U}f](\lambda, \omega) + \frac{1}{i} \sum_{j=1}^{n} [\mathcal{U}M_j f](\lambda, \omega) \\
&= \frac{n}{2i}[\mathcal{U}f](\lambda, \omega) + \left(\left[2 \left(\frac{\mathrm{d}}{\mathrm{d}\lambda} \otimes \mathrm{Id} \right) \mathcal{U}f \right] (\lambda, \omega) - \frac{n-2}{2i} [\mathcal{U}f](\lambda, \omega) \right) \\
&= 2 \left[(D_+ \otimes \mathrm{Id}) \mathcal{U}f \right] (\lambda, \omega)
\end{aligned}$$

and so $\mathcal{U}D_n\mathcal{U}^* = 2(D_+ \otimes \mathrm{Id})$. The final claim now follows from the definition $F_0 = \mathcal{U}\mathcal{F}$. □

Corollary 2.2.27. *We have* $\sigma(D_n) = \sigma_{ac}(D_n) = \mathbb{R}$.

Proof. Lemma 2.2.26 shows that D_n is unitarily equivalent to $D_+ \otimes \mathrm{Id}_{\mathcal{P}}$ (where $\mathcal{P} = L^2(\mathbb{S}^{n-1})$), which is in turn unitarily equivalent to $D \otimes \mathrm{Id}_{\mathcal{P}}$ by Lemma 2.2.20. Thus we find that D_n has purely absolutely continuous spectrum and $\sigma_{ac}(D_n) = \sigma_{ac}(D \otimes \mathrm{Id}_{\mathcal{P}}) = \mathbb{R}$. □

Corollary 2.2.28. *Let* $B = \frac{1}{2}\ln(H_0)$ *acting on* $\mathcal{H} = L^2(\mathbb{R}^n)$. *Then we have* $[D_n, B] = i\mathrm{Id}$.

Proof. It is well-known that the operator $M : \mathrm{Dom}(D) \to L^2(\mathbb{R})$ defined for $f \in C_c^\infty(\mathbb{R})$ and $\xi \in \mathbb{R}$ by $[Mf](\xi) = \xi f(\xi)$ satisfies the relation $[D, M] = -i\mathrm{Id}$ on $\mathrm{Dom}(D)$. Define for $g \in C_c^\infty(\mathbb{R}^+)$ and $\lambda \in \mathbb{R}^+$ the operator $M_{\ln}$ on $C_c^\infty(\mathbb{R}^+)$ by $[M_{\ln}g](\lambda) = \ln(\lambda)g(\lambda)$. We can compute that

$$\begin{aligned}[D_n, B] &= F_0^*F_0[D_n, B]F_0^*F_0 = F_0^*[F_0D_nF_0^*, F_0BF_0^*]F_0 \\ &= F_0^*[-2(D_+ \otimes \mathrm{Id}), \frac{1}{2}(M_{\ln} \otimes \mathrm{Id})]F_0 = -F_0^*([D_+, M_{\ln}] \otimes \mathrm{Id})F_0.\end{aligned}$$

Conjugating by the unitary L of Lemma 2.2.19 we find

$$\begin{aligned}[D_n, B] &= -F_0^*([D_+, M_{\ln}] \otimes \mathrm{Id})F_0 = -F_0^*(L \otimes \mathrm{Id})[L^*D_+L, L^*M_{\ln}L](L^* \otimes \mathrm{Id})F_0 \\ &= -F_0^*(L \otimes \mathrm{Id})[D, M](L^* \otimes \mathrm{Id})F_0 = i\mathrm{Id},\end{aligned}$$

as claimed. □

Corollary 2.2.28 shows that the operators B and D_n are canonically conjugate and thus we can use Stone-von Neumann theorem methods of [151, Chapter 4] (with some modifications, see Lemma 4.2.6) to deduce the compactness of operators of the form $f(D_n)g(B)$. The basic result is the following.

Theorem 2.2.29 ([151, Theorem 4.1])**.** *If* $f, g \in L^p(\mathbb{R}^n)$ *with* $p \in [2, \infty)$ *then we have the inclusion* $f(X)g(D) \in \mathcal{L}^p(\mathcal{H})$ *(the p-th Schatten class)*

$$||f(X)g(D)||_p \leq (2\pi)^{-\frac{n}{p}} ||f||_p ||g||_p .$$

We can use the structure of the dilation group to obtain a useful form of the functional calculus for D_n in an analogous manner to the functional calculus for D_+ in Lemma 2.2.21

Lemma 2.2.30. *Suppose that* $\varphi \in \mathcal{S}(\mathbb{R})$. *Then for* $f \in \mathrm{Dom}(D_n)$ *we have*

$$[\varphi(D_n)f](x) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\varphi](t)[U_n(t)f](x)\,\mathrm{d}t.$$

Definition 2.2.31. We denote by $P_\pm$ the positive and negative spectral projections of D_n, so that $P_+ = \chi_{[0,\infty)}(D_n)$, $P_- = \chi_{(-\infty,0)}(D_n)$ and $P_+ + P_- = \mathrm{Id}$.

The spectral projections $P_\pm$ will be used in the proof of the asymptotic completeness of the wave operators for the pair (H, H_0) and the absence of singular continuous spectrum of H in Section 2.3.

2.3 Existence and completeness for Schrödinger operators

In this section we demonstrate both the existence and asymptotic completeness of the wave operators for Schrödinger operators with potentials satisfying Assumption 2.2.14. The generator of dilations is used in a rather remarkable way to demonstrate the asymptotic completeness of the wave operators for a short range potential. This geometric approach to asymptotic completeness is due to Enss [58, 59, 60]. There are other methods of obtaining asymptotic completeness, for example the method of H_0-smoothness discussed in [164, Chapter 1.6]. The technique we present here follows closely that of Perry [128] (see also [127, Chapter 12] for more details in dimension $n = 3$).

We first apply Cook's criterion in the manner described in [106, Section 3.4] to obtain the existence of the wave operators.

Theorem 2.3.1. *Let $H = H_0 + V$ with V satisfying Assumption 2.2.14. Then the wave operators $W_\pm(H, H_0)$ exist.*

Proof. By Cook's criterion it suffices to show that

$$\int_{\mathbb{R}} \left|\left|V e^{-itH_0} f\right|\right|_2 \, dt < \infty \tag{2.26}$$

for $\mathcal{F}f \in C_c^\infty(\mathbb{R}^n \setminus \{0\})$. Suppose that $[\mathcal{F}f](\xi) = 0$ for $|\xi| \leq r$ and let P_r denote the projection onto functions supported on the ball of radius r in $\mathbb{R}^n$. Then we have

$$\left|\left|V e^{-itH_0} f\right|\right|_2 \leq ||V||_\infty \left|\left|P_{r|t|} e^{-iH_0 t} f\right|\right|_2 + \left|\left|V(\mathrm{Id} - P_{r|t|})\right|\right|_\infty ||f||_2 .$$

The method of stationary phase (see [78, Lemma A.1]) and [164, Lemma 1.2.5] show that the first term on the right hand side is bounded by any positive integer power of $|t|^{-1}$. Since V satisfies Assumption 2.2.14 for some $\rho > 1$, the second term on the right hand side is $O(|t|^{-\rho})$ and thus the integral in Equation (2.26) is finite. □

To deduce the compactness of certain operators, we need the following result, which can be found as [128, Lemma 4].

Theorem 2.3.2. *Suppose that $f \in C_0(\mathbb{R})$ and that V satisfies Assumption 2.2.14 for some $\rho > \frac{n}{2}$. Then the operator $f(H) - f(H_0)$ is compact.*

Proof. The assumption $\rho > \frac{n}{2}$ guarantees that $R(z) - R_0(z) \in \mathcal{L}^p(\mathcal{H})$ for all $p > n$ and $z \in \mathbb{C} \setminus \mathbb{R}$ and is thus compact. By analogous arguments to [150, Lemma 4] one can show that $R(-i)^j R(i)^\ell - R_0(-i)^j R_0(i)^\ell$ is compact for all $j, \ell \in \mathbb{N}$ and thus by Stone-Weierstrass the conclusion follows for arbitrary $f \in C_0(\mathbb{R})$. □

We now proceed to the proof of asymptotic completeness of the wave operators, following closely the method of Perry [128]. The key tool in the following argument is the dilation operator D_n and the Mellin transform diagonalising D_n.

Definition 2.3.3. The *Mellin transform* $\mathcal{M} : C_c^\infty(\mathbb{R}^n \setminus \{0\}) \to L^2(\mathbb{R}) \otimes \mathcal{P}$ is defined for $f \in C_c^\infty(\mathbb{R}^n \setminus \{0\})$, $s \in \mathbb{R}$ and $\omega \in \mathbb{S}^{n-1}$ by

$$[\mathcal{M}f](s,\omega) = (2\pi)^{-\frac{1}{2}} \int_0^\infty \lambda^{\frac{n-2}{2} - is} f(\lambda\omega)\, \mathrm{d}\lambda.$$

The Mellin transform extends to a unitary operator $\mathcal{M} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}) \otimes \mathcal{P}$ which satisfies $\mathcal{M} D_n \mathcal{M}^* = M_s$, the operator of multiplication by the first variable on $L^2(\mathbb{R}) \otimes \mathcal{P}$. Recall the non-negative and negative spectral projections $P_\pm$ for D_n of Definition 2.2.31. As usual for $z \in \mathbb{C} \setminus \mathbb{R}$ we write $R(z) = (H - z)^{-1}$ and $R_0(z) = (H_0 - z)^{-1}$.

Lemma 2.3.4. *Let $g \in C_c^\infty(\mathbb{R}^+)$ have support in an interval $[a,b]$ and let $\delta \in (0,a)$. Let $\tilde{\chi}_A$ denote the characteristic function of a set $A \subset \mathbb{R}^n$. Let $k \in \mathbb{N}$ and $t \in (0, \pm\infty)$. For $|x| < \delta|t|$ define $K_{x,t} \in C_c^\infty(\mathbb{R}^n \setminus \{0\})$ by*

$$K_{x,t}(\xi) = \mathrm{e}^{i|\xi|^2 t - i\langle \xi, x\rangle} \overline{g(|\xi|^2)}. \tag{2.27}$$

Then we have for $\pm t > 0$ the estimate

$$||P_\mp K_{x,t}|| \le C_k (1 + |t|)^{-k + \frac{1}{2}}$$

for some constant C_k.

Proof. We show only the case $t > 0$, since the case $t < 0$ is similar. Using the unitarity of the Mellin transform we have $||P_- K_{x,t}|| = \left|\left|\chi_{(-\infty,0)} \mathcal{M} K_{x,t}\right|\right|$. Since $K_{x,t} \in C_c^\infty(\mathbb{R}^n \setminus \{0\})$, we have for $s \in \mathbb{R}$ and $\omega \in \mathbb{S}^{n-1}$ that

$$[\mathcal{M} K_{x,t}](s,\omega) = (2\pi)^{-\frac{1}{2}} \int_0^\infty \lambda^{\frac{n-2}{2}} \mathrm{e}^{it\lambda^2 - i\langle \lambda\omega, x\rangle - is\log(\lambda)} \overline{g(\lambda^2)}\, \mathrm{d}\lambda.$$

The function $f : (0,\infty) \to \mathbb{C}$ defined by $f(\lambda) = \lambda^{\frac{n-2}{2}} \overline{g(\lambda^2)}$ is smooth and compactly supported. The phase function $\phi_{x,s,t} = \phi : \mathbb{R}^+ \times \mathbb{S}^{n-1} \to \mathbb{R}$, defined by $\phi(\lambda,\omega) = t\lambda^2 - i\langle \lambda x, \omega\rangle - is\log(\lambda)$, has derivative $\frac{\partial \phi}{\partial \lambda} = 2\lambda t - \langle x, \omega\rangle - \frac{s}{\lambda}$ has no stationary points for the allowed range of x, t, s. The method of stationary phase [78, Lemma A.3] then gives the pointwise estimate

$$|[\mathcal{M}K_{x,t}](s,\omega)| < C_{N,g}(1+|t|+|s|)^{-k}.$$

Integrating this estimate in s and ω gives directly the statement of the lemma. □

Lemma 2.3.5. *Let $g \in C_c^\infty(\mathbb{R}^+)$ have support in an interval $[a^2, b^2]$ and let $\delta \in (0,a)$. Let χ_A denote the characteristic function of a set $A \subset \mathbb{R}^n$. Then for any $k \in \mathbb{N}$ and $t \in (0, \pm\infty)$ we have*

$$\left|\left|\chi_{B(\delta|t|)} \mathrm{e}^{-itH_0} g(H_0) P_\pm \right|\right| \le C_{N,g}(1+|t|)^{-k+n+1},$$

where $B(\delta|t|) = \{y \in \mathbb{R}^n : |y| < \delta|t|\}$, the open ball of radius $\delta|t|$.

Proof. For $x \in \mathbb{R}^n$, $g \in C_c^\infty(\mathbb{R}^+)$ and $\psi \in C_c^\infty(\mathbb{R}^n)$ define

$$\psi_{t\pm}(x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{i\langle \xi, x\rangle - i|\xi|^2 t} g(|\xi|^2)[P_\pm \mathcal{F}\psi](\xi)\, \mathrm{d}\xi.$$

We consider the equality $\psi_{t\pm}(x) = \langle K_{x,t}, P_\mp \mathcal{F}\psi\rangle$. The Cauchy-Schwarz inequality then gives us

$$|\psi_{t\pm}(x)| = |\langle K_{x,t}, P_\mp \mathcal{F}\psi\rangle| = |\langle P_\mp K_{x,t}, \mathcal{F}\psi\rangle| \le ||P_\mp K_{x,t}||\, ||\psi||\,.$$

By Lemma 2.3.4 we find $||P_\mp K_{x,t}|| \le C_{k,g}(1+|t|)^{-k+\frac{1}{2}}$ and thus

$$|\psi_{t\pm}(x)| \le C_{k,g}(1+|t|)^{-k+\frac{1}{2}}\, ||\psi||\,.$$

We thus find

$$\begin{aligned}
\left|\left|\chi_{B(\delta|t|)} \mathrm{e}^{-itH_0} g(H_0) P_\pm \right|\right|^2 &= \sup_{||\psi||=1} \int_{|x|\le\delta|t|} \left|\left[\mathrm{e}^{-itH_0} g(H_0) P_\pm \psi\right](x)\right|^2 \mathrm{d}x \\
&= \sup_{||\psi||=1} \int_{|x|<\delta|t|} |\psi_{t\pm}(x)|^2 \,\mathrm{d}x \\
&\le C_{k,g}^2 \int_{|x|<\delta|t|} (1+|t|)^{-2k+1}\,\mathrm{d}x \\
&= \tilde{C}\delta^n |t|^n (1+|t|)^{-2k+1} \\
&\le \tilde{C}\delta^n (1+|t|)^{-2k+n+1},
\end{aligned}$$

from which the claim follows. □

Lemma 2.3.6. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > n$. Let $\alpha \ge 1$ and $g \in C_c^\infty(\mathbb{R}^+)$. Then the operator $B = (H+i)^{-\alpha}(W_\mp - \mathrm{Id})g(H_0)P_\pm$ is compact.*

Proof. We show that B is the norm limit of compact operators. Consider for $\pm t > 0$ the equality

$$R(-i)^\alpha(\mathrm{e}^{itH}\mathrm{e}^{-itH_0} - \mathrm{Id})g(H_0)P_\pm = \int_0^t R(-i)^\alpha \mathrm{e}^{isH} V \mathrm{e}^{-isH_0} g(H_0)P_\pm \,\mathrm{d}s. \tag{2.28}$$

Since the family $s \mapsto \mathrm{e}^{isH}$ is strongly continuous, $s \mapsto \mathrm{e}^{-isH_0}g(H_0)$ is norm continuous and the operator $R(-i) - R_0(-i)$ is compact (see the proof of Theorem 2.3.2), we find that the right-hand side of Equation (2.28) defines a compact operator for finite t. It therefore suffices to show that the map $s \mapsto \left|\left|R(-i)^\alpha \mathrm{e}^{isH} V \mathrm{e}^{-isH_0} g(H_0)P_\pm\right|\right|$ defines an integrable function on $(0, \pm\infty)$. So we make for $\beta \geq 1$ the estimate

$$\begin{aligned}\left|\left|R(-i)^\alpha V \mathrm{e}^{-itH_0} g(H_0)P_\pm\right|\right| \leq \left|\left|R(-i)^\alpha V R_0(-i)^\beta\right|\right| \left|\left|\chi_{B(\delta|t|)}\mathrm{e}^{-itH_0}R_0(-i)^{-\beta}g(H_0)P_\pm\right|\right| \\ + C\left|\left|R(-i)^\alpha V R_0(-i)^\beta \chi_{B(\delta|t|)^c}\right|\right|.\end{aligned}$$

By Lemma 2.3.5 the first term decays rapidly in t and is thus integrable. The second term is integrable by our assumption on the potential. Thus we have shown that the operator B is the norm limit of compact operators and is hence compact. □

Theorem 2.3.7. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. Then the wave operators $W_\pm$ are asymptotically complete.*

Proof. We first show that H has no singular continuous spectrum. Let $P_A(H)$ be the proejection onto the spectral subspace of H associated to the Borel set $A \subset \mathbb{R}$. For an interval I, let $P_{sc,I} = P_{sc}(H)P_I(H)$, where $P_{sc}(H)$ denotes the projection onto the singular continuous spectrum of H. Let $\alpha, \beta \geq 1$ and $g \in C_c^\infty(\mathbb{R}^+)$. By Proposition 2.1.3 we have $W_\pm W_\pm^* = P_{ac}(H)$ and $W_\pm^* W_\pm = \mathrm{Id}$. So we find

$$P_{sc}(H)W_\pm = P_{sc}(H)W_\pm W_\pm^* W_\pm = P_{sc}(H)P_{ac}(H)W_\pm = 0.$$

By an adjoint calculation we have $W_\pm^* P_{sc}(H) = 0$. The operators $P_\mp g(H_0)(W_\pm^* - \mathrm{Id})R(-i)^\alpha$ are compact. Thus we find

$$\begin{aligned} g(H_0)(H+i)^{-\alpha}P_{sc,I} &= g(H_0)R(-i)^\alpha P_{sc}(H)P_I(H) \\ &= (P_+ + P_-)g(H_0)R(-i)^\alpha P_{sc}(H)P_I(H) \\ &= -(P_+ + P_-)g(H_0)(W_\pm^* - \mathrm{Id})R(-i)^\alpha P_{sc}(H)P_I(H), \end{aligned}$$

so that $g(H_0)R(-i)^\alpha P_{sc,I}$ is compact. Define the function $\tilde{g}$ by $\tilde{g}(\lambda) = g(\lambda)(\lambda + i)^{-1}$ and choose g such that $\tilde{g} = 1$ on I. Then $P_{sc,I}$ is a compact projection, so is finite rank and hence is zero.

We next show that W_- is complete, with the proof for W_+ being similar. Suppose that $f \in \mathcal{H}_{ac}(H)$ with $f \in \mathrm{Range}(W_-)^\perp$. Without loss of generality we may suppose that there exists $g \in C_c^\infty(\mathbb{R}^+)$ with $g(H)f = f$. Then the vectors $f_t = \mathrm{e}^{-itH} f$ converge weakly to 0 as $t \to \infty$. For $\alpha \geq 1$ we thus have

$$||f||^2 = \langle f_t, f_t \rangle = \langle R(-i)^\alpha f_t, R(-i)^{-\alpha} f_t \rangle,$$

since $f \in \mathrm{Dom}(R(-i)^{-\alpha})$. The compactness of $R(-i)^\alpha (W_\mp - \mathrm{Id}) g(H_0) P_\pm$ and Theorem 2.3.2 then give

$$R(-i)^\alpha f_t - [R(-i)^\alpha W_+ g(H_0) P_- f_t + R(-i)^\alpha W_- g(H_0) P_+ f_t] \to 0$$

strongly as $t \to \infty$. So

$$||f||^2 = \lim_{t\to\infty} [\langle f_t, W_+ g(H_0) P_- f_t \rangle + \langle f_t, W_- g(H_0) P_+ f_t \rangle].$$

Since e^{-itH} leaves $\mathrm{Range}(W_-)$ invariant and $f \in \mathrm{Range}(W_-)^\perp$ we have that the second term vanishes. As $t \to \infty$, the first vanishes since

$$\langle f_t, W_+ g(H_0) P_- f_t \rangle = \langle P_- g(H_0) \mathrm{e}^{-itH_0} W_+^* f, f_t \rangle$$

and $P_- g(H_0) \mathrm{e}^{-itH_0} \to 0$ strongly as $t \to \infty$ by an adjoint estimate to Lemma 2.3.5. □

Remark 2.3.8. Theorem 2.3.7 can be proved under the weaker assumption that V satisfies Assumption 2.2.14 for some $\rho > 1$ (see [164, Theorem 1.6.2]), however the proof method we have provided emphasises the key role of the generator of dilations in scattering theory.

Proposition 2.3.9. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 1$. The wave operators $W_\pm(H, H_0)$ are Fredholm and the number of bound states (eigenvalues counted with multiplicity) of $H = H_0 + V$, denoted by N, is given by*

$$\mathrm{Index}(W_\pm) = -N.$$

Proof. Note first that by Theorem 2.2.18 the projection P_p onto the eigenspace of H is finite rank. If $f \in \mathrm{Ker}(W_\pm)$ then the relation $W_\pm^* W_\pm = \mathrm{Id}$ shows $f = 0$. Suppose $f \in \mathrm{Ker}(W_\pm^*)$. By Theorem 2.3.7 we have that H has no singular continuous spectrum and thus $P_{ac}(H) = \mathrm{Id} - P_p(H)$. The relation $W_\pm W_\pm^* = P_{ac}(H) = \mathrm{Id} - P_p(H)$ then shows $P_p f = f$ and thus f is an eigenfunction for H. Conversely, if f is an eigenfunction for H we have $W_\pm^* f = 0$ and thus $f \in \mathrm{Ker}(W_\pm^*)$, so that $\mathrm{Ker}(W_\pm^*) = P_p \mathcal{H}$. Hence $W_\pm$ are Fredholm operators and we can compute

$$\mathrm{Index}(W_\pm) = \mathrm{Dim}(\mathrm{Ker}(W_\pm)) - \mathrm{Dim}(\mathrm{Ker}(W_\pm^*)) = 0 - N = -N.$$ □

2.4 Spectral properties of the perturbed Hamiltonian

The existence and asymptotic completeness of the wave operators proved in the previous section shows that $\sigma_{ac}(H) = \sigma_{ac}(H_0) = [0, \infty)$. In this section we first describe the point spectrum of the perturbed Hamiltonian. Then we describe the limiting absorption principle for boundary values of the resolvent and use this to define a family of generalised eigenfunctions for H. The limiting absorption principle also allows us to obtain explicit stationary formulas for the wave and scattering operators in terms of generalised eigenfunctions.

We shall regularly use the well known fact [110, p. 44] that a function in $H^{s,0}$ with $s > \frac{1}{2}$ has a trace (in the sense of restriction) on any smooth $(n-1)$-dimensional manifold embedded in $\mathbb{R}^n$.

Theorem 2.4.1. *Let Ω be a smooth compact $(n-1)$-dimensional manifold embedded in $\mathbb{R}^n$ and let $\mathrm{d}\omega$ be the measure induced on Ω by Lebesgue measure. Then for any $s > \frac{1}{2}$ there exists a bounded linear map $\tau : H^{s,0} \to L^2(\Omega)$ such that $\tau f = f|_\Omega$ for $u \in H^{s,0} \cap C(\mathbb{R}^n)$.*

In particular, for $\lambda > 0$ and $s > \frac{1}{2}$ we shall often let $\Omega = \mathbb{S}^{n-1}$ and denote for $\lambda > 0$ the trace operator by $\gamma(\lambda^{\frac{1}{2}}) : H^{s,0} \to L^2(\mathbb{S}^{n-1})$, whose action on $f \in H^{s,0}$ is given by

$$[\gamma(\lambda^{\frac{1}{2}})f](\omega) = f(\lambda^{\frac{1}{2}}\omega). \tag{2.29}$$

2.4.1 The limiting absorption principle

For $z \notin \sigma(H)$ we let $R(z) = (H - z)^{-1}$. In this section we show in what sense $R(z)$ assumes boundary values along the positive real axis, as limits of values from the upper and lower half plane. Since $(0, \infty) \subset \sigma(H)$ we see that such limits cannot exist in $\mathcal{B}(\mathcal{H})$, however we will see that when considered in weaker topologies (that of $\mathcal{B}(H^{0,t}, H^{0,-t})$ for $t > \frac{1}{2}$) such limits do exist.

This fact is known as the limiting absorption principle and has its origins in the work of Ignatowski [79], who considered the propagation of electromagnetic waves in a wire, and Friedrichs [67] who established the existence of related limits to construct some explicit wave operators. The terminology limiting absorption principle was introduced by Svešnikov [156, 157]. The limiting absorption principle was used by Kato [92] and Kuroda [102, 103] and established more generally in the work of Vaĭnberg [159]. Proofs of the limiting absorption principle can be found in many texts on scattering theory, however the proof presented here follows closely those of Agmon [3, Section 4], Kuroda [106, Chapter 5] and Yafaev[164, Chapter 6].

The proof is rather long and so will be broken into a number of intermediate steps, the first of which is to prove the limiting absorption principle for H_0. We let $R_0(z) = (H_0 - z)^{-1}$

and consider $R_0(z)$ as an analytic operator valued function on $\mathbb{C} \setminus [0, \infty)$ with values in $\mathcal{B}(H^{0,t}, H^{2,-t})$ for any $t > \frac{1}{2}$.

Lemma 2.4.2. *Let $t > \frac{1}{2}$ and $f, g \in H^{0,t}$. Then for any $\lambda \in (0, \infty)$ the limits*

$$\langle R_0(\lambda \pm i0)f, g\rangle := \lim_{\varepsilon \to 0} \langle R_0(\lambda \pm i\varepsilon)f, g\rangle \tag{2.30}$$

exist. Furthermore, for any $\lambda \in (0, \infty)$ and $f \in H^{0,t}$ the limit

$$R_0(\lambda \pm i0)f := \lim_{\varepsilon \to 0} R_0(\lambda \pm i\varepsilon)f, \tag{2.31}$$

taken in the weak topology of $H^{2,-t}$, exists in $H^{2,-t}$.

Proof. Let $t > \frac{1}{2}$ and $f, g \in H^{0,t}$. We show that the function $F : \mathbb{C} \setminus [0, \infty) \to \mathbb{C}$ given by $F(z) = \langle R_0(z)f, g\rangle$ has continuous boundary values on both sides of $(0, \infty)$ (that is for $\lambda \in (0, \infty)$ the limits $\lim_{\varepsilon \to 0} F(\lambda \pm i\varepsilon)$ exist and are continuous in λ). By a version of the elliptic estimate [3, Theorem A.1] we have

$$||R_0(z)f||_{H^{2,-t}} \leq C\, ||f||_{H^{0,t}} \tag{2.32}$$

for all $f \in H^{0,t}$ and $z \in \mathbb{C} \setminus \mathbb{R}^+$ such that $K^{-1} \leq |z| \leq K$ for fixed $K > 1$. For $g \in H^{2,-t}$ we obtain

$$|F(z)| = |\langle R_0(z)f, g\rangle| \leq ||R_0(z)f||_{H^{2,-t}}\, ||g||_{H^{-2,t}} \leq C\, ||f||_{H^{0,t}}\, ||g||_{H^{0,t}} \tag{2.33}$$

for another constant C and $K^{-1} \leq |z| \leq K$. The estimate (2.33) shows that it suffices to prove that F assumes continuous boundary values on both sides of $(0, \infty)$ on a dense subset of $H^{0,t}$. So for $f, g \in C_c^\infty(\mathbb{R}^n)$ we have by Equation (2.16) that

$$\begin{aligned} F(z) = \langle R_0(z)f, g\rangle = \langle \mathcal{F}R_0(z)f, \mathcal{F}g\rangle &= \int_{\mathbb{R}^n} \frac{\overline{[\mathcal{F}f](\xi)}[\mathcal{F}g](\xi)}{|\xi|^2 - z}\, \mathrm{d}\xi \\ &= \frac{1}{2}\int_0^\infty \int_{\mathbb{S}^{n-1}} \frac{k^{\frac{n-2}{2}}}{k - z} \overline{[\mathcal{F}f](k^{\frac{1}{2}}\omega)}[\mathcal{F}g](k^{\frac{1}{2}}\omega)\, \mathrm{d}\omega\, \mathrm{d}k. \end{aligned}$$

This is a Cauchy type integral, which in the limit can be evaluated using the Plemelj formula [131, Chapter 14] (see also [161, Theorem 9.8]) to obtain

$$\begin{aligned} &\lim_{\varepsilon \to 0} \langle R_0(\lambda \pm i\varepsilon)f, g\rangle \\ &= \pm \frac{\pi i \lambda^{\frac{n-2}{2}}}{2} \int_{\mathbb{S}^{n-1}} \overline{[\mathcal{F}f](\lambda^{\frac{1}{2}}\omega)}[\mathcal{F}g](\lambda^{\frac{1}{2}}\omega)\, \mathrm{d}\omega + \text{P.V.}\left(\int_{\mathbb{R}^n} \frac{\overline{[\mathcal{F}f](\xi)}[\mathcal{F}g](\xi)}{|\xi|^2 - \lambda}\, \mathrm{d}\xi\right), \end{aligned} \tag{2.34}$$

where the last integral is singular and taken in the principal value sense. Applying [121, Theorem 20.1] (see also [17, Theorem 2]) to Equation (2.34) shows that F admits continuous boundary values on both sides of $(0, \infty)$. The existence of the limits in Equation (2.34) shows that for $f \in H^{0,t}$ the limit

$$\lim_{\varepsilon \to 0} R_0(\lambda \pm i\varepsilon) f, \tag{2.35}$$

taken in the weak topology of $H^{0,-t}$, exists in $H^{0,-t}$. Then $R_0(z)f$ is bounded near λ when considered as a function with values in $H^{2,-t}$ by the estimate (2.32). The weak compactness of the unit ball in $H^{2,-t}$ then shows that the limit (2.35) exists also in $H^{2,-t}$ and is by definition given by the function $R_0(\lambda \pm i0)f$ of Equation (2.31). $\square$

Corollary 2.4.3. *For any $t > \frac{1}{2}$ and $f \in H^{0,t}$ we have the identity*

$$\operatorname{Im}\left(\langle R_0(\lambda \pm i0)f, f\rangle\right) = \pm \frac{\pi \lambda^{\frac{1}{2}}}{2} \int_{\mathbb{S}^{n-1}} |[\gamma(\lambda^{\frac{1}{2}})\mathcal{F}f](\omega)|^2 \, \mathrm{d}\omega, \tag{2.36}$$

where γ is defined by Equation (2.29).

Proof. The result follows immediately by taking $f = g$ in Equation (2.34) and then taking the imaginary part. $\square$

Corollary 2.4.4. *For any $t > \frac{1}{2}$, $f \in H^{0,t}$ and $\lambda \in (0, \infty)$ the function $\psi = R_0(\lambda \pm i0)f$ satisfies the differential equation*

$$(H_0 - \lambda)\psi = f \tag{2.37}$$

in the sense of distributions.

Proof. For any $\varphi \in C_c^\infty(\mathbb{R}^n)$ and $z \notin \mathbb{R}$ we have the relation

$$\langle R_0(z)f, (H_0 - \overline{z})\varphi\rangle = \langle f, \varphi\rangle.$$

By Lemma 2.4.2 we thus have for $\lambda \in (0, \infty)$ the equalities

$$\langle f, \varphi\rangle = \lim_{\varepsilon \to 0} \langle R_0(\lambda \pm i\varepsilon)f, (H_0 - \lambda)\varphi\rangle = \langle \psi, (H_0 - \lambda)\varphi\rangle = \langle (H_0 - \lambda)\psi, \varphi\rangle.$$

Since this holds for all $\varphi \in C_c^\infty(\mathbb{R}^n)$, we find $(H_0 - \lambda)\psi = f$ in the sense of distributions. $\square$

We will now show that the weak limits (2.31) exist in a stronger sense.

Theorem 2.4.5 (Limiting absorption principle for H_0)**.** *Consider the resolvent operator $R_0(z) = (H_0 - z)^{-1}$. Then for any $\lambda \in (0, \infty)$ and $t > \frac{1}{2}$ the limits*

$$\lim_{\varepsilon \to 0} R_0(\lambda \pm i\varepsilon) =: R_0(\lambda \pm i0) \tag{2.38}$$

exist in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{2,-t})$

Proof. Let $\mathbb{C}_\pm = \{z \in \mathbb{C} : \pm\mathrm{Im}(z) > 0\}$ and $\overline{\mathbb{C}_\pm} = \mathbb{C}_\pm \cup (0, \infty)$. Define the operator-valued functions $R_0^\pm : \overline{\mathbb{C}_\pm} \to \mathcal{B}(H^{0,t}, H^{2,-t})$ by

$$R_0^\pm(z) = \begin{cases} R_0(z), & \text{if } \pm\,\mathrm{Im}(z) > 0, \\ R_0(\lambda \pm i0), & \text{if } z = \lambda \in (0, \infty). \end{cases} \tag{2.39}$$

From Lemma 2.4.2 we have that the $R_0^\pm$ define weak operator topology continuous operator-valued functions on $\overline{\mathbb{C}_\pm}$. We now show that $R_0^\pm$ are actually continuous on $\overline{\mathbb{C}_\pm}$ in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{2,-t})$. Since for $u \in H^{2-,t}$ we have that $||u||_{H^{2,-t}}$ is equivalent, via the elliptic estimate [76, p. 283], to $||\cdot||_{eq} = ||\cdot||_{H^{0,-t}} + ||H_0\cdot||_{H^{0,-t}}$ it suffices to show that both $R_0^\pm$ and $H_0R_0^\pm$ are continuous in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$. Since $H_0R_0^\pm(z) = \mathrm{Id} + zR_0^\pm(z)$ it further suffices to show that the operators $R_0^\pm$ are continuous in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$. We will prove this in several steps.

First we show that $R_0^\pm$ are continuous on $\overline{\mathbb{C}_\pm}$ in the strong topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$. Note that the inclusion $H^{2,-m} \hookrightarrow H^{0,-t}$ is compact for any $m < t$ (a consequence of Rellich's compactness theorem, see Theorem 2.2.5 (b)), and that for $f \in H^{0,t}$ we have $R_0(z)f \in H^{2,-m}$ for any $m > \frac{1}{2}$. Then for $z_0 \in \mathbb{C}_\pm$ we have

$$R_0^\pm(z_0)f := \lim_{z \to z_0} R_0^\pm(z)f \tag{2.40}$$

exists in $H^{0,-t}$ by the continuity of $R_0(z) \in \mathcal{B}(H^{0,t}, H^{2,-t})$ and so in $\mathcal{B}(H^{0,t}, H^{0,-t})$ by compactness of the inclusion map $H^{2,-t} \hookrightarrow H^{0,-t}$. For $z_0 \in (0, \infty)$ we use that the limit (2.31) exists to see that the limit (2.40) holds in $H^{2,-t}$ and thus $R_0(z_0)$ defines an operator in $\mathcal{B}(H^{0,t}, H^{2,-t})$ and so also in $\mathcal{B}(H^{0,t}, H^{0,-t})$ by compactness of the inclusion $H^{2,-t} \hookrightarrow H^{0,-t}$. Thus we have shown that $R_0^\pm$ are continuous on $\overline{\mathbb{C}_\pm}$ in the strong topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$.

Let $(z_k) \subset \mathbb{C}_\pm$ and $(f_j) \subset H^{0,t}$ be sequences with $z_k \to z_0 \in \mathbb{C}_\pm$ and $\lim f_j = f \in H^{0,t}$ in the weak topology of $H^{0,t}$. Then we can compute for any $g \in H^{0,t}$ that

$$\lim_{j\to\infty} \langle R_0^\mp(z_j)f_j, g\rangle = \lim_{j\to\infty} \langle f_j, R_0^\pm(\overline{z_j})g\rangle = \langle f, R_0^\pm(\overline{z_0})g\rangle = \langle R_0^\mp(z_0)f, g\rangle.$$

Hence we find the existence of the limit

$$\lim_{j\to\infty} R_0^\pm(z_j)f_j = R_0^\pm(z_0)f \tag{2.41}$$

in the weak topology of $H^{0,-t}$, considered as the dual of $H^{0,t}$. The estimate (2.32) shows that the sequence $(R_0^\pm(z_j)f_j)$ is bounded in $H^{2,-m}$ for any $m > \frac{1}{2}$. The compactness of the inclusion $H^{2,-m} \hookrightarrow H^{0,-t}$ for $m < t$ then shows that the existence of the limit (2.41) gives the existence of the limit

$$\lim_{j\to\infty} R_0^{\pm}(z_j)f_j = R_0^{\pm}(z_0)f \tag{2.42}$$

in the strong topology of $H^{0,-t}$ also. We now show that it follows from Equation (2.42) that $R_0^{\pm}$ is continuous on $\overline{\mathbb{C}_{\pm}}$ in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$. Suppose for contradiction that $R_0^{\pm}$ is not continuous on $\overline{\mathbb{C}_{\pm}}$ in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{0,-t})$. Then there exists a sequence $(z_j) \subset \overline{\mathbb{C}_{\pm}}$ with $z_j \to z_0 \in \overline{\mathbb{C}_{\pm}}$ and a sequence $(f_j) \subset H^{0,t}$ with $||f_j||_{H^{0,t}} = 1$ such that

$$\lim_{j\to\infty} \left|\left|(R_0^{\pm}(z_j) - R_0^{\pm}(z_0))f_j\right|\right|_{H^{0,-t}} > 0. \tag{2.43}$$

We can assume (after passing to a subsequence if necessary) the existence of the weak limit $\lim_{j\to\infty} f_j =: f \in H^{0,t}$ in the weak topology of $H^{0,t}$. Then by Equation (2.42) we have

$$\lim_{j\to\infty} R_0^{\pm}(z_j)f_j = R_0^{\pm}(z_0)f = \lim_{j\to\infty} R_0^{\pm}(z_0)f_j,$$

in $H^{0,-t}$ (with the limits in the strong topology), which contradicts the inequality (2.43).
□

Definition 2.4.6. A function $\psi \in H^{2,0}_{loc}$ will be called k-outgoing (for '+') or k-incoming (for '−') if for $k > 0$ the relation

$$\psi = R_0(k^2 \pm i0)f \tag{2.44}$$

holds for some $f \in H^{0,t}$ and $t > \frac{1}{2}$. Here the subscript *loc* denotes that ψ is locally integrable, that is $\psi \in H^{2,0}(K)$ for any compact $K \subset \mathbb{R}^n$,

Lemma 2.4.7. *Let $\psi \in H^{2,0}_{loc}$ be a k-outgoing (or k-incoming) function satisfying the differential equation*

$$(H_0 + V)\psi = k^2\psi \tag{2.45}$$

for some V satisfying Assumption 2.2.14. Then $\psi \in H^{0,t}$ for all $t \in \mathbb{R}$.

Proof. We shall provide a proof for ψ outgoing, the proof for ψ incoming being similar. Since ψ is outgoing there exists $t_0 > \frac{1}{2}$ and $f \in H^{0,t_0}$ such that $\psi = R_0(k^2 + i0)f$. Then we compute

$$\begin{aligned}(H_0 - k^2)\psi &= (H_0 - k^2)\left(\lim_{\varepsilon\to 0} R_0(k^2 + i\varepsilon)f\right) = \lim_{\varepsilon\to 0}(H_0 - k^2)R_0(k^2 + i\varepsilon)f \\ &= \lim_{\varepsilon\to 0}\left(f + i\varepsilon R_0(k^2 + i\varepsilon)f\right) = f,\end{aligned}$$

by Theorem 2.4.5. By Equation (2.45) we have $f = -V\psi$. By Corollary 2.4.3 and the fact that V is real-valued, evaluating $\mathcal{F}f$ on the sphere of radius k we find

$$k^{n-1}\int_{\mathbb{S}^{n-1}} |[\mathcal{F}f](k\omega)|^2 \,\mathrm{d}\omega = \frac{2k}{\pi}\mathrm{Im}\left(\langle R_0(k^2+i0)f, f\rangle\right) = -\frac{2k}{\pi}\mathrm{Im}\left(\langle \psi, V\psi\rangle\right) = 0. \quad (2.46)$$

This shows that the restriction of $\mathcal{F}f$ to the sphere of radius k vanishes and so by [3, Theorem 3.2] we have the function $h : \mathbb{R}^n \to \mathbb{C}$ defined by $h(\xi) = [\mathcal{F}f](\xi)(|\xi|^2 - k^2)^{-1}$ is such that $h \in L^1_{loc}(\mathbb{R}^n)$ (that is $h \in L^1(K)$ for all $K \subset \mathbb{R}^n$ compact). Define $\psi \in H^{0,-t_0}$ by $\psi = \lim_{\varepsilon\to 0} R_0(k^2 + i\varepsilon)f$ and let $g \in \mathcal{S}(\mathbb{R}^n)$. We compute that

$$\begin{aligned}\langle \psi, g\rangle = \lim_{\varepsilon\to 0}\langle R_0(k^2+i\varepsilon)f, g\rangle &= \lim_{\varepsilon\to 0}\int_{\mathbb{R}^n} \frac{\overline{[\mathcal{F}f](\xi)}[\mathcal{F}g](\xi)}{|\xi|^2-k^2}\frac{|\xi|^2-k^2}{|\xi|^2-k^2-i\varepsilon}\,\mathrm{d}\xi \\ &= \int_{\mathbb{R}^n}\frac{\overline{[\mathcal{F}f](\xi)}}{|\xi|^2-k^2}[\mathcal{F}g](\xi)\,\mathrm{d}\xi, \end{aligned} \quad (2.47)$$

where we have used that $\psi \in H^{0,-t_0}$, the unitarity of $\mathcal{F}$ and Lebesgue's dominated convergence theorem. Thus $\mathcal{F}\psi \in L^1_{loc}(\mathbb{R}^n)$ and since Equation (2.47) holds for all $g \in \mathcal{S}(\mathbb{R}^n)$, we find $\mathcal{F}\psi = h$ in the sense of distributions. Then by [3, Theorem 3.3] we have $\psi \in H^{2,t} \subset H^{0,t}$ for all $t \in \mathbb{R}$, which proves the result. □

We can now state and prove the limiting absorption principle for general Schrödinger operators. For $z \in \mathbb{C}\setminus\sigma(H)$ we let $R(z) = (H - z)^{-1}$ considered as an analytic operator valued function on $\mathbb{C}\setminus\sigma(H)$ with values in $\mathcal{B}(H^{0,t}, H^{2,-t})$ for any $t > \frac{1}{2}$.

Theorem 2.4.8 (Limiting absorption principle for H). *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 2$ and consider the operator $R(z) = (H - z)^{-1}$. Then for any $\lambda \in (0,\infty)$ the limits*

$$R(\lambda \pm i0) := \lim_{\varepsilon\to 0} R(\lambda \pm i\varepsilon) \quad (2.48)$$

exist in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{2,-t})$ for any $t > \frac{1}{2}$.

Proof. We prove the theorem for $R(\lambda+i0)$ since the proof for $R(\lambda-i0)$ is similar. Without loss of generality we suppose that $t \in \left(\frac{1}{2}, \frac{1}{2}+\varepsilon\right)$ for some $\varepsilon > 0$. We choose ε sufficiently small so that V defines a compact operator from $H^{2,-\frac{1}{2}-\varepsilon}$ to $H^{0,\frac{1}{2}+\varepsilon}$ (possible by Rellich's compactness theorem since $|V(x)| \leq C(1+|x|)^{-\rho}$ for some $\rho > 1$ and almost all $x \in \mathbb{R}^n$).

For any $z \in \overline{\mathbb{C}_+}$ we define $Q(z) \in \mathcal{B}(H^{2,-t}, H^{2,-t})$ by

$$Q(z)\psi = R_0(z+i0)V\psi. \quad (2.49)$$

From Theorem 2.4.5 and the compactness of V as an operator from $H^{2,-t}$ to $H^{0,t}$ we have that $Q(z)$ defines a compact operator for every $z \in \overline{\mathbb{C}_+}$, and that the operator-valued function Q is continuous on $\overline{\mathbb{C}_+}$ in the uniform operator topology of $\mathcal{B}(H^{2,-t}, H^{2,-t})$.

For $\mathrm{Im}(z) > 0$ we can use the resolvent equation

$$R(z) = R_0(z) - R_0(z)VR(z) \tag{2.50}$$

and the definition of $Q(z)$ to see that for any $f \in \mathcal{H}$ and $\psi = R(z)f \in H^{2,0}$ we have

$$(\mathrm{Id} + Q(z))\psi = R_0(z)f. \tag{2.51}$$

We see, by varying f, that $H^{2,0} \subset \mathrm{Range}(\mathrm{Id} + Q(z)) \subset H^{2,-t}$. Since the closure of the domain of the Laplacian with respect to the weight $\mathbb{R}^n \ni x \mapsto (1 + |x|^2)^{-\frac{t}{2}}$ is $H^{2,-t}$ we find $\overline{\mathrm{Range}(\mathrm{Id} + Q(z))} = H^{2,-t}$. Standard Fredholm theory (see [106, Proposition 5.2.1]) then shows that the inverse $(\mathrm{Id} + Q(z))^{-1}$ exists in $\mathcal{B}(H^{2,-t}, H^{2,-t})$.

Now we let $z = \lambda \in (0, \infty)$. Then the analytic Fredholm alternative says that $\mathrm{Id}+Q(\lambda)$ is invertible if and only if -1 is not an eigenvalue of $Q(\lambda)$. We now show that for $\lambda > 0$, -1 is an eigenvalue of $Q(\lambda)$ if and only if λ is an eigenvalue of H.

So we suppose that -1 is an eigenvalue of $Q(\lambda)$ and that $\psi \in H^{2,-t}$ is a corresponding eigenfunction. The definition of Q shows that $\psi = -R_0(\lambda + i0)V\psi$ which implies that ψ is a $\lambda^{\frac{1}{2}}$-outgoing solution of the equation $(H_0 + V)\psi = \lambda\psi$. By Lemma 2.4.7 we see that $\psi \in H^{0,t_0}$ for all $t_0 \in \mathbb{R}$. So $\mathcal{F}f \in C^\infty(\mathbb{R}^n)$ and hence f has rapid decay. Thus $f \in \mathrm{Dom}(H_0)$ and λ is an eigenvalue of H, contradicting the fact that H has no positive eigenvalues.

Conversely, we suppose that $\lambda > 0$ is an eigenvalue of H with corresponding eigenfunction $\psi \in \mathrm{Dom}(H)$. Using Equation (2.50) we find that $\psi + R_0(z)V\psi = (\lambda - z)R_0(z)\psi$ for $z \in \mathbb{C}_+$. Taking the limit as $z \to \lambda$ we find $\psi + R_0^+(\lambda)V\psi = 0$ and thus -1 is an eigenvalue of $Q(\lambda)$. Since H has no positive eigenvalues we find that $(\mathrm{Id} + Q(z))^{-1}$ exists for all $z \in \overline{\mathbb{C}_+}$.

Since Q is continuous on $\overline{\mathbb{C}_+}$ in the uniform operator topology of $\mathcal{B}(H^{2,-t}, H^{2,-t})$, it follows that the operator-valued function $(\mathrm{Id} + Q(z))^{-1}$ is also continuous on $\overline{\mathbb{C}_+}$ in the uniform operator topology of $\mathcal{B}(H^{2,-t}, H^{2,-t})$. The resolvent equation (2.50) and the definition of Q give us that

$$R(z) = (\mathrm{Id} + Q(z))^{-1}R_0(z) \tag{2.52}$$

for $\mathrm{Im}(z) > 0$. Using the continuity properties of $(\mathrm{Id} + Q(z))^{-1}$ and $R_0(z)$ it follows that the limits

$$\lim_{\varepsilon \to 0} R(\lambda + i\varepsilon) = (\mathrm{Id} + Q(\lambda))^{-1}R_0(\lambda + i0) \tag{2.53}$$

exist in the uniform operator topology of $\mathcal{B}(H^{0,t}, H^{2,-t})$. □

Corollary 2.4.9. *For any* $t > \frac{1}{2}$ *and* $f \in H^{0,t}$ *we have*

$$R(\lambda \pm i0)f = R_0(\lambda \pm i0)f - R_0(\lambda \pm i0)VR(\lambda \pm i0)f. \tag{2.54}$$

In particular, $\psi_+ = R(\lambda + i0)f$ *is a* $\lambda^{\frac{1}{2}}$*-outgoing solution and* $\psi_- = R(\lambda - i0)f$ *is a* $\lambda^{\frac{1}{2}}$*-incoming solution of the differential equation*

$$(H_0 + V)\psi = f. \tag{2.55}$$

Proof. Using the continuity properties of $R(z)$ established in Theorem 2.4.8 we obtain Equation (2.54) immediately from Equation (2.50). The fact that $\psi_+ = R(\lambda + i0)f$ is a $\lambda^{\frac{1}{2}}$-outgoing solution was established and used in the proof of Theorem 2.4.8. □

We conclude this section by using similar methods to determine the high energy behaviour of the resolvent. The result is the following.

Lemma 2.4.10. *Suppose that* $\rho > \frac{n+1}{2}$ *in Assumption* (2.2.14) *and define the complex domain* $C_+ = \{z \in \mathbb{C} : \mathrm{Re}(z) \geq 1 \text{ and } \mathrm{Im}(z) > 0\}$ *and* $t \in (\frac{1}{2}, \rho - \frac{1}{2})$*. Then* $VR_0(z)$ *and* $(\mathrm{Id} + VR_0(z))^{-1}$ *can be extended to continuous and uniformly bounded functions from* C_+ *to* $\mathcal{B}(H^{0,t}, H^{0,t})$*. Similarly,* $R_0(z)V$ *and* $(\mathrm{Id} + R_0(z)V)^{-1}$ *can be extended to continuous and uniformly bounded functions from* C_+ *to* $\mathcal{B}(H^{0,-t}, H^{0,-t})$*.*

Proof. Since for any $\rho > \frac{n+1}{2}$ and $t \in (\frac{1}{2}, \rho - \frac{1}{2})$ we have $R_0(z) \in \mathcal{B}(H^{0,t}, H^{0,t-\rho})$ is continuous in $z \in C_+$ by [85, proof of Lemma 3.1], and since $V \in \mathcal{B}(H^{0,t-\rho}, H^{0,t})$ by assumption, we find that $VR_0(z) \in \mathcal{B}(H^{0,t}, H^{0,t})$ for any $t \in (\frac{1}{2}, \rho - \frac{1}{2})$.

Since $VR_0(z)$ is compact and has no eigenvalue -1 for $z \in C_+$ (see the discussion in the proof of Theorem 2.4.8), the operator $(\mathrm{Id} + VR_0(z))^{-1} \in \mathcal{B}(H^{0,t}, H^{0,t})$ exists and is continuous in $z \in C_+$. By [120, Theorem 1] we have that $VR_0(z) \to 0$ as $|z| \to \infty$ in C_+ in the norm of $\mathcal{B}(H^{0,t}, H^{0,t})$ for any $t > \frac{1}{2}$, so that the operator $(\mathrm{Id} + VR_0(z))^{-1}$ is uniformly bounded. A similar computation (or duality) can be used to prove the second claim. □

2.4.2 Generalised eigenfunctions and stationary wave operators

In this section we use the spectral properties of H_0 in conjunction with the limiting absorption principle to define a family of 'generalised eigenfunctions' for the operator H.

Definition 2.4.11. For each $\lambda > 0$ and $\omega \in \mathbb{S}^{n-1}$ the function $\psi_0(\cdot, \omega, \lambda) : \mathbb{R}^n \to \mathbb{C}$ defined by

$$\psi_0(x, \omega, \lambda) = \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle x, \omega\rangle}$$

satisfies the relation $[H_0\psi_0(\cdot,\omega,\lambda)](x) = \lambda\psi_0(x,\omega,\lambda)$ and thus defines a 'generalised eigenfunction' for the continuous spectrum of H_0.

We now demonstrate how the generalised eigenfunctions give rise to Stone's formula, relating the spectral measure for H_0 to the limiting absorption principle.

Theorem 2.4.12. *For $\lambda > 0$ we have for $t > \frac{1}{2}$, the operator $B(\lambda) \in \mathcal{B}(H^{0,t}, H^{0,-t})$ by $B(\lambda) = R_0(\lambda + i0) - R_0(\lambda - i0)$ is an integral operator with kernel*

$$R_0(x,y,\lambda + i0) - R_0(x,y,\lambda - i0) = \frac{i}{2}\lambda^{\frac{n-2}{2}}(2\pi)^{-(n-1)} \int_{\mathbb{S}^{n-1}} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle\omega,x-y\rangle}\,\mathrm{d}\omega, \tag{2.56}$$

for $x, y \in \mathbb{R}^n$.

Proof. Fix $\lambda > 0$. From Corollary 2.4.3 we have for any $f \in H^{0,t}$ with $t > \frac{1}{2}$ the relation

$$\frac{1}{2i}\langle (R_0(\lambda + i0) - R_0(\lambda - i0))\, f, f\rangle = \frac{\pi\lambda^{\frac{n-2}{2}}}{4} \int_{\mathbb{S}^{n-1}} |[\gamma(\lambda^{\frac{1}{2}})\mathcal{F}f](\omega)|^2\,\mathrm{d}\omega.$$

So we compute that

$$\begin{aligned}
&\int_{\mathbb{S}^{n-1}} |[\gamma(\lambda^{\frac{1}{2}})\mathcal{F}f](\omega)|^2\,\mathrm{d}\omega \\
&= (2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} \overline{f(x)}\mathrm{e}^{i\lambda^{\frac{1}{2}}\langle x,\omega\rangle}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n} f(y)\mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle y,\omega\rangle}\,\mathrm{d}y\right)\mathrm{d}\omega \\
&= (2\pi)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \overline{f(x)}f(y)\left(\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle y-x,\omega\rangle}\,\mathrm{d}\omega\right)\mathrm{d}y\,\mathrm{d}x.
\end{aligned}$$

We next note that

$$\begin{aligned}
\langle (R_0(\lambda + i0) - R_0(\lambda - i0))\, f, f\rangle &= \int_{\mathbb{R}^n} \overline{[(R_0(\lambda + i0) - R_0(\lambda - i0))\, f]\,(x)} f(y)\,\mathrm{d}y \\
= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} &(R_0(x,y,\lambda - i0) - R_0(x,y,\lambda + i0))\,\overline{f(x)}f(y)\,\mathrm{d}y\,\mathrm{d}x.
\end{aligned}$$

Since $f \in H^{0,t}$ was arbitrary, the claim follows. □

Using the limiting absorption principle, one can define analogous generalised eigenfunctions for the operator H.

Proposition 2.4.13 (Lippmann-Schwinger)**.** *Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. Then for all $\lambda > 0$, $\omega \in \mathbb{S}^{n-1}$ and $m \in \left(\frac{n}{2}, \rho - \frac{n}{2}\right)$ there is a unique solution $\psi_\pm \in H^{0,-m}$ to*

$$\psi_\pm(x,\omega,\lambda) = \psi_0(x,\omega,\lambda) - [R_0(\lambda \pm i0)V\psi_\pm(\cdot,\omega,\lambda)](x), \quad x \in \mathbb{R}^n. \tag{2.57}$$

This solution is given by the equation

$$\psi_\pm(x,\omega,\lambda) = \psi_0(x,\omega,\lambda) - [R(\lambda \pm i0)V\psi_0(\cdot,\omega,\lambda)](x). \tag{2.58}$$

Furthermore, for each fixed $\lambda > 0$ and $\omega \in \mathbb{S}^{n-1}$ we have

$$[H\psi_\pm(\cdot,\omega,\lambda)](x) = \lambda\psi_\pm(x,\omega,\lambda). \tag{2.59}$$

Proof. First note that for all $s \in (\frac{1}{2}, \rho - \frac{n}{2})$ we have $V\psi_0(\cdot,\omega,\lambda) \in H^{0,s}$. So defining $\psi_\pm$ by Equation (2.58) we find that $\psi_\pm(\cdot,\omega,\lambda) \in H^{0,-m}$ for all $m > \frac{n}{2}$. Apply the operator $\mathrm{Id}+R_0(\lambda\mp i0)V$ to both sides of Equation (2.58) in conjunction with the resolvent identity

$$(\mathrm{Id} + R_0(z)V)(\mathrm{Id} - R(z)V) = \mathrm{Id} \tag{2.60}$$

gives that $\psi_\pm(\cdot,\omega,\lambda)$ satisfies Equation (2.57). If $\varphi_\pm(\cdot,\omega,\lambda) \in H^{0,-m}$ were another solution to Equation (2.57), we apply the operator $\mathrm{Id} - R(\lambda \mp i0)V$ to both sides of Equation (2.57) in conjunction with (the adjoint of) Equation (2.60) to see that $\varphi_\pm = \psi_\pm$. Equation (2.59) then follows from Corollary 2.4.9. □

Equations (2.57) and (2.58) are known as the Lippmann-Schwinger equations and were first introduced in a different form in [111, 112]. Equation (2.59) shows that the $\psi_\pm$ define generalised eigenfunctions of the continuous spectrum of H. We now consider the asymptotics of the generalised eigenfunctions $\psi_\pm$ as $|x| \to \infty$. To do so requires the introduction of the following operator.

Definition 2.4.14. Define for $\lambda > 0$ and $t > \frac{1}{2}$ the operator $\Gamma_0(\lambda) : H^{0,t} \to \mathcal{P}$ by

$$[\Gamma_0(\lambda)f](\omega) = [F_0 f](\lambda,\omega) = 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}}[\mathcal{F}f](\lambda^{\frac{1}{2}}\omega), \quad \omega \in \mathbb{S}^{n-1},$$

with F_0 from Definition 2.2.7.

Proposition 2.4.15. *For $\lambda > 0$ and $t > \frac{1}{2}$ the operator $\Gamma_0(\lambda) : H^{0,t} \to \mathcal{P}$ and its formal adjoint $\Gamma_0(\lambda)^* : \mathcal{P} \to H^{0,-t}$ are uniformly bounded on compact intervals. Moreover, the operator-valued function $\Gamma_0(\lambda)$ is strongly continuous in $\lambda > 0$.*

Proof. For $f \in H^{0,t}$ and $\lambda > 0$ we use the estimate (2.32) to obtain for λ in some compact interval the bound

$$||\Gamma_0(\lambda)f||^2 = \lim_{\varepsilon\to 0} \varepsilon\, ||R_0(\lambda \pm i\varepsilon)f||^2 \le C\, ||f||_{H^{0,t}}{}^2,$$

and thus $\Gamma_0(\lambda)$ is uniformly bounded. To see that $\Gamma_0(\lambda)$ is strongly continuous in $\lambda > 0$ we fix $\mu, \lambda > 0$ and compute that

$$|[(\Gamma_0(\mu) - \Gamma_0(\lambda))f](\omega)|^2 = |[\Gamma_0(\mu)f](\omega)|^2 + |[\Gamma_0(\lambda)f](\omega)|^2 - 2\mathrm{Re}([\Gamma_0(\mu)f](\omega)\overline{[\Gamma_0(\lambda)f](\omega)}).$$

So we write

$$[\Gamma_0(\mu)f](\omega)\overline{[\Gamma_0(\lambda)f](\omega)} = \frac{(\lambda\mu)^{\frac{n-2}{4}}}{2(2\pi)^n}\left(\int_{\mathbb{R}^n} \mathrm{e}^{-i\mu^{\frac{1}{2}}\langle x,\omega\rangle} f(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle x,\omega\rangle} f(x)\,\mathrm{d}x\right),$$

which converges to $|[\Gamma_0(\lambda)f](\omega)|^2$ as $\mu \to \lambda$. Thus we find

$$||(\Gamma_0(\mu) - \Gamma_0(\lambda))f||^2 = \int_{\mathbb{S}^{n-1}} |[(\Gamma_0(\mu) - \Gamma_0(\lambda))f](\omega)|^2\,\mathrm{d}\omega \to 0$$

as $\mu \to \lambda$, so that $\Gamma_0(\lambda)$ is strongly continuous in λ. □

We can use the operator $\Gamma_0(\lambda)$ to obtain the asymptotics of $\psi_\pm$ in terms of scattering data. To do so requires the following definition.

Definition 2.4.16. For $r, \lambda > 0$ we define the *outgoing and incoming spherical waves* by

$$w_\pm(r,\lambda) = r^{-\frac{n-1}{2}}\mathrm{e}^{\pm i\lambda^{\frac{1}{2}}r \mp i\pi\frac{n-3}{2}}. \tag{2.61}$$

Theorem 2.4.17. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. Then for fixed $\omega \in \mathbb{S}^{n-1}$ and $\lambda > 0$, with $\psi_\pm(\cdot,\omega,\lambda)$ as in Proposition 2.4.13, we have as $|x| \to \infty$ that*

$$\psi_\pm(x,\omega,\lambda) = \psi_0(x,\omega,\lambda) + a_\pm(\hat{x},\omega,\lambda)w_\mp(|x|,\lambda) + o_{av}(|x|^{-\frac{n+1}{2}}), \tag{2.62}$$

where for $x \neq 0$ we have defined $\hat{x} = |x|^{-1}x$. The coefficient $a_\pm$ can be recovered by the formula

$$a_\pm(\theta,\omega,\lambda) = -\pi^{\frac{1}{2}}\lambda^{-\frac{1}{4}}[\Gamma_0(\lambda)V\psi_\pm(\cdot,\omega,\lambda)](\mp\theta), \tag{2.63}$$

with $\theta,\omega \in \mathbb{S}^{n-1}$ and $\lambda > 0$.

Here o_{av} denotes a Cesaro averaged asymptotics. We refer to 2.4.17 [164, Theorem 6.7.4] for the proof, which relies on the method of stationary phase. Our only use of Theorem 2.4.17 is in Section 4.2 to develop intuition for the form of the wave operator and thus the details are not necessary here.

Definition 2.4.18. For fixed $\omega \in \mathbb{S}^{n-1}$ and $\lambda > 0$ the coefficient $a_-(\cdot,\omega,\lambda) : \mathbb{S}^{n-1} \to \mathbb{C}$ of the outgoing spherical wave in the asymptotics (2.62) is called the *scattering amplitude* for the energy λ and direction ω.

We will justify the name scattering amplitude in Lemma 2.4.33.

For $\lambda > 0$, the operator $\Gamma_0(\lambda)$ is related to the limiting absorption principle via Stone's formula 2.4.12.

Lemma 2.4.19. *For $\lambda > 0$ and $t > \frac{1}{2}$ the operator $\Gamma_0(\lambda)^*\Gamma_0(\lambda) : H^{0,t} \to H^{0,-t}$ satisfies*

$$2\pi i\Gamma_0(\lambda)^*\Gamma_0(\lambda) = R_0(\lambda + i0) - R_0(\lambda - i0).$$

In particular, $2\pi i\Gamma_0(\lambda)^*\Gamma_0(\lambda)$ is an integral operator with kernel given by Equation (2.56).

Proof. For $t > \frac{1}{2}$, $\lambda > 0$, $f \in H^{0,t}$ and $x \in \mathbb{R}^n$ we check that

$$\begin{aligned}
[\Gamma_0(\lambda)^*\Gamma_0(\lambda)f](x) &= 2^{-\frac{1}{2}}(2\pi)^{-\frac{n}{2}}\lambda^{\frac{n-2}{4}} \int_{\mathbb{S}^{n-1}} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle\omega,x\rangle}[\Gamma_0(\lambda)f](\omega)\,\mathrm{d}\omega \\
&= 2^{-1}(2\pi)^{-n}\lambda^{\frac{n-2}{2}} \int_{\mathbb{S}^{n-1}} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle x,\omega\rangle} \left(\int_{\mathbb{R}^n} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle y,\omega\rangle} f(y)\,\mathrm{d}y\right) \mathrm{d}\omega \\
&= \frac{\lambda^{\frac{n-2}{2}}}{2(2\pi)^n} \int_{\mathbb{R}^n} \left(\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle y-x,\omega\rangle}\,\mathrm{d}\omega\right) f(y)\,\mathrm{d}y.
\end{aligned}$$

Since $f \in H^{0,t}$ was arbitrary, a comparison with Equation (2.56) gives the result. □

We now factorise the potential V in order to use the integral kernels defined by Theorem 2.4.12 and Lemma 2.4.19 to define trace class operators, which we shall use extensively in Chapter 5. For $x \in \mathbb{R}^n$ we introduce the notation

$$v(x) = |V(x)|^{\frac{1}{2}}, \quad U(x) = \begin{cases} 1, & \text{if } V(x) \geq 0, \\ -1, & \text{if } V(x) < 0, \end{cases} \tag{2.64}$$

so that $V = vUv$.

Lemma 2.4.20. *Suppose that $g_1, g_2 : \mathbb{R}^n \to \mathbb{C}$ are compactly supported with $g = g_1g_2$. For $\lambda > 0$ define the operator $B(\lambda) \in \mathcal{B}(\mathcal{H})$ by $B(\lambda) = g_1\left(R_0(\lambda + i0) - R_0(\lambda - i0)\right)g_2$. Then $B(\lambda) \in \mathcal{L}^1(\mathcal{H})$ and*

$$\mathrm{Tr}\left(B(\lambda)\right) = \frac{(2\pi i)\lambda^{\frac{n-2}{2}}\mathrm{Vol}(\mathbb{S}^{n-1})}{2(2\pi)^n} \int_{\mathbb{R}^n} g(x)\,\mathrm{d}x.$$

Furthermore, for $t > \frac{1}{2}$ and $\lambda > 0$ we have the equality $R_0(\lambda + i0) - R_0(\lambda - i0) = 2\pi i\Gamma_0(\lambda)^*\Gamma_0(\lambda)$ as operators in $\mathcal{B}(H^{0,t}, H^{0,-t})$.

Proof. Fix $t > \frac{1}{2}$ and $\lambda > 0$. As an operator in $\mathcal{B}(H^{0,t}, H^{0,-t})$ we have (see [3, Equation 4.3] and [6, Equation 15]) that $A(\lambda) = R_0(\lambda + i0) - R_0(\lambda - i0)$ is an integral operator with integral kernel

$$A(\lambda, x, y) = \frac{(2\pi i)}{2(2\pi)^n}\lambda^{\frac{n-2}{2}} \int_{\mathbb{S}^{n-1}} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle\omega,x-y\rangle}\,\mathrm{d}\omega,$$

for $x, y \in \mathbb{R}^n$. Direct computation shows that the integral kernel of $(2\pi i)\Gamma_0(\lambda)^*\Gamma_0(\lambda)$ is the same as that of $A(\lambda)$.

That $B(\lambda)$ is trace class is proved in [73, Lemma III.2] (see also the comments on the bottom of page 32), however we provide an alternative proof. For any $t > \frac{1}{2}$ direct computation shows that $g_1\Gamma_0(\lambda)^* \in \mathcal{L}^2(\mathcal{P},\mathcal{H})$ and $\Gamma_0(\lambda)g_2 \in \mathcal{L}^2(\mathcal{H},\mathcal{P})$ and thus $B(\lambda) \in \mathcal{L}^1(\mathcal{H})$.

We can then compute the trace of $B(\lambda)$ by integrating along the diagonal, which completes the proof. □

Remark 2.4.21. The assumption of compact support on the potential V is stronger than necessary to guarantee that the operator $B(\lambda)$ is trace class. It is sufficient that the multiplication operators corresponding to g_1, g_2 map $\mathcal{H}$ into $H^{0,t}$ for some $t > \frac{1}{2}$. The computation of the trace of $B(\lambda)$ was first done by Buslaev [36] (see also Newton [124] and Bollé and Osborn [31]).

In fact we can differentiate $B(\lambda)$ arbitrarily in λ in the trace norm.

Lemma 2.4.22. *Suppose that g_1, g_2 are compactly supported and $g = g_1g_2$. For $\lambda > 0$ define the operator $B(\lambda) \in \mathcal{L}^1(\mathcal{H})$ by $B(\lambda) = g_1\left(R_0(\lambda + i0) - R_0(\lambda - i0)\right)g_2$. Then $B(\lambda)$ is differentiable in λ in the norm of $\mathcal{L}^1(\mathcal{H})$ and for all $\ell \in \mathbb{N}$ we have*

$$\frac{\mathrm{d}^{\ell-1}}{\mathrm{d}\lambda^{\ell-1}}B(\lambda) = (\ell-1)!g_1\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_2. \tag{2.65}$$

In particular for $\lambda > 0$ and $\ell \in \mathbb{N}$ we have that $g_1\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_2$ has for $x, y \in \mathbb{R}^n$ the integral kernel

$$\frac{(2\pi i)\Gamma\left(\frac{n}{2}\right)\lambda^{\frac{n}{2}-\ell}}{2(\ell-1)!\Gamma\left(\frac{n}{2}+1-\ell\right)(2\pi)^n}g_1(x)g_2(y)\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle\omega,y-x\rangle}\,\mathrm{d}\omega + \tilde{A}(\lambda,x,y)$$

where $\tilde{A}(\lambda,\cdot,\cdot)$ vanishes on the diagonal and thus

$$\operatorname{Tr}\left(g_1\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_2\right) = \frac{(2\pi i)\Gamma\left(\frac{n}{2}\right)\lambda^{\frac{n}{2}-\ell}\mathrm{Vol}(\mathbb{S}^{n-1})}{2(\ell-1)!\Gamma\left(\frac{n}{2}+1-\ell\right)(2\pi)^n}\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x. \tag{2.66}$$

Proof. That $B(\lambda)$ is differentiable is proved in [164, Lemma 8.1.8] and so we obtain Equation (2.65). Differentiating $(\ell-1)$ times the integral kernel for $B(\lambda)$ we obtain

$$\frac{\mathrm{d}^{\ell-1}}{\mathrm{d}\lambda^{\ell-1}}B(\lambda,x,y) = \frac{(2\pi i)}{2(2\pi)^n}g_1(x)g_2(y)\sum_{j=0}^{\ell-1}\binom{\ell-1}{j}\left(\frac{\mathrm{d}^j}{\mathrm{d}\lambda^j}\lambda^{\frac{n-2}{2}}\right)\frac{\mathrm{d}^{\ell-1-j}}{\mathrm{d}\lambda^{\ell-1-j}}\int_{\mathbb{S}^{n-1}}\mathrm{e}^{i\lambda^{\frac{1}{2}}\langle\omega,x-y\rangle}\,\mathrm{d}\omega.$$

By factoring as the product of two Hilbert-Schmidt operators as in Lemma 2.4.20, each term in the sum is individually trace class. All terms except the $j = \ell - 1$ term vanish on the diagonal since they contain an $\langle\omega, x-y\rangle^j$ term, so integrating over the diagonal gives Equation (2.66). □

Remark 2.4.23. The differentiability of $B(\lambda)$ and Equation (2.65) can be checked directly at the level of kernels. Doing so demonstrates that again the assumption of compact support is stronger than necessary, it is enough that the multiplication operators $(1+|\cdot|)^\ell g_1, (1+|\cdot|)^\ell g_2$ map $\mathcal{H}$ into $H^{0,t}$ for some $t > \frac{1}{2}$.

In fact we can easily generalise the above result to all positive integer powers of $A(\lambda)$ and $B(\lambda)$ as follows.

Lemma 2.4.24. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 2n$. For $\lambda > 0$ define the operators $A(\lambda) \in \mathcal{B}(\mathcal{H})$ and $B(\lambda) \in \mathcal{B}(\mathcal{P})$ by $A(\lambda) = (\Gamma_0(\lambda)V\Gamma_0(\lambda)^*$ and $B(\lambda) = v(R_0(\lambda+i0) - R_0(\lambda-i0))Uv$. Then we have*

$$\mathrm{Tr}(A(\lambda)^\ell) = (2\pi i)^{-\ell}\mathrm{Tr}(B(\lambda)^\ell)$$

for all $\ell \in \mathbb{N}$.

Proof. That $A(\lambda)^\ell$ and $B(\lambda)^\ell$ are trace class follows from the fact that $A(\lambda)$ and $B(\lambda)$ are. We first write down the integral kernels explicitly and then integrate to show the traces are the same. Fix $\lambda > 0$ and compute for any $f \in H^{s,t}$ that

$$\begin{aligned}
[\Gamma_0(\lambda)^*\Gamma_0(\lambda)f](x) &= 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}}(2\pi)^{-\frac{n}{2}}\int_{\mathbb{S}^{n-1}} \mathrm{e}^{i\lambda^{\frac{1}{2}}\langle x,\omega\rangle}[\Gamma_0(\lambda)f](\omega)\,\mathrm{d}\omega \\
&= 2^{-1}\lambda^{\frac{n-2}{4}}(2\pi)^{-n}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^n} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle \omega,y-x\rangle}f(y)\,\mathrm{d}y\,\mathrm{d}\omega \\
&= \frac{1}{2\pi i}[(R_0(\lambda+i0) - R_0(\lambda-i0))f](x),
\end{aligned}$$

where we have applied Theorem 2.4.12 for the final equality. We can thus determine the expression

$$\begin{aligned}
A(\lambda)^\ell &= (\Gamma_0(\lambda)V\Gamma_0(\lambda)^*)^\ell \\
&= \Gamma_0(\lambda)V(\Gamma_0(\lambda)^*\Gamma_0(\lambda)V)^{\ell-1}\Gamma_0(\lambda)^* \\
&= (2\pi i)^{-(\ell-1)}\Gamma_0(\lambda)V((R_0(\lambda+i0) - R_0(\lambda-i0))V)^{\ell-1}\Gamma_0(\lambda)^* \\
&= (2\pi i)^{-(\ell-1)}\Gamma_0(\lambda)VB(\lambda)^{\ell-1}\Gamma_0(\lambda)^*.
\end{aligned}$$

Noting the identity $\Gamma_0(\lambda)^*\Gamma_0(\lambda) = (2\pi i)^{-1}(R_0(\lambda+i0) - R_0(\lambda-i0))$ we find using cyclicity of the trace that

$$\mathrm{Tr}(A(\lambda)^\ell) = (2\pi i)^{-(\ell-1)}\mathrm{Tr}(\Gamma_0(\lambda)VB(\lambda)^{\ell-1}\Gamma_0(\lambda)^*) = (2\pi i)^{-\ell}\mathrm{Tr}(B(\lambda)^\ell).$$

We can also show the equality of traces at the level of integral kernels, however this is not necessary. □

We now use the operator $\Gamma_0(\lambda)$ to construct a generalised Fourier transform which diagonalises the perturbed Hamiltonian H.

Definition 2.4.25. Define for $\lambda > 0$ and $t > \frac{1}{2}$ the operators $\Gamma_\pm(\lambda) : H^{0,t} \to \mathcal{P}$ by

$$\Gamma_\pm(\lambda) = \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda \pm i0)).$$

Proposition 2.4.26. *For $\lambda > 0$ and $t > \frac{1}{2}$ the operators $\Gamma_\pm(\lambda) : H^{0,t} \to \mathcal{P}$ and their formal adjoints $\Gamma_\pm(\lambda)^* : \mathcal{P} \to H^{0,-t}$ are uniformly bounded on compact intervals. Moreover, the operator-valued functions $\Gamma_\pm(\lambda)$ are strongly continuous in $\lambda > 0$.*

Proof. This follows from Lemma 2.4.15 and the limiting absorption principle for H (Theorem 2.4.8). □

Definition 2.4.27. For $s \in \mathbb{R}$ and $t > \frac{1}{2}$ we define the *generalised Fourier transforms* $F_\pm : H^{s,t} \to \mathcal{H}_{spec}$ by

$$[F_\pm f](\lambda, \omega) = [\Gamma_\pm(\lambda) f](\omega).$$

Theorem 2.4.28. *Suppose that V satsifies Assymption 2.2.14. Then the operators $F_\pm$ extend by continuity to bounded operators $F_\pm : \mathcal{H} \to \mathcal{H}_{ac}$ which satisfy $F_\pm F_\pm^* = \mathrm{Id}$ and $F_\pm^* F_\pm = P_{ac}(H)$. The operators $F_\pm$ diagonalise H in the sense that for $f \in \mathrm{Dom}(H)$ and $\varphi : \mathbb{R}^+ \to \mathbb{C}$ measurable we have*

$$[F_\pm \varphi(H) F_\pm^* f](\lambda, \omega) = \varphi(\lambda) f(\lambda, \omega), \quad \lambda \in \mathbb{R}^+, \omega \in \mathbb{S}^{n-1}. \tag{2.67}$$

Proof. First note that for $f \in H^{0,t}$ and $\lambda > 0$ we have the limits

$$\pi^{-1} \lim_{\varepsilon \to 0} \varepsilon \, ||R_0(\lambda \pm i\varepsilon) f||^2 = \lim_{\varepsilon \to 0} \langle (R_0(\lambda + i\varepsilon) - R_0(\lambda - i\varepsilon)) f, f \rangle = |\Gamma_0(\lambda) f|^2.$$

The limiting absorption principle also gives us for $\lambda > 0$ the limit

$$\lim_{\varepsilon \to 0} ||VR(\lambda + i\varepsilon) f - VR(\lambda + i0) f||_{H^{0,t}} = 0.$$

Combining these, we find for any $f \in H^{0,t}$ and $\lambda > 0$ that

$$\begin{aligned} |\Gamma_\pm(\lambda) f|^2 &= |\Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda \pm i0)) f|^2 \\ &= \pi^{-1} \lim_{\varepsilon \to 0} \varepsilon \, ||R_0(\lambda \pm i\varepsilon)(\mathrm{Id} - VR(\lambda \pm i\varepsilon)) f||^2 \\ &= \pi^{-1} \lim_{\varepsilon \to 0} \varepsilon \, ||R(\lambda \pm i\varepsilon) f||^2 \\ &= \frac{\mathrm{d}\langle P_\lambda f, f \rangle}{\mathrm{d}\lambda}, \end{aligned}$$

by Stone's theorem (see [164, Equation (0.1.10)]. Integrating over $\mathbb{R}^+$ we find

$$||F_\pm f||^2 = \int_{\mathbb{R}^+} |\Gamma_\pm(\lambda)f|^2 \,\mathrm{d}\lambda = \int_{\mathbb{R}^+} \frac{\mathrm{d}\langle P_\lambda f, f\rangle}{\mathrm{d}\lambda} \,\mathrm{d}\lambda = ||P_{ac}(H)f||^2,$$

which implies $F_\pm^* F_\pm = P_{ac}(H)$. For the second partial isometry relation, we proceed by contradiction. Supposing that $F_\pm F_\pm^* \neq \mathrm{Id}$, we find there exists $g \in \mathcal{H}_{spec}$ such that all $f \in H^{0,t}$ and intervals $I \subset \mathbb{R}^+$ we have $\langle F_\pm P_I f, g\rangle = 0$, which further implies

$$\int_I \langle \Gamma_\pm(\lambda)f, g\rangle \,\mathrm{d}\lambda = 0.$$

Since I is an arbitrary interval we find $\langle \Gamma_\pm(\lambda)f, g(\lambda,\cdot)\rangle = \langle f, \Gamma_\pm(\lambda)^* g(\lambda,\cdot)\rangle = 0$ for almost every $\lambda > 0$. Since $f \in H^{0,t}$ is arbitrary we have $\Gamma_\pm(\lambda)^* g(\lambda,\cdot) = 0$ and thus by [164, Lemma 6.6.4] we find $g(\lambda,\cdot) = 0$ for almost all $\lambda > 0$.

To prove the intertwining relation of Equation (2.67), it suffices to check that for all $f \in C_c^\infty(\mathbb{R}^n)$ and $g \in C_c(\mathbb{R}^+) \otimes L^2(\mathbb{S}^{n-1})$ that

$$0 = \int_{\mathbb{R}^+} \langle \Gamma_\pm(\lambda)(H-\lambda)f, g(\lambda,\cdot)\rangle \,\mathrm{d}\lambda = \int_{\mathbb{R}^+} \langle f, (H-\lambda)\Gamma_\pm(\lambda)^* g(\lambda,\cdot)\rangle \,\mathrm{d}\lambda. \tag{2.68}$$

We readily check that $[H_0\Gamma_0(\lambda)^* g(\lambda,\cdot)](x) = \lambda g(\lambda,x)$ and so

$$\begin{aligned}
[(H-\lambda)\Gamma_\pm(\lambda)^* g(\lambda,\cdot)](x) &= [(H-\lambda)(\mathrm{Id} - R(\lambda \mp i0)V)\Gamma_0(\lambda)^* g(\lambda,\cdot)](x) \\
&= [(H_0 + V - \lambda)\Gamma_0(\lambda)^* g(\lambda,\cdot)](x) \\
&\quad - [(H-\lambda)R(\lambda \mp i0)V\Gamma_0(\lambda)^* g(\lambda,\cdot)](x) \\
&= 0,
\end{aligned}$$

which shows that the final integrand of Equation (2.68) is zero. □

Theorem 2.4.29. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 1$. Then for all $t > \frac{1}{2}$ and $f, g \in H^{0,t}$ we have*

$$\langle W_\pm f, g\rangle = \int_0^\infty \langle \Gamma_0(\lambda)f, \Gamma_\pm(\lambda)f\rangle \,\mathrm{d}\lambda = \langle F_0 f, F_\pm g\rangle.$$

That is the wave operators are given by $W_\pm = F_\pm^* F_0$.

Proof. We first compute for $f, g \in H^{0,t}$ with $t > \frac{1}{2}$ that

$$\begin{aligned}
\langle \Gamma_0(\lambda)f, \Gamma_\pm(\lambda)g\rangle &= \langle \Gamma_0(\lambda)f, \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda \pm i\varepsilon))g\rangle \\
&= (2\pi i)^{-1} \lim_{\varepsilon\to 0} \langle (R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon))f, (\mathrm{Id} - VR(\lambda \pm \varepsilon))g\rangle \\
&= \pi^{-1} \lim_{\varepsilon\to 0} \varepsilon \langle R_0(\lambda \pm i\varepsilon)f, R(\lambda \pm i\varepsilon)g\rangle.
\end{aligned}$$

Then by [164, Lemma 6.6.8] we can compute by bringing the limit inside the integral that

$$\pi^{-1} \lim_{\varepsilon \to 0} \int_{\mathbb{R}} \langle R_0(\lambda \pm i\varepsilon) f, R(\lambda \pm \varepsilon) g \rangle \, \mathrm{d}\lambda = \int_0^\infty \langle \Gamma_0(\lambda) f, \Gamma_\pm(\lambda) g \rangle \, \mathrm{d}\lambda. \tag{2.69}$$

One readily checks using Theorem 2.1.11 that

$$\int_0^\infty \langle \Gamma_0(\lambda) f, \Gamma_\pm(\lambda) g \rangle \, \mathrm{d}\lambda = \lim_{\varepsilon \to 0} 2\varepsilon \int_0^\infty \mathrm{e}^{-2\varepsilon t} \langle \mathrm{e}^{itH_0} f, \mathrm{e}^{\pm itH} g \rangle \, \mathrm{d}t$$

which gives the result. □

Definition 2.4.30. Suppose V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. We define the operators $\mathcal{F}_\pm : \mathcal{H} \to \mathcal{H}$ by $\mathcal{F}_\pm = F_\pm \mathcal{U}^*$, where $\mathcal{U}$ is as in Definition 2.2.7.

For $0 \neq \xi \in \mathbb{R}^n$ we use the notation

$$\mathbb{S}^{n-1} \ni \hat{\xi} = |\xi|^{-1} \xi \tag{2.70}$$

for the unit vector in the direction of ξ.

Lemma 2.4.31. *Suppose V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. Let $\psi_\pm$ be the generalised eigenfunctions for H of Proposition 2.4.13. For $f, g \in C_c^\infty(\mathbb{R}^n)$ and $x, \xi \in \mathbb{R}^n$ we have*

$$[\mathcal{F}_\pm f](\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \overline{\psi_\pm(x, \hat{\xi}, |\xi|^2)} f(x) \, \mathrm{d}x, \quad \xi \in \mathbb{R}^n, \tag{2.71}$$

and

$$[\mathcal{F}_\pm^* g](x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \psi_\pm(x, \hat{\xi}, |\xi|^2) g(\xi) \, \mathrm{d}\xi, \quad x \in \mathbb{R}^n. \tag{2.72}$$

Proof. For $t > \frac{n+1}{2}$, $f \in H^{0,t}$, $\omega \in \mathbb{S}^{n-1}$ and $\lambda > 0$ we note that

$$\begin{aligned} 2^{\frac{1}{2}} \lambda^{-\frac{n-2}{4}} (2\pi)^{\frac{n}{2}} [\Gamma_\pm(\lambda) f](\omega) &= \langle (\mathrm{Id} - VR(\lambda \pm i0)) f, \psi_0(\cdot, \omega, \lambda) \rangle \\ &= \langle f, (\mathrm{Id} - R(\lambda \mp i0) V) \psi_0(\cdot, \omega, \lambda) \rangle \\ &= \langle f, \psi_\pm(\cdot, \omega, \lambda) \rangle. \end{aligned}$$

Since $\psi_\pm \in H^{0,t}$, this immediately implies the formula for $\mathcal{F}_\pm$. To determine the adjoint, we let $t > \frac{n+1}{2}$ and fix $f \in H^{0,t}$ and $g \in \mathcal{H}$ with compact support in $\mathbb{R}^n \setminus \{0\}$. Then we have

$$\langle \mathcal{F}_\pm^* f, g \rangle = \langle g, \mathcal{F}_\pm f \rangle = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} g(\xi) \left(\int_{\mathbb{R}^n} \overline{f(x)} \psi_\pm(x, \hat{\xi}, |\xi|^2) \, \mathrm{d}x \right) \mathrm{d}\xi.$$

Since the integral is absolutely convergent, Fubini's theorem allows us to interchange the order of integration and obtain the formula for $\mathcal{F}_\pm^*$ as claimed. For arbitrary $g \in \mathcal{H}$ and $x \in \mathbb{R}^n$ one should use the formula

$$[\mathcal{F}_\pm^* g](x) = (2\pi)^{-\frac{n}{2}} \lim_{r\to\infty} \int_{r^{-1}\leq|\xi|\leq r} g(\xi)\psi_\pm(x, \hat{\xi}, |\xi|^2)\, \mathrm{d}\xi,$$

where the limit is taken in $\mathcal{H}$. □

The operators $\mathcal{F}_\pm$ can be considered as 'generalised Fourier transforms' which diagonalise the operator $H = H_0 + V$ in the sense that $\mathcal{F}_\pm H \mathcal{F}_\pm^* = M$, and share many interesting properties with the Fourier transform. In particular we note that if $V = 0$ we recover the standard Fourier transform and we have the for $f \in C_c^\infty(\mathbb{R}^n)$ and $\xi \in \mathbb{R}^n$ the relation

$$\begin{aligned} f(\xi) = [\mathcal{F}_\pm \mathcal{F}_\pm^* f](\xi) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \overline{\psi_\pm(x, \hat{\xi}, |\xi|^2)} [\mathcal{F}_\pm^* f](x)\, \mathrm{d}x \\ &= (2\pi)^{-n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \overline{\psi_\pm(x, \hat{\xi}, |\xi|^2)} \psi_\pm(x, \hat{\rho}, |\rho|^2) f(\rho)\, \mathrm{d}\rho\, \mathrm{d}x \\ &= \int_{\mathbb{R}^n} \left((2\pi)^{-n} \int_{\mathbb{R}^n} \overline{\psi_\pm(x, \hat{\xi}, |\xi|^2)} \psi_\pm(x, \hat{\rho}, |\rho|^2)\, \mathrm{d}x \right) f(\rho)\, \mathrm{d}\rho, \end{aligned}$$

so that the generalised eigenfunctions $\psi_\pm$ gives rise to a delta function, as in the case of the plane waves ψ_0 and the standard Fourier transform.

2.4.3 The scattering matrix

Let S be the scattering operator for the pair (H, H_0) as defined in Definition 2.1.9. Since the scattering operator S satisfies $[S, H_0] = 0$ the spectral theorem asserts that there exists a family $\{S(\lambda)\}_{\lambda\in\mathbb{R}^+}$ of unitary operators on $\mathcal{P} = L^2(\mathbb{S}^{n-1})$ such that for all $\lambda \in \mathbb{R}^+$ we have $[F_0 S F_0^* f](\lambda, \omega) = S(\lambda) f(\lambda, \omega)$. For $\lambda \in \mathbb{R}^+$ the operator $S(\lambda)$ is referred to as the scattering matrix at energy λ and was first studied by Wheeler [162] and Heisenberg [75]. The term 'scattering matrix' is historical and due to the fact that in dimension $n = 1$ we have $L^2(\mathbb{S}^0) = \mathbb{C}^2$, so that the scattering matrix is a bona fide matrix-valued function $S : \mathbb{R}^+ \to M_2(\mathbb{C})$.

For potentials decaying sufficiently fast, Kuroda [104, 105] used stationary scattering theory to establish an expression for the scattering matrix in terms of the potential and resolvent using the limiting absorption principal.

Theorem 2.4.32 ([164, Theorem 6.10])**.** *Suppose that V satisfies Assumption 2.2.14. Then the scattering matrix is given for all $\lambda \in (0, \infty)$ by the equation*

$$S(\lambda) = \mathrm{Id} - 2\pi i \Gamma_0(\lambda)(V - VR(\lambda + i0)V)\Gamma_0(\lambda)^*. \tag{2.73}$$

The operator $S(\lambda)$ is unitary in $L^2(\mathbb{S}^{n-1})$ and depends norm continuously on $\lambda \in (0, \infty)$.

Proof. By Theorem 2.4.29 we can write the wave operators in terms of generalised Fourier transforms and thus $S = W_+^* W_- = (F_+^* F_0)^* (F_-^* F_0) = F_0^* (F_+ F_-^*) F_0$. Thus the scattering matrix is given by $S = F_+ F_-^*$. So to prove that Equation (2.73) defines the scattering matrix it suffices to check for any $t > \frac{1}{2}$ and $f \in H^{0,t}$ that $S(\lambda)$ defined by Equation (2.73) satisfies

$$[F_+ f](\lambda, \omega) = S(\lambda)[F_- f](\lambda, \omega), \quad \lambda \in \mathbb{R}^+, \omega \in \mathbb{S}^{n-1},$$

which by Definition 2.4.27 is equivalent to the relation

$$\Gamma_+(\lambda) f = S(\lambda) \Gamma_-(\lambda) f. \tag{2.74}$$

So we compute the right hand side of Equation (2.74) as

$$\begin{aligned} S(\lambda)\Gamma_-(\lambda) f &= \Gamma_-(\lambda) f - 2\pi i \Gamma_0(\lambda)(V - VR(\lambda + i0)V)\Gamma_0(\lambda)^* \Gamma_-(\lambda) f \\ &= \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda - i0)) f \\ &\quad - 2\pi i \Gamma_0(\lambda)(V - VR(\lambda + i0)V)\Gamma_0(\lambda)^* \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda - i0)) f \\ &= \Gamma_0(\lambda) f - \Gamma_0(\lambda) VR(\lambda - i0) f \\ &\quad - 2\pi i \Gamma_0(\lambda)(V - VR(\lambda + i0)V)\Gamma_0(\lambda)^* \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda - i0)) f \end{aligned}$$

The left hand side of Equation (2.74) can be written as

$$\Gamma_+(\lambda) f = \Gamma_0(\lambda) f - \Gamma_0(\lambda) VR(\lambda + i0) f.$$

Taking the difference of the two expressions shows that Equation (2.74) is equivalent to

$$\begin{aligned} &\Gamma_0(\lambda)(R(\lambda - i0) - R(\lambda + i0)) f \\ &= -2\pi i \Gamma_0(\lambda)(V - VR(\lambda + i0)V)\Gamma_0(\lambda)^* \Gamma_0(\lambda)(\mathrm{Id} - VR(\lambda - i0)) f. \end{aligned}$$

We recall the identity $2\pi i \Gamma_0(\lambda)\Gamma_0(\lambda)^* = R_0(\lambda + i0) - R_0(\lambda - i0)$ (see Lemma 2.4.19) and thus it suffices to check

$$R(\lambda + i0) - R(\lambda - i0) = V(\mathrm{Id} - R(\lambda + i0)V)(R_0(\lambda + i0) - R_0(\lambda - i0))(\mathrm{Id} - VR(\lambda - i0)), \tag{2.75}$$

where both sides are considered as mappings from $H^{0,t}$ to $H^{0,-t}$. For $z \in \rho(H)$, Equation (2.75) follows from resolvent identities (see Equation (2.50)) and for $z = \lambda + i0$ the result follows by the limiting absorption principle (Theorems 2.4.5 and 2.4.8). □

We can use the Lippmann-Schwinger equation to explicitly determine the integral kernel of the scattering matrix in terms of the scattering amplitude of Definition 2.4.18.

Lemma 2.4.33. *[164, Theorem 6.7.8] Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$. Then for $\lambda > 0$ the operator $S(\lambda) - \mathrm{Id} \in \mathcal{B}(\mathcal{P})$ is an integral operator with integral kernel*

$$\tilde{S}(\theta, \omega, \lambda) = (2\pi i)(2\pi)^{-\frac{n+1}{2}} \lambda^{\frac{n-1}{4}} a_-(\theta, \omega, \lambda),$$

where a_- is the scattering amplitude of Definition 2.4.18.

Proof. Note that for $t > \frac{n}{2}$ and $f \in H^{0,t}$ we can write

$$[\Gamma_0(\lambda) f](\omega) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} (2\pi)^{-\frac{n}{2}} \langle f, \psi_0(\cdot, \omega, \lambda) \rangle,$$

where here we are considering $\langle \cdot, \cdot \rangle$ as the duality between $H^{0,t}$ and $H^{0,-t}$. Thus by Equation (2.63) we have the scattering amplitude $a_\pm$ given by the absolutely convergent integral

$$\begin{aligned} a_-(\theta, \omega, \lambda) &= -2^{-1} (2\pi)^{-\frac{n-1}{2}} \lambda^{\frac{n-3}{4}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\lambda^{\frac{1}{2}} \langle \theta, x \rangle} V(x) \psi_\pm(x, \omega, \lambda) \, \mathrm{d}x \\ &= -2^{-1} (2\pi)^{-\frac{n-1}{2}} \lambda^{\frac{n-3}{4}} \langle (V - VR(\lambda + i0)V) \psi_0(\cdot, \omega, \lambda), \psi_0(\cdot, \theta, \lambda) \rangle. \end{aligned}$$

Comparing with Equation (2.73) completes the proof. □

Birman and Kreĭn [25] note that for trace class perturbations V the operator $S(\lambda) - \mathrm{Id}$ defines a compact operator on $\mathcal{P}$ for all $\lambda \in \mathbb{R}^+$. In fact much stronger summability conditions for the scattering operator are known. The following can be found as [164, Proposition 8.1.5], we omit the proof since it requires substantial techniques from the method of H_0-smoothness.

Theorem 2.4.34. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 1$. Then for all $\lambda > 0$ and $p > \frac{n-1}{\rho - 1}$ we have $S(\lambda) - \mathrm{Id} \in \mathcal{L}^p(\mathcal{P})$, the p-th Schatten class . In particular, if $\rho > n$ then $S(\lambda) - \mathrm{Id}$ is trace class.*

In fact the proof of Theorem 2.4.34 can be used to establish differentiability of the scattering matrix in the Schatten norms also. The following is [164, Proposition 8.1.9].

Proposition 2.4.35. *Let $\ell \in \mathbb{N} \cup \{0\}$ and $p \geq 1$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > \ell + 1 + \frac{n-1}{p}$. Then the scattering matrix $S : \mathbb{R}^+ \to \mathcal{L}^p(\mathcal{P})$ is ℓ times continuously differentiable in $\mathcal{L}^p(\mathcal{H})$. In particular, if $\rho > \ell + n$ then S is ℓ times differentiable in trace norm.*

2.5 Levinson's theorem

Levinson's theorem [108] is a fundamental result in scattering theory relating the number of bound states of a Hamiltonian $H = H_0 + V$ to a quantity related to the 'total phase shift'. The original proof of Levinson's theorem uses classical ODE theory, complex analysis and the subtleties of a scattering object known as the Jost function. As such the proof is specific to one dimension. In this section we describe the time-delay operator and the spectral shift function, important quantities in scattering theory which can be used to prove and generalise Levinson's theorem to higher dimensions. We discuss the high energy behaviour of the time-delay operator and spectral shift function and how they relate to Levinson's theorem. We conclude with several simple examples.

2.5.1 Time delay

In this section we describe intuitively the time delay of a quantum mechanical system and construct an operator, known as the Eisenbud-Wigner time delay operator which is defined to be the time delay in the spectral representation and can be explicitly described in terms of the scattering matrix. The time delay of particles was first considered by Eisenbud [57] and Wigner [163] in a stationary manner.

To define the time delay, we consider for $r > 0$ the orthogonal projection P_r onto the functions with support in the ball of radius r in $\mathcal{H}$. For $f \in \mathcal{H}$ a measure of the total time spent in $P_r\mathcal{H}$ is given by

$$\int_{\mathbb{R}} \left|\left|P_r \mathrm{e}^{-itH} f\right|\right|^2 \, \mathrm{d}t. \tag{2.76}$$

For any $f \in \mathcal{H}$, the quantities $\mathrm{e}^{-itH_0} f$ and $\mathrm{e}^{-itH} W_- f$ agree in the limit as $t \to -\infty$. The difference of times spent in $P_r\mathcal{H}$ of these states is given by

$$\Delta T_r(f) = \int_{\mathbb{R}} \left(\left|\left|P_r \mathrm{e}^{-itH} W_- f\right|\right|^2 - \left|\left|P_r \mathrm{e}^{-itH_0} f\right|\right|^2 \right) \mathrm{d}t. \tag{2.77}$$

As $r \to \infty$ one expects a finite limit (at least for a dense set of $f \in \mathcal{H}$). We will show that there exists a self-adjoint operator T, called the Eisenbud-Wigner time delay operator, which satisfies

$$\langle f, Tf \rangle := \lim_{r \to \infty} \Delta T_r(f). \tag{2.78}$$

This time-dependent definition of the time-delay operator was introduced in [82] and further discussed in [83]. Proofs of Equations (2.77) and (2.78) were first given in [114] in the case that the scattering matrix is scalar and later extended in [86]. An alternative definition of time delay is provided in [122]. A thorough and physically motivated discussion of the time delay operator is given in [115], see also [48]. The operator T is given explicitly in terms of the scattering matrix. To prove such a result requires some intermediary results on the differentiability of the scattering matrix.

Recall from Theorem 2.4.1 for $\mu > 0$ the trace operator $\gamma(\mu) : C_c^\infty(\mathbb{R}^n) \to \mathcal{P}$ defined by $[\gamma(\mu)f](\omega) = f(\mu\omega)$. It is well-known that for any $s > \frac{1}{2}$ and $m \in \mathbb{R}$ the operator $\gamma(\mu)$ extends to an element of $\mathcal{B}(H^{s,m}, \mathcal{P})$. The following result, which demonstrates the differentiability of the trace map, is due to Jensen [86, Lemma 3.3].

Lemma 2.5.1. *Let $m \in \mathbb{R}$, $k \geq 0$ an integer and $s > k + \frac{1}{2}$. Then $\mu \mapsto \gamma(\mu)$ is k times continuously differentiable in norm on $\mathcal{B}(H^{s,m}, \mathcal{P})$.*

To construct the time delay operator we also need differentiability properties of the boundary values of the free resolvent along the positive real axis. The following result is a combination of [86, Lemma 3.4].

Lemma 2.5.2. *Suppose that V satsifies Assumption 2.2.14 for some $\rho > 2$. Suppose that $s, m > \frac{3}{2}$. Then $\lambda \mapsto R(\lambda + i0)$ is continuously differentiable as a map from $(0, \infty)$ to $\mathcal{B}(H^{-1,s}, H^{1,-m})$.*

With the differentiability of the trace and free resolvent established, we can use the stationary formula for the scattering matrix of Theorem 2.4.32 to determine the differentiability of the scattering matrix.

We are now ready to construct the time delay operator as in [86, Theorem 3.7].

Theorem 2.5.3. *Let V satisfy Assumption 2.2.14 for some $\varepsilon > 0$ and $\rho > 2 + \varepsilon$ and let T be defined by*

$$\mathrm{Dom}(T) = \{f \in \mathcal{H} : P_{[a,b]}(H_0)f = f \text{ for some } [a, b] \subset (0, \infty)\} \subset \mathrm{Dom}(H_0)$$

with $T = -iF_0^* S(\cdot)^* S'(\cdot)F_0$. The operator T is essentially self-adjoint on $\mathrm{Dom}(T)$ *and T commutes with H_0.*

Proof. By Proposition 2.4.35 we have that the scattering matrix is differentiable in the pth Schatten class $\mathcal{L}^p(\mathcal{P}) \subset \mathcal{B}(\mathcal{P})$ for all $p > \frac{n-1}{\varepsilon}$. Unitarity of the scattering matrix then implies the relation

$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda}(S(\lambda)^* S(\lambda)) = S(\lambda)^* S'(\lambda) + (S'(\lambda))^* S(\lambda)$$

and thus for each $\lambda \in (0, \infty)$ we find $-iS(\lambda)^* S'(\lambda)$ is a bounded self-adjoint operator in $\mathcal{B}(\mathcal{P})$. So T is densely-defined, symmetric and for each $[a, b] \subset (0, \infty)$ we have $TP_{[a,b]}$ is a bounded self-adjoint operator. So T is essentially self-adjoint on $\mathrm{Dom}(T)$. That T commutes with H_0 follows from the definition in terms of S. □

We refer to T as the Eisenbud-Wigner time delay operator, or simply the time delay. The explicit representation of T in Theorem 2.5.3 was first given in [152]. We note that here we have only discussed time delay for Euclidean Schrödinger operators, however time delay is a more fundamental concept of a scattering system and its definition generalises to a more abstract setting. We refer to [139] for a discussion of such topics.

Lemma 2.5.4. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > n+1$. Then for all $\lambda \in \mathbb{R}^+$ the operator $S(\lambda)^* S'(\lambda)$ is trace class on $\mathcal{P}$.*

Proof. By Theorem 2.4.34 the operator $S'(\lambda)$ is trace class. Since the trace class operators form an ideal, the product $S(\lambda)^* S'(\lambda)$ is trace class also. □

2.5.2 The spectral shift function

The spectral shift function was first introduced by Lifshits to study the size of the eigenvalue shift for finite rank perturbations B of a lattice model operator A_0 in quantum mechanics and later extended in [109] to computing the trace of $f(A_0+B) - f(A_0)$ for a large class of functions. Lifshits suggested the formula

$$\mathrm{Tr}(f(A_0+B) - f(A_0)) = \int_{\mathbb{R}} f'(\lambda)\xi(\lambda, A_0+B, A_0)\,\mathrm{d}\lambda \tag{2.79}$$

where the function $\xi(\cdot, A_0+B, A_0)$ depends only on the self-adjoint operators A_0 and A_0+B. The extension from discrete models to continuous models was first studied by Kreĭn [100], who provided a suitable class of perturbations for which the spectral shift function ξ exists and Equation (2.79) holds. In [101] Kreĭn showed that the spectral shift function exists and satisfies Equation (2.79) if the operator $(A_0+B-z)^{-1} - (A_0-z)^{-1}$ is trace class for some (and hence all) $z \in \mathbb{C} \setminus \mathbb{R}$. The approach of Kreĭn is based on the theory of perturbation determinants as in Definition 2.5.5 (see [33], [99], [70, Section IV.3] and [151, Chapter 5] for more details).

Definition 2.5.5. Suppose that $\mathcal{H}$ is a Hilbert space and A is a trace class operator on $\mathcal{H}$. Then we define

$$\mathrm{Det}(\mathrm{Id} + A) = \prod_{j=1}^{\infty} (1 + \mu_j(A)),$$

where the μ_j denote the eigenvalues of A. The absolute convergence of the product is guaranteed by the assumption that A is trace class. If $A \in \mathcal{L}^p(\mathcal{H})$ (the p-th Schatten class) for some $p \in \mathbb{N}$ then we can define the regularised determinant by

$$\mathrm{Det}_p(\mathrm{Id} + A) = \prod_{j=1}^{\infty} \left((1 + \mu_j(A)) \exp\left(\sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mu_j(A)^\ell \right) \right).$$

Definition 2.5.6. Let A and $B = A + \tilde{V}$ be self-adjoint operators on $\mathcal{H}$ such that $\tilde{V}(A-z)^{-1}$ defines a trace class operator for some (and hence all) $z \in \rho(A)$. Then we define for $z \in \rho(A)$ the function

$$D(z) = \mathrm{Det}(\mathrm{Id} + \tilde{V}(A-z)^{-1}).$$

The analytic Fredholm alternative tells us that $D(z)$ is defined and holomorphic on the set $\rho(A)$ and that $D(z) \neq 0$ for all $z \in \rho(A) \cap \rho(B)$. Furthermore for $z \in \rho(A) \cap \rho(B)$ we have [164, Equation 0.9.3] the equality

$$D^{-1}(z)D'(z) = \mathrm{Tr}((A-z)^{-1} - (B-z)^{-1}).$$

The first theorem of Kreĭn demonstrates the existence of the spectral shift function for a trace class perturbation $\tilde{V}$.

Theorem 2.5.7. *[164, Theorem 0.9.1] Let A and B be self-adjoint operators on $\mathcal{H}$ such that $\tilde{V} := B - A$ is trace class. Then for almost all $\lambda \in \mathbb{R}$ the limit*

$$\xi(\lambda, A, B) := \pi^{-1} \lim_{\varepsilon \to 0} \mathrm{Arg}(D(\lambda + i\varepsilon)) \tag{2.80}$$

exists and satisfies

$$\int_{\mathbb{R}} |\xi(\lambda, A, B))| \,\mathrm{d}\lambda \leq \left|\left|\tilde{V}\right|\right|_1, \quad \text{and} \quad \int_{\mathbb{R}} \xi(\lambda, A, B) \,\mathrm{d}\lambda = \mathrm{Tr}(\tilde{V}).$$

Proposition 2.5.8. *[164, Proposition 0.9.1] Let A and B be self-adjoint operators on $\mathcal{H}$ such that $\tilde{V} := B - A$ is trace class. On component intervals of the set $\rho(A) \cap \rho(B)$ of common regular points of the operators A and B the spectral shift function $\xi(\lambda, A, B)$ assumes constant integer values. If λ is an isolated eigenvalue of finite multiplicity $M_A(\lambda)$ of the operator A and $M_B(\lambda)$ of the operator B, then*

$$\xi(\lambda + 0, A, B) - \xi(\lambda - 0, A, B) = M_A(\lambda) - M_B(\lambda).$$

The second theorem of Kreĭn establishes Equation (2.79) for trace class perturbations $\tilde{V}$.

Theorem 2.5.9. *[164, Theorem 0.9.3] Let A and B be self-adjoint operators on $\mathcal{H}$ such that $\tilde{V} := B - A$ is trace class and suppose that $f \in C^1(\mathbb{R})$ and its derivative admits the representative*

$$f'(\lambda) = \int_{\mathbb{R}} \mathrm{e}^{-i\lambda t} \mathrm{d}m(t)$$

for a finite (complex) measure m and almost all $\lambda \in \mathbb{R}$. Then $f(B) - f(A) \in \mathcal{L}^1(\mathcal{H})$ and we have the trace formula

$$\mathrm{Tr}(f(B) - f(A)) = \int_{\mathbb{R}} f'(\lambda)\xi(\lambda, A, B) \,\mathrm{d}\lambda. \tag{2.81}$$

We now specialise again to the operators H_0 and $H = H_0 + V$. The following statement gives a relationship between the spectral shift function, the scattering matrix and the time delay operator.

Theorem 2.5.10. *Suppose $V \in \mathcal{L}^1(\mathcal{H})$. Then we have*

$$\mathrm{Det}(S(\lambda)) = \mathrm{e}^{-2\pi i \xi(\lambda)} \tag{2.82}$$

for almost all $\lambda \in \sigma_{ac}(H_0)$. Furthermore, we have

$$\mathrm{Tr}(S(\lambda)^* S'(\lambda)) = -2\pi i \xi'(\lambda). \tag{2.83}$$

Equation (2.82) dates back to an observation of Beth and Uhlenbeck [22] relating a phase shift to the second virial coefficient, and was first proved in the context of the spectral shift function by Birman and Kreĭn [25]. Unfortunately the above definition needs some modification since our multiplication operator V is not usually compact. To fix this, we consider relatively trace class perturbations.

Lemma 2.5.11. *[73, Proposition III.1] Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{n+1}{2}$ and fix $c > |\inf \sigma_p(H)|$. Then the operators $H_0 + c$ and $H + c$ are positive definite and we have the difference $R(-c)^m - R_0(-c)^m$ is trace class for any integer $m \geq \rho$.*

Define the operators $G = R(-c)^m$ and $G_0 = R_0(-c)^m$. Then we can use Theorem 2.5.7 to define the spectral shift function for the pair (G, G_0) and lead us to the following definition.

Definition 2.5.12. Suppose that V satisfies Assumption 2.2.14 for some $\rho > n$. We define the *spectral shift function* for the pair (H, H_0) to be the function

$$\xi(\lambda, H, H_0) = \begin{cases} -\xi((\lambda + c)^{-m}, G, G_0), & \text{if } \lambda > -c, \\ 0 & \text{if } \lambda - \leq c. \end{cases}$$

The spectral shift function is determined uniquely by the constraint $\xi(\lambda, H, H_0) = 0$ for $\lambda \leq -c$. We will often just write $\xi(\lambda)$ for the spectral shift function of the pair (H, H_0) and drop the reference to these operators.

The spectral shift function satisfies the following properties.

Theorem 2.5.13. *[164, Theorem 0.9.7] Suppose that V satisfies Assumption 2.2.14 for some $\rho > n$. Then the spectral shift function ξ of Definition 2.5.12 satisfies the estimate*

$$m \int_{\mathbb{R}} |\xi(\lambda)|(1 + |\lambda|)^{-m-1} \, \mathrm{d}\lambda \leq ||R(-c)^m - R_0(-c)^m||_1 < \infty$$

and is related to the scattering matrix by Equation (2.82). Furthermore, if $f : \mathbb{R} \to \mathbb{C}$ has *two locally bounded derivatives and for some $\varepsilon > 0$ we have*

$$(\lambda^{m+1} f'(\lambda))' = O(\lambda^{-1-\varepsilon}) \tag{2.84}$$

as $\lambda \to \infty$ then the trace formula of Equation (2.81) *holds. The conclusion of Proposition 2.5.8 holds also.*

In Chapter 5 we will use Equation (2.82) to determine the value of the spectral shift function as $\lambda \to 0$ from above.

We have the following statement regarding the properties of $\mathrm{Det}(S(\lambda))$ due to Guillopé [73, Theorem III.1].

Lemma 2.5.14. *Suppose that $V = q_1 q_2$ with $q_1, q_2 \in C_c^\infty(\mathbb{R}^n)$. Then for all $\lambda > 0$ and $p \geq \lfloor \frac{n}{2} \rfloor$ we have*

$$\mathrm{Det}\,(S(\lambda)) \\ = \frac{\mathrm{Det}_p\,(\mathrm{Id} + q_1 R_0(\lambda - i0) q_2)}{\mathrm{Det}_p\,(\mathrm{Id} + q_1 R_0(\lambda + i0) q_2)} \exp\left(\sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0) q_2)^\ell - (q_1 R_0(\lambda - i0) q_2)^\ell\right)\right).$$

Remark 2.5.15. If $n = 1$ and $p = 1$ or $n = 2, 3$ and $p = 2$ we only require that V satisfies Assumption 4.3.1 to obtain the statement of Lemma 2.5.14 (see [164, Section 9.1]).

We also recall the following [164, Proposition 9.1.3].

Lemma 2.5.16. *Suppose that ρ satisfies Assumption 4.3.1. If $n = 1$, let $p \geq 1$, if $n = 2, 3$ let $p \geq 2$ and if $n \geq 4$ let $p \geq n$. Define for $z \in \mathbb{C} \setminus \mathbb{R}$ the function*

$$D_p(z) = \mathrm{Det}_p(\mathrm{Id} + q_1 R_0(z) q_2).$$

Then we have

$$\lim_{|z| \to \infty} D_p(z) = 1$$

uniformly in $\mathrm{Arg}(z)$*. By the limiting absorption principle this limit extends to the positive real axis also.*

Combining the results of Lemmas 2.5.14 and 2.5.16 with Theorem 2.5.13 we can determine the high-energy behaviour of the spectral shift function.

Lemma 2.5.17. *Suppose that $V = q_1 q_2$ with $q_1, q_2 \in C_c^\infty(\mathbb{R}^n)$. If $n = 1$, let $p \geq 1$, if $n = 2, 3$ let $p \geq 2$ and if $n \geq 4$ let $p \geq n$. Then we have the limit*

$$\lim_{\lambda \to \infty} \left(-2\pi i \xi(\lambda) + \sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0) q_2)^\ell - (q_1 R_0(\lambda - i0) q_2)^\ell\right)\right) = 2\pi m$$

for some $m \in \mathbb{Z}$.

Proof. Using Lemma 2.5.14 and Theorem 2.5.13 we have

$$\begin{aligned}
&\frac{\mathrm{Det}_p\left(\mathrm{Id} + q_1 R_0(\lambda - i0) q_2\right)}{\mathrm{Det}_p\left(\mathrm{Id} + q_1 R_0(\lambda + i0) q_2\right)} \\
&= \mathrm{Det}(S(\lambda)) \exp\left(\sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0) q_2)^\ell - (q_1 R_0(\lambda - i0) q_2)^\ell\right)\right) \\
&= \exp\left(-2\pi i \xi(\lambda) + \sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0) q_2)^\ell - (q_1 R_0(\lambda - i0) q_2)^\ell\right)\right).
\end{aligned}$$

By Lemma 2.5.16 we have

$$\lim_{\lambda \to \infty} \frac{\mathrm{Det}_p\left(\mathrm{Id} + q_1 R_0(\lambda - i0) q_2\right)}{\mathrm{Det}_p\left(\mathrm{Id} + q_1 R_0(\lambda + i0) q_2\right)} = 1,$$

from which the result follows. □

Remark 2.5.18. We can fix a branch of the meromorphic function $\ln \mathrm{Det}_p(\mathrm{Id} + q_1 R_0(z) q_2)$ by the condition

$$\lim_{|z| \to \infty} \arg \mathrm{Det}_p(\mathrm{Id} + q_1 R_0(z) q_2) = 0.$$

Fixing this branch gives $m = 0$ in Lemma 2.5.17 and we take this convention for the results of Chapter 5.

We now demonstrate some further special properties of the spectral shift function for Schrödinger operators. We enumerate the eigenvalues of H in increasing order as $\lambda_K < \cdots < \lambda_2 < \lambda_1 \leq 0$ and write $M(\lambda_k)$ for the multiplicity of the eigenvalue λ_k. We also write $N_0 = M(0)$.

Theorem 2.5.19 (Birman-Kreĭn)**.** *Suppose that V satisfies Assumption 2.2.14 for some $\rho > n$. Then for any differentiable f such that Equation* (2.81) *holds we have*

$$\begin{aligned}
\mathrm{Tr}(f(H) - f(H_0)) = &\sum_{k=1}^{K} f(\lambda_k) M(\lambda_k) + f(0)\big(\xi(0-) - \xi(0+) - N_0\big) \\
&+ \frac{1}{2\pi i} \int_0^\infty f(\lambda) \mathrm{Tr}(S(\lambda)^* S'(\lambda))\, \mathrm{d}\lambda.
\end{aligned} \tag{2.85}$$

Proof. Suppose that 0 is an eigenvalue of H, so that when enumerated the distinct eigenvalues of H are $\lambda_K < \cdots < \lambda_2 < \lambda_1 = 0$. The case when 0 is not an eigenvalue is similar.

We begin by applying Proposition 2.5.8 and the trace formula (2.81) to note that

$$\begin{aligned}\mathrm{Tr}(f(H)-f(H_0)) &= \int_{\mathbb{R}} f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda = \int_{-\infty}^{0} f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda \\ &= \int_{-\infty}^{\lambda_K} f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda + \sum_{k=2}^{K-1}\int_{\lambda_{k+1}}^{\lambda_k} f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda + \int_{\lambda_2}^{0} f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda \\ &\quad + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda.\end{aligned}$$

The spectral shift function is constant in intervals between eigenvalues by Proposition 2.5.8 and so we obtain

$$\begin{aligned}\mathrm{Tr}(f(H)-f(H_0)) &= \xi(\lambda_K-)(f(\lambda_K)-f(-\infty)) + \sum_{k=2}^{K-1}\left(f(\lambda_k)\xi(\lambda_k-) - f(\lambda_{k+1})\xi(\lambda_{k+1}+)\right) \\ &\quad + (f(0)\xi(0-) - f(\lambda_2)\xi(\lambda_2+)) + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda \\ &= \sum_{k=2}^{K} f(\lambda_k)(\xi(\lambda_k-)-\xi(\lambda_k+)) + f(0)\xi(0-) + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda \\ &= \sum_{k=1}^{K} f(\lambda_k)M(\lambda_k) - f(0)N_0 + f(0)\xi(0-) + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda.\end{aligned}$$

We note that by [164, Lemma 9.1.20] we have $\xi|_{(0,\infty)} \in C^1((0,\infty))$ provided $\rho > n$. We integrate by parts and apply Equation (2.83) (valid by Theorem 2.5.13) to obtain

$$\begin{aligned}\mathrm{Tr}(f(H)-f(H_0)) &= \sum_{k=1}^{K} f(\lambda_k)M(\lambda_k) - f(0)N_0 + f(0)\xi(0-) + \int_0^\infty f'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda \\ &= \sum_{k=1}^{K} f(\lambda_k)M(\lambda_k) - f(0)N_0 + f(0)\xi(0-) \\ &\quad + (f(\infty)\xi(\infty) - f(0)\xi(0+)) + \frac{1}{2\pi i}\int_0^\infty f(\lambda)\mathrm{Tr}(S(\lambda)^*S'(\lambda))\,\mathrm{d}\lambda.\end{aligned}$$

Noting that $f(\infty) = 0$ completes the proof. □

We will discuss further in Chapter 5 how the value of $\xi(0+)$ depends on the existence of resonances in each dimension after developing the relevant low energy expansions of the resolvent. Such results have been discussed in dimension $n \neq 2, 4$ in [73, Theorem III.2] using perturbation determinant methods and the low energy behaviour of the resolvent discussed in Chapter 3. The Birman-Kreĭn formula can also be obtained (in odd dimensions) using the Helffer-Sjöstrand functional calculus, see [56, Theorem 3.51] for example. The Birman-Kreĭn formula can also be shown to hold in other scattering contexts, such as for massive Dirac operators in $\mathbb{R}^3$ [51, Theorem 4.2] and for obstacle scattering [155, Theorem 6.1]. A discussion of the spectral shift function and Birman-Kreĭn formula for scattering on asymptotically cylindrical manifolds can be found in [119]. A discussion of the spectral shift function in supersymmetric scattering can be found in [32] and [118].

2.5.3 Trace class properties of the scattering matrix

In this section we describe the high-energy behaviour of the scattering operator in the trace norm using the expression for $\mathrm{Det}(S(\lambda))$ of Lemma 2.5.14. As a result we determine, using pseudodifferential expansions of the resolvent and the limiting absorption principle, the leading order high-energy asymptotics of the spectral shift function ξ and its derivative. These leading order asymptotics are related to the heat kernel expansion as $t \to 0^+$ of the trace of the difference $\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0}$.

To evaluate some further traces, we need to be able to integrate polynomials over $\mathbb{S}^{n-1}$. We use the following result [65].

Lemma 2.5.20. *Let α be a multi-index of length n and let $P_\alpha : \mathbb{R}^n \to \mathbb{C}$ be given by $P_\alpha(x) = x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. Then*

$$\int_{\mathbb{S}^{n-1}} P_\alpha(\omega)\,\mathrm{d}\omega = \begin{cases} 0, & \text{if some } \alpha_j \text{ is odd,} \\ \frac{2\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)}{\Gamma\left(\frac{n+|\alpha|}{2}\right)}, & \text{if all } \alpha_j \text{ are even.} \end{cases}$$

Lemma 2.5.21. *Suppose that α is a multi-index of length n, $g \in C_c^\infty(\mathbb{R}^n)$ and let $X = g\partial^\alpha$, a differential operator of order $|\alpha|$. Then for $t > 0$ we have*

$$\mathrm{Tr}\left(X\mathrm{e}^{-tH_0}\right) = \frac{(-i)^{|\alpha|}\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)t^{-\frac{n+|\alpha|}{2}}}{(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right)$$

if all α_j are even and $\mathrm{Tr}\left(X\mathrm{e}^{-tH_0}\right) = 0$ otherwise.

Proof. We compute the trace as

$$\mathrm{Tr}\left(X\mathrm{e}^{-tH_0}\right) = \frac{(-i)^{|\alpha|}}{(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n} y^\alpha \mathrm{e}^{-t|y|^2}\,\mathrm{d}y\right).$$

If any of the components α_j is odd, then by changing to polar coordinates we find that $\mathrm{Tr}\left(X\mathrm{e}^{-tH_0}\right) = 0$ by Lemma 2.5.20. If all of the α_j are even we obtain

$$\begin{aligned}\mathrm{Tr}\left(X\mathrm{e}^{-tH_0}\right) &= \frac{2(-i)^{|\alpha|}\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)}{(2\pi)^n\Gamma\left(\frac{n+|\alpha|}{2}\right)}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right)\left(\int_0^\infty r^{|\alpha|+n-1}\mathrm{e}^{-tr^2}\,\mathrm{d}r\right) \\ &= \frac{(-i)^{|\alpha|}\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)t^{-\frac{n+|\alpha|}{2}}}{(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right),\end{aligned}$$

where we have used polar coordinates and Lemma 2.5.20 to compute the spherical integral.
□

Lemma 2.5.22. *Suppose that α is a multi-index of length n, $g_1, g_2 \in C_c^\infty(\mathbb{R}^n)$ and let $g = g_1 g_2$. Let $X = g_2\partial^\alpha$ be a differential operator of order $|\alpha|$. Fix $\ell \in \mathbb{N}$ with $\ell \leq \frac{n+|\alpha|}{2}$ if n is even. Then for $\lambda > 0$ we have*

$$\begin{aligned}&\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right)\\ &= \frac{(-i)^{|\alpha|}(2\pi i)\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)\lambda^{\frac{n+|\alpha|}{2}-\ell}}{(\ell-1)!\Gamma\left(\frac{n}{2}+1-\ell+\frac{|\alpha|}{2}\right)(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right)\end{aligned}$$

if all α_j are even and $\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right) = 0$ otherwise. If n is even and $\ell > \frac{n+|\alpha|}{2}$ then $\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right) = 0$ also.

Proof. Fix $\lambda > 0$. The integral kernel of $B(\lambda) = \left(R_0(\lambda+i0) - R_0(\lambda-i0)\right)g_1$ is given by

$$B(\lambda,x,y) = \frac{(2\pi i)\lambda^{\frac{n}{2}-1}}{2(2\pi)^n}g_1(y)\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle\omega,y-x\rangle}\,\mathrm{d}\omega.$$

Letting $A(\lambda) = X\left(R_0(\lambda+i0) - R_0(\lambda-i0)\right)g_1$ we see by Lemma 2.4.20 that $A(\lambda)$ has integral kernel

$$A(\lambda,x,y) = \frac{(-i)^{|\alpha|}(2\pi i)\lambda^{\frac{n+|\alpha|}{2}-1}}{2(2\pi)^n}g_2(x)g_1(y)\int_{\mathbb{S}^{n-1}} \omega_1^{\alpha_1}\cdots\omega_n^{\alpha_n}\mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle\omega,y-x\rangle}\,\mathrm{d}\omega.$$

Applying now the techniques of Lemma 2.4.22 we differentiate $(\ell-1)$ times to find that the operator $A_\ell(\lambda) = X(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell)g_1$ has integral kernel

$$\begin{aligned}A_\ell(\lambda,x,y) = &\frac{(-i)^{|\alpha|}(2\pi i)\Gamma\left(\frac{n+|\alpha|}{2}\right)\lambda^{\frac{n+|\alpha|}{2}-1}}{2\Gamma\left(\frac{n}{2}+1-\ell+\frac{|\alpha|}{2}\right)(2\pi)^n}g_2(x)g_1(y)\int_{\mathbb{S}^{n-1}} \omega_1^{\alpha_1}\cdots\omega_n^{\alpha_n}\mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle\omega,y-x\rangle}\,\mathrm{d}\omega\\ &+\tilde{A}(\lambda,x,y),\end{aligned}$$

where $\tilde{A}(\lambda,\cdot,\cdot)$ has vanishing trace. Integrating over the diagonal gives that

$$\begin{aligned}&\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right)\\ &= \frac{(-i)^{|\alpha|}(2\pi i)\Gamma\left(\frac{n+|\alpha|}{2}\right)\lambda^{\frac{n+|\alpha|}{2}-\ell}}{2(\ell-1)!\Gamma\left(\frac{n}{2}+1-\ell+\frac{|\alpha|}{2}\right)(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{S}^{n-1}} \omega_1^{\alpha_1}\cdots\omega_n^{\alpha_n}\,\mathrm{d}\omega\right).\end{aligned}$$

If some α_j is odd we find $\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right) = 0$ by Lemma 2.5.20. If all α_j are even we have

$$\begin{aligned}&\operatorname{Tr}\left(X\left(R_0(\lambda+i0)^\ell - R_0(\lambda-i0)^\ell\right)g_1\right)\\&=\frac{(-i)^{|\alpha|}(2\pi i)\Gamma\left(\frac{\alpha_1+1}{2}\right)\cdots\Gamma\left(\frac{\alpha_n+1}{2}\right)\lambda^{\frac{n+|\alpha|}{2}-\ell}}{(\ell-1)!\Gamma\left(\frac{n}{2}+1-\ell+\frac{|\alpha|}{2}\right)(2\pi)^n}\left(\int_{\mathbb{R}^n} g(x)\,\mathrm{d}x\right),\end{aligned}$$

again by Lemma 2.5.20. □

For the next statement, we introduce for $m \in \mathbb{N}\cup\{0\}$ and $f \in C_c^\infty(\mathbb{R}^n)$ the notation $f^{(m)} = [H_0, [H_0, [\cdots, [H_0, f]\cdots]]]$ (where the expression has m commutators). Note that $f^{(m)}$ is a differential operator of order m.

Lemma 2.5.23. *Suppose that $q_1, q_2 \in C_c^\infty(\mathbb{R}^n)$ with $V = q_1 q_2$. Then for all $z \in \mathbb{C}\setminus\mathbb{R}$, $\ell \in \mathbb{N}$ and $K \in \mathbb{N}\cup\{0\}$ we have*

$$(q_1 R_0(z) q_2)^\ell = q_1\left(\sum_{|k|=0}^{K}(-1)^{|k|+1}C_{\ell-1}(k)V^{(k_1)}\cdots V^{(k_{\ell-1})}R_0(z)^{\ell+|k|}\right)q_2 + q_1 P_{K,\ell}(z) q_2, \tag{2.86}$$

where $P_{K,\ell}(z)$ is of order at most $-2\ell-K-1$, k is a multi-index of length $(\ell-1)$ and

$$C_\ell(k) = \frac{(|k|+\ell)!}{k_1!k_2!\cdots k_\ell!(k_1+1)(k_1+k_2+2)\cdots(|k|+\ell)}.$$

When $\ell = 1$ we have no remainder term. For all $z \in \mathbb{C}\setminus\mathbb{R}$, $M \in \mathbb{N}$ and $K \in \mathbb{N}\cup\{0\}$ we have

$$\begin{aligned}R(z)-R_0(z) = \sum_{m=1}^{M}&\left(\sum_{|k|=0}^{K}(-1)^{m+|k|}C_m(k)V^{(k_1)}\cdots V^{(k_m)}R_0(z)^{m+|k|+1} + P_{K,m}(z)\right)\\&+(-1)^{M+1}(R_0(z)V)^{M+1}R(z),\end{aligned} \tag{2.87}$$

where $P_{K,m}(z)$ has order (at most) $-2m-K-3$ and k is a multi-index of length m.

Proof. Equation (2.86) follows from the pseudodifferential calculus of [46, Lemma 6.11]. For Equation (2.87), we write

$$R(z)-R_0(z) = \sum_{m=1}^{M}(-1)^m(R_0(z)V)^m R_0(z) + (-1)^{M+1}(R_0(z)V)^{M+1}R(z).$$

Applying again [46, Lemma 6.11] we have

$$R(z) - R_0(z) = \sum_{m=1}^{M} \left(\sum_{|k|=0}^{K} (-1)^{m+|k|} C_m(k) V^{(k_1)} \cdots V^{(k_m)} R_0(z)^{m+|k|+1} + P_{K,m}(z) \right) + (-1)^{M+1} (R_0(z)V)^{M+1} R(z),$$

where $P_{K,m}(z)$ has order (at most) $-2m - K - 3$. □

Since $V \in C_c^\infty(\mathbb{R}^n)$ and for $\ell \in \mathbb{N}$ and k a multi-index of length ℓ we have $V^{(k_1)} \cdots V^{(k_\ell)}$ is a differential operator of order $|k|$ with smooth compactly supported coefficients, we can write

$$V^{(k_1)} \cdots V^{(k_\ell)} = \sum_{|r|=0}^{|k|} g_{k,r} \partial^r, \tag{2.88}$$

with r a multi-index with n components and $g_{r,k} \in C_c^\infty(\mathbb{R}^n)$. With this notation, we obtain the following heat kernel expansion due to Colin de Verdière [160] in odd dimensions (see also [56, Theorem 3.64] for a general proof and [15] for explicit computations of some coefficients). We provide a detailed proof using the pseudodifferential expansion of Lemma 2.5.23 and the trace formulae of Lemma 2.5.21. As a result we obtain an expression for the coefficients which differs from [56, Theorem 3.64] or [15], although is equivalent. This new expression is necessary for a comparison with the high-energy behaviour of the scattering operator, as we show in Theorem 2.5.29.

Proposition 2.5.24. *Suppose that $V \in C_c^\infty(\mathbb{R}^n)$. Then for any $J \in \mathbb{N}$ we have the expansion*

$$\mathrm{Tr}\left(\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0}\right) = \sum_{j=1}^{J} a_j(n,V) t^{j-\frac{n}{2}} + E_J(t),$$

where $E_J(t) = O\left(t^{J+1-\frac{n}{2}}\right)$ as $t \to 0^+$. For $j \in \mathbb{N}$ we define the set

$$Q_{M,K}(j) = \Big\{ (m,k,r) \in \{0,1,\dots,M\} \times \{0,1,\dots,K\}^m \times \{0,1,\dots,K\}^n : |r| \le |k|, \text{ all } r_j \text{ are even and } m + |k| + 1 - \frac{|r|}{2} = j \Big\}.$$

The constants $a_j(n,V)$ are given by

$$a_j(n,V) = \sum_{(m,k,r) \in Q_{M,K}(j)} \frac{(-i)^{|r|} C_m(k) (-1)^{m+|k|+1} \Gamma\left(\frac{r_1+1}{2}\right) \cdots \Gamma\left(\frac{r_n+1}{2}\right)}{(2\pi)^n (m+1)(m+|k|)!} \left(\int_{\mathbb{R}^n} V(x) g_{k,r}(x) \, \mathrm{d}x \right),$$

where we have used the notation of Equation (2.88).

Proof. Fix $t > 0$. By [56, Theorem 3.64] we have $\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0} \in \mathcal{L}^1(\mathcal{H})$. Choose $a > 0$ such that $a > |\lambda|$ for all $\lambda \in \sigma_p(H)$ and define the vertical line $\gamma_t = \{-a - \frac{1}{t} + iv : v \in \mathbb{R}\}$. We write

$$\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0} = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{-t(H_0+sV)}\,\mathrm{d}s = -t\int_0^1 V\mathrm{e}^{-t(H_0+sV)}\,\mathrm{d}s.$$

Cauchy's integral theorem tells us that for all $s \in [0,1]$ we have

$$\mathrm{e}^{-t(H_0+sV)} = \frac{1}{2\pi i}\int_{\gamma_t} \mathrm{e}^{-tz}(z - H_0 - sV)^{-1}\,\mathrm{d}z = -\frac{1}{2\pi i}\int_{\gamma_t} \mathrm{e}^{-tz}R_s(z)\,\mathrm{d}z,$$

where we have introduced the notation $R_s(z) = (H_0 + sV - z)^{-1}$. An application of Lemma 2.5.23 gives us for all $M, K \in \mathbb{N}\cup\{0\}$ the expansion

$$\begin{aligned}R_s(z) = \sum_{m=0}^{M}\left(\sum_{|k|=0}^{K}(-1)^{m+|k|}s^m C_m(k)V^{(k_1)}\cdots V^{(k_m)}R_0(z)^{m+|k|+1} + s^m P_{K,m}(z)\right)\\ + (-1)^{M+1}s^{M+1}(R_0(z)V)^{M+1}R_s(z).\end{aligned}$$

Thus we write

$$\begin{aligned}&\mathrm{Tr}\left(V\mathrm{e}^{-t(H_0+sV)}\right) = -\mathrm{Tr}\left(\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}R_s(z)\,\mathrm{d}z\right)\\ &= -\mathrm{Tr}\left(\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}\sum_{m=0}^{M}\sum_{|k|=0}^{K}(-1)^{m+|k|}s^m C_m(k)VV^{(k_1)}\cdots V^{(k_m)}R_0(z)^{m+|k|+1}\,\mathrm{d}z\right)\\ &- \mathrm{Tr}\left(\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}\sum_{m=0}^{M}s^m VP_{K,m}(z)\mathrm{d}z - \frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}(-1)^{M+1}s^{M+1}V(R_0(z)V)^{M+1}R_s(z)\mathrm{d}z\right)\\ &:= -\mathrm{Tr}\left(\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}\sum_{m=0}^{M}\sum_{|k|=0}^{K}(-1)^{m+|k|}s^m C_m(k)VV^{(k_1)}\cdots V^{(k_m)}R_0(z)^{m+|k|+1}\,\mathrm{d}z\right)\\ &\quad + e_{M,K}(t,s).\end{aligned}$$

We now apply Cauchy's integral formula again to obtain

$$\begin{aligned}\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}R_0(z)^{m+|k|+1}\,\mathrm{d}z &= (-1)^{m+|k|+1}\frac{1}{2\pi i}\int_{\gamma_t}\mathrm{e}^{-tz}(z - H_0)^{-m-|k|-1}\,\mathrm{d}z\\ &= \frac{(-1)^{m+|k|+1}}{(m+|k|)!}\frac{\mathrm{d}^{m+|k|}}{dz^{m+|k|}}\left(\mathrm{e}^{-tz}\right)|_{z=H_0} = -\frac{t^{m+|k|}}{(m+|k|)!}\mathrm{e}^{-tH_0}.\end{aligned}$$

Hence we find

$$\operatorname{Tr}\left(V\mathrm{e}^{-t(H_0+sV)}\right) = \sum_{m=0}^{M}\sum_{|k|=0}^{K}(-1)^{m+|k|}s^m\frac{C_m(k)}{(m+|k|)!}t^{m+|k|}\operatorname{Tr}\left(VV^{(k_1)}\cdots V^{(k_m)}\mathrm{e}^{-tH_0}\right) + e_{M,K}(t,s).$$

Integrating out the s variable we have

$$\begin{aligned}\operatorname{Tr}\left(\mathrm{e}^{-tH}-\mathrm{e}^{-tH_0}\right) &= -t\int_0^1 \operatorname{Tr}\left(V\mathrm{e}^{-t(H_0+sV)}\right)\mathrm{d}s\\ &= \sum_{m=0}^{M}\sum_{|k|=0}^{K}\frac{(-1)^{m+|k|+1}C_m(k)}{(m+1)(m+|k|)!}t^{m+|k|+1}\operatorname{Tr}\left(VV^{(k_1)}\cdots V^{(k_m)}\mathrm{e}^{-tH_0}\right)\\ &\quad - t\int_0^1 e_{M,K}(t,s)\,\mathrm{d}s.\end{aligned}$$

We now use Lemma 2.5.21 to write

$$\begin{aligned}&\sum_{m=0}^{M}\sum_{|k|=0}^{K}\frac{(-1)^{m+|k|+1}C_m(k)}{(m+1)(m+|k|)!}t^{m+|k|+1}\operatorname{Tr}\left(VV^{(k_1)}\cdots V^{(k_m)}\mathrm{e}^{-tH_0}\right)\\ &= \sum_{m=0}^{M}\sum_{|k|=0}^{K}\sum_{\substack{|r|=0\\ r\text{ even}}}^{|k|}\frac{(-i)^{|r|}(-1)^{\ell+m+|k|}C_m(k)\Gamma\left(\frac{r_1+1}{2}\right)\cdots\Gamma\left(\frac{r_n+1}{2}\right)t^{m+|k|+1-\frac{n+|r|}{2}}}{(m+1)(m+|k|)!(2\pi)^n}\\ &\times\left(\int_{\mathbb{R}^n}V(x)g_{k,r}(x)\,\mathrm{d}x\right),\end{aligned}$$

where the sum is over all multi-indices r of length n such that all r_j are even. We now collect together powers of t. For $j\in\mathbb{N}$ we define the set

$$\begin{aligned}Q_{M,K}(j) = \Big\{&(m,k,r)\in\{0,1,\dots,M\}\times\{0,1,\dots,K\}^m\times\{0,1,\dots,K\}^n : |r|\le|k|,\\ &\text{all } r_j \text{ are even and } m+|k|+1-\frac{|r|}{2}=j\Big\}\end{aligned}$$

and the coefficients

$$a_j(n,V) = \sum_{(m,k,r)\in Q_{M,K}(j)}\frac{(-i)^{|r|}(-1)^{m+|k|+1}C_m(k)\Gamma\left(\frac{r_1+1}{2}\right)\cdots\Gamma\left(\frac{r_n+1}{2}\right)}{(m+1)(m+|k|)!(2\pi)^n}\left(\int_{\mathbb{R}^n}V(x)g_{k,r}(x)\,\mathrm{d}x\right).$$

The $a_j(n,V)$ allow us to write

$$\sum_{m=0}^{M}\sum_{|k|=0}^{K}\frac{(-1)^{m+|k|+1}C_m(k)}{(m+1)(m+|k|)!}t^{m+|k|+1}\operatorname{Tr}\left(VV^{\{k_1\}}\cdots V^{\{k_m\}}\mathrm{e}^{-tH_0}\right) = \sum_{j=1}^{M+1}a_j(n,V)t^{-\frac{n}{2}+j}+G(t),$$

where $G(t) = O(t^{M+2-\frac{n}{2}})$ as $t \to 0^+$. Thus we have the expansion

$$\operatorname{Tr}\left(\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0}\right) = \sum_{j=1}^{M+1} a_j(n,V) t^{-\frac{n}{2}+j} + G(t) - t\int_0^1 e_{M,K}(t,s).$$

It remains to check the behaviour of the final remainder term, which consists of two types of terms. Recall that the operator $P_{K,m}(z)$ has order (at most) $-2m-K-3$. By [46, Lemma 6.12] there exists a constant C (depending on V, m and K but not z) such that

$$\left|\left|R_0(z)^{-m-\frac{K}{2}-\frac{1}{2}} q_2 P_{K,m}(z)\right|\right| \leq C.$$

Choose $K = n - m$, large enough so that $q_1 R_0(z)^{m+\frac{K}{2}+\frac{1}{2}}$ defines a trace-class operator. So we use Hölder's inequality for Schatten classes to find

$$||VP_{K,m}(z)||_1 \leq C\left|\left|q_1 R_0(z)^{m+\frac{K}{2}+\frac{1}{2}}\right|\right|_1.$$

We can now estimate the remainder term via

$$\begin{aligned}\left|\left|\int_0^1 s^m \int_{\gamma_t} \mathrm{e}^{-tz} P_{K,m}(z)\,\mathrm{d}z\,\mathrm{d}s\right|\right|_1 &\leq \frac{C}{m+1}\int_{\mathbb{R}} \mathrm{e}^{at+1}\left|\left|q_1 R_0(z)^{m+\frac{K}{2}+\frac{1}{2}}\right|\right|_1 \mathrm{d}v\\ &\leq \tilde{C}\mathrm{e}^{at+1}\int_{\mathbb{R}}\left(\left(a+\frac{1}{t}\right)^2 + v^2\right)^{-\frac{m}{2}-\frac{K}{4}-\frac{1}{4}+\frac{n}{4}} \mathrm{d}v.\end{aligned}$$

Make the substitution $v = \left(a + \frac{1}{t}\right) w$ to find

$$\begin{aligned}\left|\left|\int_0^1 s^m \int_{\gamma_t} \mathrm{e}^{-tz} P_{K,m}(z)\,\mathrm{d}z\,\mathrm{d}s\right|\right|_1 &\leq \tilde{C}\mathrm{e}^{at+1}\int_{\mathbb{R}}\left(\left(a+\frac{1}{t}\right)^2 + v^2\right)^{-\frac{m}{2}-\frac{K}{4}-\frac{1}{4}+\frac{n}{4}} \mathrm{d}v\\ &= \tilde{C}\mathrm{e}^{at}\left(a+\frac{1}{t}\right)^{-m-\frac{K}{2}-\frac{1}{2}+\frac{n}{2}}\int_{\mathbb{R}}(1+w^2)^{-\frac{m}{2}-\frac{K}{4}-\frac{1}{4}+\frac{n}{4}}\,\mathrm{d}w\\ &\leq C\mathrm{e}^{at} t^{m+\frac{K}{2}+\frac{1}{2}-\frac{n}{2}}\int_{\mathbb{R}}(1+w^2)^{-\frac{m}{2}-\frac{K}{4}-\frac{1}{4}+\frac{n}{4}}\,\mathrm{d}w\\ &= O\left(t^{m+\frac{K+1}{2}-\frac{n}{2}}\right)\end{aligned}$$

as $t \to 0+$. A similar estimate shows that

$$\left|\left|\int_0^1 s^{M+1}\int_{\gamma_t} V(R_0(z)V)^{M+1} R_s(z)\mathrm{e}^{-tz}\,\mathrm{d}z\,\mathrm{d}s\right|\right|_1 = O\left(t^{M+2-\frac{n}{2}}\right)$$

as $t \to 0^+$. Taking $J = M+1$ completes the proof. □

Remark 2.5.25. The heat kernel coefficients $a_j(n,V)$ are well-known and have been computed for small j by many authors, see for example [15] and [160] in this context. The first few are

$$a_1(n,V) = -\frac{\Gamma\left(\frac{n}{2}\right)\mathrm{Vol}(\mathbb{S}^{n-1})}{2(2\pi)^n}\int_{\mathbb{R}^n} V(x)\,\mathrm{d}x,$$
$$a_2(n,V) = \frac{\Gamma\left(\frac{n}{2}\right)\mathrm{Vol}(\mathbb{S}^{n-1})}{4(2\pi)^n}\int_{\mathbb{R}^n} V(x)^2\,\mathrm{d}x,$$
$$a_3(n,V) = -\frac{\Gamma\left(\frac{n}{2}\right)\mathrm{Vol}(\mathbb{S}^{n-1})}{6(2\pi)^n}\int_{\mathbb{R}^n} \left(V(x)^3 + \frac{1}{2}|[\nabla V](x)|^2\right)\mathrm{d}x.$$

The expression for the $a_j(n,V)$ provided by Proposition 2.5.24 provides a systematic way of computing these coefficients.

Truncating the heat kernel expansion of Proposition 2.5.24 at $J = \lfloor\frac{n}{2}\rfloor$ we can write for $t > 0$ the expression

$$\begin{aligned}\mathrm{Tr}\left(\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0}\right) &= \sum_{j=1}^{\lfloor\frac{n}{2}\rfloor} a_j(n,V)t^{j-\frac{n}{2}} + E_{\lfloor\frac{n}{2}\rfloor}(t) \qquad (2.89)\\ &= \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\frac{a_j(n,V)}{\Gamma\left(\frac{n}{2}-j\right)}\int_0^\infty \lambda^{\frac{n}{2}-j-1}\mathrm{e}^{-t\lambda}\,\mathrm{d}\lambda + \frac{(-1)^n+1}{2}a_{\lfloor\frac{n}{2}\rfloor}(n,V) + E_{\lfloor\frac{n}{2}\rfloor}(t),\end{aligned}$$

where we have separated out the constant term in even dimensions as

$$\beta_n(V) = \frac{(-1)^n+1}{2}a_{\lfloor\frac{n}{2}\rfloor}(n,V). \qquad (2.90)$$

Definition 2.5.26. We define the *high-energy polynomial for* ξ' to be $p_n : (0,\infty) \to \mathbb{C}$ given for $\lambda \in (0,\infty)$ by

$$p_n(\lambda) = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} c_j(n,V)\lambda^{\frac{n}{2}-j-1} := \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\frac{(2\pi i)a_j(n,V)}{\Gamma\left(\frac{n}{2}-j\right)}\lambda^{\frac{n}{2}-j-1}.$$

By [144, Theorem 1.2] the high-energy polynomial p_n is related to the spectral shift function by $\lim_{\lambda\to\infty}(-2\pi i\xi'(\lambda) - p_n(\lambda)) = 0$.

We can explicitly determine p_n for small n as $p_1 = p_2 = 0$,

$$p_3(\lambda) = -\frac{(2\pi i)\lambda^{-\frac{1}{2}}\mathrm{Vol}(\mathbb{S}^2)}{4(2\pi)^3}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x = \frac{(2\pi i)\lambda^{-\frac{1}{2}}a_1(3,V)}{\Gamma\left(\frac{1}{2}\right)},$$
$$p_4(\lambda) = -\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^3)}{2(2\pi)^4}\int_{\mathbb{R}^4} V(x)\,\mathrm{d}x = (2\pi i)a_1(4,V).$$

We can use Proposition 2.5.24 and the Birman-Kreĭn trace formula to analyse the integrability of the (derivative of) the spectral shift function on $\mathbb{R}^+$.

Lemma 2.5.27. *If $n = 1, 2, 3$ suppose that V satisfies Assumption 4.3.1. If $n \geq 4$ suppose that $V \in C_c^\infty(\mathbb{R}^n)$. Then the function* $\mathrm{Tr}\,(S(\cdot)^* S'(\cdot)) - p_n$ *is integrable on $\mathbb{R}^+$. In particular, if $n = 1, 2$ we have* $\mathrm{Tr}\,(S(\cdot)^* S'(\cdot)) \in L^1(\mathbb{R}^+)$.

Proof. Since $\xi|_{(0,\infty)} \in C^1((0,\infty))$ by [164, Lemma 9.1.20] it suffices to check integrability in a neighbourhood of zero and a neighbourhood of infinity. The lowest power in the high-energy polynomial p_n is $\lambda^{-\frac{1}{2}}$ and thus p_n is integrable in a neighbourhood of zero. That ξ' is integrable in a neighbourhood of zero is the statement of [90, Theorem 5.2]. This can also be proved directly by using the resolvent expansions of [88, 85, 87, 89] and Equation (2.73) to analyse the small λ behaviour of $\mathrm{Tr}\,(S(\lambda)^* S'(\lambda))$ as in [52, Lemma 5.1].

For the claim regarding the integrability in a neighbourhood of infinity, we use the high-energy asymptotics of [132, Theorem 1]. The result is that as $\lambda \to \infty$ we have the expansion

$$\mathrm{Tr}\,(S(\lambda)^* S'(\lambda)) - p_n(\lambda) \sim \sum_{j=\lfloor \frac{n}{2} \rfloor + 1}^{\infty} c_j(n, V) \lambda^{\frac{n}{2} - j - 1}. \tag{2.91}$$

We note also that there is no coefficient of λ^{-1} in even dimensions by [90, Theorem 5.3]. The expansion (2.91) implies that for sufficiently large λ we have the estimate

$$|\mathrm{Tr}\,(S(\lambda)^* S'(\lambda)) - p_n(\lambda)| \leq C \lambda^{\frac{n}{2} - \lfloor \frac{n}{2} \rfloor - 2},$$

from which the integrability of $\mathrm{Tr}\,(S(\cdot)^* S'(\cdot)) - p_n$ in a neighbourhood of infinity follows. □

We now analyse the high-energy behaviour of the (determinant of the) scattering matrix using the limiting absorption principle and the pseudodifferential expansion of Lemma 2.5.23. To do so we define the following high-energy polynomial.

Definition 2.5.28. We define the *high-energy polynomial for ξ* to be $P_n : (0, \infty) \to \mathbb{C}$ given for $\lambda \in (0, \infty)$ by

$$P_n(\lambda) = 2\pi i \beta_n(V) + \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \frac{c_j(n, V)}{\frac{n}{2} - j} \lambda^{\frac{n}{2} - j} = \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} \frac{(2\pi i) a_j(n, V)}{\Gamma\left(\frac{n}{2} - j + 1\right)} \lambda^{\frac{n}{2} - j}.$$

We note also that $P_n' = p_n$, with p_n the high-energy polynomial for ξ' of Definition 2.5.26.

We can explicitly compute the lowest order polynomials, finding $P_1 = 0$,

$$
\begin{aligned}
P_2(\lambda) &= -\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^1)}{2(2\pi)^2}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x = -\frac{2\pi i}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x = (2\pi i)\beta_2(V),\\
P_3(\lambda) &= -\frac{(2\pi i)\lambda^{\frac{1}{2}}\mathrm{Vol}(\mathbb{S}^2)}{2(2\pi)^3}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x = -\frac{(2\pi i)\lambda^{\frac{1}{2}}}{4\pi^2}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x = \frac{(2\pi i)a_1(3,V)\lambda^{\frac{1}{2}}}{\Gamma\left(\frac{3}{2}\right)},\\
P_4(\lambda) &= -\frac{(2\pi i)\lambda\mathrm{Vol}(\mathbb{S}^3)}{2(2\pi)^4}\int_{\mathbb{R}^4} V(x)\mathrm{d}x + \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^3)}{4(2\pi)^4}\int_{\mathbb{R}^4} V(x)^2\mathrm{d}x.
\end{aligned}
$$

Theorem 2.5.29. *Suppose that $q_1, q_2 \in C_c^\infty(\mathbb{R}^n)$ with $V = q_1 q_2$. Then for all $\lambda > 0$ and $J \in \mathbb{N}$ we have*

$$
\sum_{\ell=1}^{J}\left(\frac{(-1)^\ell}{\ell}\mathrm{Tr}\left((q_1 R_0(\lambda+i0)q_2)^\ell - (q_1 R_0(\lambda-i0))^\ell q_2\right)\right) = -\sum_{j=1}^{J} C_j(n,V)\lambda^{\frac{n}{2}-j} + E_J(\lambda), \tag{2.92}
$$

where $E_J(\lambda) = O\left(\lambda^{\frac{n}{2}-J-3}\right)$ as $\lambda \to \infty$ and E_J is differentiable. If n is even we have $C_j(n,V) = 0$ for all $j > \frac{n}{2}$. If n is even and $j \le \frac{n}{2}$ or n is odd the coefficients $C_j(n,V)$ are given by

$$
C_j(n,V) = \frac{(2\pi i)a_j(n,V)}{\Gamma\left(\frac{n}{2}-j+1\right)}, \tag{2.93}
$$

with the $a_j(n,V)$ the heat kernel coefficients of Proposition 2.5.24. Note also that for n even we have $C_{\frac{n}{2}}(n,V) = 2\pi i\beta_n(V)$.

Proof. For $\lambda > 0$, we have

$$
\begin{aligned}
\mathrm{Tr}\left(q_1\left(R_0(\lambda+i0) - R_0(\lambda-i0)\right)q_2\right) &= \frac{(2\pi i)\lambda^{\frac{n-2}{2}}\mathrm{Vol}(\mathbb{S}^{n-1})}{2(2\pi)^n}\int_{\mathbb{R}^n} V(x)\,\mathrm{d}x\\
&= -\frac{(2\pi i)a_1(n,V)\lambda^{\frac{n}{2}-1}}{\Gamma\left(\frac{n}{2}\right)}.
\end{aligned}
$$

by Lemma 2.4.20, with no need for any kind of expansion. We now consider the $\ell \geq 2$ terms in the sum. For $z \in \mathbb{C}\setminus\mathbb{R}$ we use Lemma 2.5.23 to obtain the expansion

$$
\begin{aligned}
&\frac{(-1)^\ell}{\ell}(q_1 R_0(z) q_2)^\ell\\
&= \left(\frac{(-1)^\ell}{\ell}q_1\left(\sum_{|k|=0}^{K}(-1)^{|k|+1}C_{\ell-1}(k)V^{(k_1)}\cdots V^{(k_{\ell-1})}R_0(z)^{\ell+|k|}\right)q_2 + \frac{(-1)^\ell}{\ell}q_1 P_{K,\ell}(z)q_2\right),
\end{aligned}
$$

where $P_{K,\ell}(z)$ is of order (at most) $-2\ell - K - 1$. By the limiting absorption principle, this equality extends to $z = \lambda \pm i0$ for $\lambda \in (0, \infty)$ and thus we find

$$\begin{aligned}
&\frac{(-1)^\ell}{\ell}\mathrm{Tr}\left((q_1(R_0(\lambda+i0)q_2)^\ell - (q_1R_0(\lambda-i0))q_2)^\ell\right)\\
&= \mathrm{Tr}\left(q_1\left(\sum_{|k|=0}^{K}\frac{(-1)^{\ell+|k|+1}}{\ell}C_{\ell-1}(k)V^{(k_1)}\cdots V^{(k_{\ell-1})}\left(R_0(\lambda+i0)^{\ell+|k|} - R_0(\lambda-i0)^{\ell+|k|}\right)\right)q_2\right.\\
&\quad\left. + \frac{(-1)^\ell}{\ell}q_1\left(P_{K,\ell}(\lambda+i0) - P_{L,\ell}(\lambda-i0)\right)q_2\right).
\end{aligned}$$

We now use the expansion of Equation (2.88) to write

$$\begin{aligned}
&\frac{(-1)^\ell}{\ell}\mathrm{Tr}\left(q_1(R_0(\lambda+i0)q_2)^\ell - (q_1R_0(\lambda-i0)q_2)^\ell\right)\\
&= \mathrm{Tr}\left(q_1\left(\sum_{|k|=0}^{K}\sum_{|r|=0}^{|k|}\frac{(-1)^{\ell+|k|+1}}{\ell}C_{\ell-1}(k)q_1g_{k,r}\partial^r\left(R_0(\lambda+i0)^{\ell+|k|} - R_0(\lambda-i0)^{\ell+|k|}\right)\right)q_2\right.\\
&\quad\left. + \frac{(-1)^\ell}{\ell}q_1\left(P_{L,\ell}(\lambda+i0) - P_{L,\ell}(\lambda-i0)\right)q_2\right).
\end{aligned}$$

Ignoring for a moment the remainder term we find using Lemma 2.4.22 that

$$\begin{aligned}
&\mathrm{Tr}\left(\frac{(-1)^\ell}{\ell}q_1\left(\sum_{|k|=0}^{K}\sum_{|r|=0}^{|k|}(-1)^{|k|+1}C_{\ell-1}(k)g_{k,r}\partial^r\left(R_0(\lambda+i0)^{\ell+|k|} - R_0(\lambda-i0)^{\ell+|k|}\right)\right)q_2\right)\\
&= \sum_{|k|=0}^{K}\sum_{|r|=0}^{|k|}\frac{(-1)^{\ell+|k|}(2\pi i)C_{\ell-1}(k)(-i)^{|r|}\Gamma\left(\frac{r_1+1}{2}\right)\cdots\Gamma\left(\frac{r_n+1}{2}\right)\lambda^{\frac{n+|r|}{2}-\ell-|k|}}{\ell(\ell+|k|-1)!\Gamma\left(\frac{n}{2}+1-\ell-|k|+\frac{|r|}{2}\right)(2\pi)^n}\int_{\mathbb{R}^n}V(x)g_{k,r}(x)\,\mathrm{d}x.
\end{aligned}$$

Lemma 2.4.22 also gives that for n even all terms with $\ell + |k| - \frac{|r|}{2} > \frac{n}{2}$ vanish. We now collect together the powers of λ. For $j \in \mathbb{N}$ we define the set

$$\begin{aligned}
Q_{L,K}(j) = \Big\{&(\ell, k, r) \in \{1, \dots, L\} \times \{0, \dots, K\}^\ell \times \{0, \dots, K\}^n : |r| \le |k| \le K,\\
&\text{all } r_j \text{ are even, and } \ell + |k| - \frac{|r|}{2} = j\Big\}
\end{aligned}$$

So we write

$$\begin{aligned}
&\sum_{\ell=2}^{L}\mathrm{Tr}\left(\frac{(-1)^\ell}{\ell}q_1\left(\sum_{|k|=0}^{K}\sum_{|r|=0}^{|k|}(-1)^{|k|+1}C_{\ell-1}(k)q_1g_{r,k}\partial^r\left(R_0(\lambda+i0)^{\ell+|k|} - R_0(\lambda-i0)^{\ell+|k|}\right)\right)q_2\right)\\
&= -\sum_{j=2}^{J}C_j(n,V)\lambda^{\frac{n}{2}-j},
\end{aligned}$$

where the coefficients $C_j(n,V)$ are given by

$$C_j(n,V) = \sum_{(\ell,k,r)\in Q_{L,K}(j)} \frac{(-1)^{\ell+|k|}(2\pi i)C_{\ell-1}(k)(-i)^{|r|}\Gamma\left(\frac{r_1+1}{2}\right)\cdots\Gamma\left(\frac{r_n+1}{2}\right)}{\ell(\ell+|k|-1)!\Gamma\left(\frac{n}{2}+1-\ell-|k|+\frac{|r|}{2}\right)(2\pi)^n}\int_{\mathbb{R}^n} V(x)g_{r,k}(x)\,\mathrm{d}x.$$

Direct comparison with Proposition 2.5.24 shows that we have the relation

$$C_j(n,V) = \frac{(2\pi i)a_j(n,V)}{\Gamma\left(\frac{n}{2}+1-j\right)}.$$

We now return to the remainder term. Due to the form of the remainder terms $P_{K,\ell}(\lambda \pm i0)$ the difference $q_1\left(P_{K,\ell}(\lambda+i0) - P_{K,\ell}(\lambda-i0)\right)q_2$ is always trace-class, as we now show. The proof of [46, Lemma 6.12] shows that $P_{K,\ell}(\lambda \pm i0)$ is a linear combination of terms of the form

$$\prod_{m=1}^{M} A_m R_0(\lambda \pm i0)^{\alpha_m},$$

for some $M, \alpha_m \in \mathbb{N}$ and differential operators A_m of order $a_m < 2\alpha_m$ with smooth compactly supported coefficients and

$$\sum_{m=1}^{M}\left(\alpha_m - \frac{a_m}{2}\right) \geq -2\ell - L - 1.$$

Each A_m can be factored as $f_m\tilde{A}_m g_m$ for $f_m, g_m \in C_c^\infty(\mathbb{R}^n)$ and $\tilde{A}_m$ also of order a_m. Taking the difference and factorising we find

$$\begin{aligned}
&\left(\prod_{m=1}^{M} A_m R_0(\lambda+i0)^{\alpha_m} - \prod_{m=1}^{M} A_m R_0(\lambda-i0)^{\alpha_m}\right)\\
=&\sum_{p=1}^{M}\left(\prod_{m<p} A_m R_0(\lambda-i0)^{\alpha_m}\right)\left(A_p(R_0(\lambda+i0)^{\alpha_p} - R_0(\lambda-i0)^{\alpha_p})\right)\left(\prod_{m>p} A_m R_0(\lambda+i0)^{\alpha_m}\right),
\end{aligned}$$

each term of which is trace-class by Lemma 2.4.22. Hölder's inequality for the trace norm then shows that

$$\begin{aligned}
&\left\|q_1\left(\prod_{m=1}^{M} A_m R_0(\lambda+i0)^{\alpha_m} - \prod_{m=1}^{M} A_m R_0(\lambda-i0)^{\alpha_m}\right)q_2\right\|_1\\
\leq &\sum_{p=1}^{M}\left\|q_1 f_1\left(\prod_{m<p}\tilde{A}_m g_m R_0(\lambda-i0)^{\alpha_m} f_{m+1}\right)\right\|\left\|\tilde{A}_p g_p\left(R_0(\lambda+i0)^{\alpha_p} - R_0(\lambda-i0)^{\alpha_p}\right)f_{p+1}\right\|_1\\
&\times\left\|\tilde{A}_{p+1}g_{p+1}\left(\prod_{p<m\leq M} R_0(\lambda+i0)^{\alpha_m} f_{m+1}\right)q_2\right\|,
\end{aligned}$$

where we use the convention $f_{M+1} = 1$. By [3, Theorem A.1] (see also [120, Theorem 1]) we have for any $\alpha > 0$ and differential operator A of order $a < 2\alpha$ the estimate

$$||q_1 A R_0(\lambda \pm i0)^\alpha q_2|| = O\left(\lambda^{-\frac{1}{2}\alpha + \frac{a}{4}}\right)$$

as $\lambda \to \infty$. By Lemma 2.5.22 we have the estimate

$$||q_1 A \left(R_0(\lambda + i0)^\alpha - R_0(\lambda - i0)^\alpha\right) q_2||_1 \leq C\lambda^{\frac{n}{2} - \alpha + \frac{a}{2}}.$$

Combining these we obtain

$$\begin{aligned}
&\left|\left| q_1 \left(\prod_{m=1}^{M} q_1 A_m q_2 R_0(\lambda + i0)^{\alpha_m} - \prod_{m=1}^{M} q_1 A_m q_2 R_0(\lambda - i0)^{\alpha_m} \right) q_2 \right|\right|_1 \\
&= C \sum_{p=1}^{M} \lambda^{\frac{n}{2} - \alpha_p + \frac{a_p}{2}} \left(\prod_{m \neq p} O\left(\lambda^{-\frac{1}{2}\alpha_m + \frac{a_m}{4}}\right) \right) \leq O\left(\lambda^{\frac{n}{2} - \ell - \frac{L+1}{2}}\right)
\end{aligned}$$

as $\lambda \to \infty$. By varying K we obtain Equation (2.92). That E_L is differentiable follows from the observation that the left-hand side of Equation (2.92) is differentiable, as is each power of λ on the right-hand side. □

Remark 2.5.30. Choosing $J \geq \lfloor \frac{n}{2} \rfloor$ in Theorem 2.5.29 gives

$$\sum_{\ell=1}^{J} \left(\frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0) q_2)^\ell - (q_1 R_0(\lambda - i0) q_2)^\ell \right) \right) = -P_n(\lambda) - E(\lambda),$$

with $E(\lambda) = O(\lambda^{-\frac{1}{2}})$ as $\lambda \to \infty$ with E differentiable. A comparison with Lemma 2.5.17 and using the convention of Remark 2.5.18 gives the relation

$$\lim_{\lambda \to \infty} \left(-2\pi i \xi(\lambda) - P_n(\lambda)\right) = 0,$$

justifying the terminology of P_n being the high-energy polynomial for ξ.

2.5.4 Levinson's theorem

Levinson's original theorem [108] gives, in one dimension, a relation between the number of bound states of a system and a quantity related to the scattering data of the system. The original proof makes use of the Jost functions [91] and relies heavily on complex analysis. Such techniques are specific to one dimension and not easily generalisable to higher dimensions, except in the case of spherically symmetric potentials which can essentially be reduced to a one dimensional problem, see [123, Section 5] and [137, Theorem XI.59]. We will present in Chapter 5 a proof based based on the index of the wave operator, which will allow us to obtain analogous statements in higher dimensions. Statements of Levinson's theorem require slight modification when certain obstructions, called resonances, exist at zero energy. The nature of these obstructions depends on the parity of the dimension, and they cannot occur for dimension $n \geq 5$. We will develop the required machinery to motivate definitions of resonances in Chapter 3, however for now we make reference to them without providing a precise definition.

Theorem 2.5.31 (Levinson's theorem in one dimension)**.** *Let $n = 1$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > 2$. Then the number of bound states (eigenvalues counted with multiplicity) N of the operator $H = H_0 + V$ is given by*

$$-N = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2}\left(M_R(0) - 1\right), \tag{2.94}$$

where $M_R(0) = 1$ if there exists a resonance or $H = H_0$, and $M_R(0) = 0$ otherwise.

Levinson's theorem is more complicated in even dimensions due to the nature of the logarithmic singularity of the perturbed resolvent $R(z) = (H - z)^{-1}$ near $z = 0$.

Theorem 2.5.32 (Levinson's theorem in two dimensions)**.** *Let $n = 2$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > 11$. Then the number of bound states (eigenvalues counted with multiplicity) of $H = H_0 + V$ is given by*

$$-N = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + M_p(0) + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x, \tag{2.95}$$

where $M_p(0) \in \{0, 1, 2\}$ is the number of p-resonances.

Theorem 2.5.32 was originally proved in [26, Theorem 6.3], although the proof is rather complicated and requires a good deal of supplementary arguments from the reader. In Chapter 5 we provide a new proof based on the index of the wave operator in the case of no p-resonances. The extra term involving the integral of the potential in Equation (2.95) is related to the high energy behaviour of the scattering matrix via

$$\frac{1}{2\pi i}\mathrm{Log}(\mathrm{Det}(S(\infty))) = \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x. \tag{2.96}$$

The intricate behaviour of the scattering matrix at infinity plays a role in Levinson's theorem in all dimensions and is rather subtle. The fact that the term on the right hand side of Equation (2.96) does not appear under the λ integral with $\mathrm{Tr}(S(\lambda)^* S'(\lambda))$ is peculiar to even dimensions.

In three dimensions (and all higher dimensions), the large λ behaviour of the scattering matrix means that the function $\mathrm{Tr}(S(\cdot)^* S'(\cdot))$ is no longer integrable (see Theorem 2.5.34) and thus we require additional correction terms to Levinson's theorem. Such correction terms are a feature for all $n \geq 3$, however quickly become very difficult to compute (see for example [73, Section V], [143, Theorem 1.2] and [56, Section 3.11]). The following statement is due to [31] and can be deduced also from [124] under the assumption that the spectral shift function belongs to $C^1(\mathbb{R}^+)$, although as in the dimension $n = 2$ case a good deal of additional argument from the reader is required to make the proofs work.

Theorem 2.5.33 (Levinson's theorem in three dimensions)**.** *Let $n = 3$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > 5$. Then the number of bound states (eigenvalues counted with multiplicity) of $H = H_0 + V$ is given by*

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda))) - c_1(3,V)\lambda^{-\frac{1}{2}}\right) \mathrm{d}\lambda + \frac{1}{2}M_R(0),$$

where $M_R(0) = 1$ if there is a zero-energy resonance and $M_R(0) = 0$ otherwise. The constant c_1 is given by

$$c_1(3,V) = -\frac{i}{4\pi}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x.$$

A higher dimensional version of Levinson's theorem can be obtained from the Birman-Kreĭn trace formula with knowledge of heat asymptotics, although as in lower dimensions requires knowledge of the spectral shift function at zero. We have the following, due in odd dimensions to Guillopé [73, Theorem IV.5] (see also [56, Theorem 3.66]). We provide only a sketch of the proof as there are many subleties.

Theorem 2.5.34. *[Levinson's theorem in higher dimensions] Suppose that $V \in C_c^\infty(\mathbb{R}^n)$. Then the number of bound states of $H = H_0 + V$ is given by*

$$\begin{aligned} -N = \frac{1}{2\pi i}\int_0^\infty &\left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2}\rfloor} c_j(n,V)\lambda^{\frac{n-2}{2}-j}\right) \mathrm{d}\lambda - N_0 \\ &- (\xi(0+) - \xi(0-)) - \beta_n(V), \end{aligned}$$

where the $c_j(n,V)$ and $\beta_n(V)$ are constants depending on V and its derivatives with $b_n = 0$ for n odd.

Proof sketch. From Proposition 2.5.24 we have the limit

$$0 = \lim_{t\to 0^+}\left(\mathrm{Tr}\left(\mathrm{e}^{-tH} - \mathrm{e}^{-tH_0}\right) - \sum_{j=1}^{\lfloor \frac{n}{2}\rfloor} a_j(n,V)t^{k-\frac{n}{2}}\right).$$

Using Equation (2.89) and the Birman-Kreĭn trace formula in the form of Theorem 2.5.19

we obtain

$$\begin{aligned} 0 &= \lim_{t\to 0^+}\left(\frac{1}{2\pi i}\int_0^\infty \mathrm{e}^{-t\lambda}\mathrm{Tr}\left(S(\lambda)^*S'(\lambda)\right)\,\mathrm{d}\lambda + \sum_{k=1}^{K}\mathrm{e}^{-t\lambda_k}M(\lambda_k)\right.\\ &\quad\left. - N - \xi(0+) - \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\frac{a_j(n,V)}{\Gamma\left(\frac{n}{2}-k\right)}\int_0^\infty \lambda^{\frac{n}{2}-k-1}\mathrm{e}^{-t\lambda}\,\mathrm{d}\lambda - \beta_n(V)\right)\\ &= \lim_{t\to 0^+}\left(\frac{1}{2\pi i}\int_0^\infty \mathrm{e}^{-t\lambda}\left(\mathrm{Tr}\left(S(\lambda)^*S'(\lambda)\right) - \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\frac{(2\pi i)a_j(n,V)\lambda^{\frac{n}{2}-k-1}}{\Gamma\left(\frac{n}{2}-k\right)}\right)\mathrm{d}\lambda\right.\\ &\quad\left. + \sum_{k=1}^{K}\mathrm{e}^{-t\lambda_k}M(\lambda_k) - N - \xi(0+) - \beta_n(V)\right)\\ &= \lim_{t\to 0^+}\frac{1}{2\pi i}\int_0^\infty \mathrm{e}^{-t\lambda}\left(\mathrm{Tr}\left(S(\lambda)^*S'(\lambda)\right) - p_n(\lambda)\right)\mathrm{d}\lambda - \xi(0+) - \beta_n(V). \end{aligned}$$

Here the constant $\beta_n(V)$ is as in Equation (2.90). An application of Lemma 2.5.27 and the dominated convergence theorem then allows us to bring the limit as $t\to 0^+$ inside the integral to obtain

$$\xi(0+) = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}\left(S(\lambda)^*S'(\lambda)\right) - p_n(\lambda)\right)\mathrm{d}\lambda - \beta_n(V).$$

□

The key element missing in Theorem 2.5.34 is the difference $\xi(0+)-\xi(0-)$ of the spectral shift function from the left and right at zero. The value $\xi(0-) = -N + N_0$ is determined by Theorem 2.5.13 and thus the only unknown element in statements of Levinson's theorem is the value $\xi(0+)$, which we determine in Chapter 5 to be dependent on the existence of resonances. In fact we can rewrite Levinson's theorem as

$$\xi(0+) = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} c_j(n,V)\lambda^{\frac{n}{2}-j-1}\right)\mathrm{d}\lambda - \beta_n(V). \tag{2.97}$$

We shall not have occasion to use any higher order terms, although they can be computed if necessary (see [56, Theorem 3.64] for more details). These coefficients will return in Chapter 5 when we study high energy corrections to the scattering operator and in Chapter 6 when we study spectral flow.

An interesting point to note is that in all even dimensions, Levinson's theorem has an additional term outside of the integral expression. This additional term is given in low dimensions by

$$\begin{aligned}\beta_2(V) &= -\frac{\mathrm{Vol}(\mathbb{S}^1)}{2(2\pi)^2}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x,\\ \beta_4(V) &= \frac{\mathrm{Vol}(\mathbb{S}^3)}{4(2\pi)^4}\int_{\mathbb{R}^4} V(x)^2\,\mathrm{d}x,\\ \beta_6(V) &= -\frac{\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\int_{\mathbb{R}^6}\left(V(x)^3+\frac{1}{2}|[\nabla V](x)|^2\right)\mathrm{d}x.\end{aligned}$$

Here we have used the coefficients $c_j(n, V)$ to determine the $\beta_n(V)$.

2.5.5 Examples

In this section we demonstrate some explicit low dimensional examples, explicitly computing the scattering operator and describing the bound states and any anomalous behaviour.

In dimension $n = 1$, we see that for fixed energy $\lambda \in \mathbb{R}^+$ we have the unitary scattering matrix $S(\lambda) \in \mathcal{B}(L^2(\mathbb{S}^0)) = M_2(\mathbb{C})$. In our definition of $\mathcal{U}$ we have made a choice of basis of $\mathbb{C}^2$. Some authors use a different convention which leads to different forms of the scattering matrix. Recall that $\mathcal{U} : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+, \mathbb{C}^2)$ is unitary and defined by

$$[\mathcal{U}f](r) = 2^{-\frac{1}{2}}\lambda^{-\frac{1}{2}}\begin{pmatrix} f(\lambda^{\frac{1}{2}}) \\ f(-\lambda^{\frac{1}{2}})\end{pmatrix}.$$

Some authors prefer to use the map $\mathcal{V} : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+, \mathbb{C}^2)$ defined by

$$[\mathcal{V}f](r) = 2^{-\frac{1}{2}}\lambda^{-\frac{1}{2}}\begin{pmatrix} \frac{f(\lambda^{\frac{1}{2}})+f(-\lambda^{\frac{1}{2}})}{2} \\ \frac{f(\lambda^{\frac{1}{2}})-f(-\lambda^{\frac{1}{2}})}{2}\end{pmatrix}.$$

The operator $\mathcal{V}$ is unitary and related to $\mathcal{U}$ by the change of basis,

$$B = 2^{-\frac{1}{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}.$$

which satisfies $B^{-1}\mathcal{U}(\lambda, \cdot)B = \mathcal{V}(\lambda, \cdot)$.

The first example we consider is the finite square well in dimension $n = 1$.

Example 2.5.35. We fix $E_0, L > 0$ and define the function $V : \mathbb{R} \to \mathbb{R}$ by

$$V(x) = \begin{cases} 0, & \text{if } |x| > L, \\ -E_0, & \text{if } |x| \le L.\end{cases}$$

The potential V is a step function which is only non-zero inside the region $[-L, L]$ with depth $-E_0$. We note that V satisfies Assumption 2.2.14 for any $\rho > 1$ and thus all of our results apply. In particular, the operator $H = H_0 + V$ has finitely many non-positive eigenvalues.

Recall the change of basis matrix $B = 2^{-\frac{1}{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ from the standard polar decomposition of $L^2(\mathbb{R}^+, \mathbb{C}^2)$ into the basis provided by the operator $\mathcal{V}$. The scattering matrix is given explicitly by

$$B^{-1}S(\lambda)B = -\mathrm{e}^{-2i\lambda^{\frac{1}{2}}L} \begin{pmatrix} \frac{\left(\frac{\lambda+E_0}{\lambda}\right)^{\frac{1}{2}} \tan\left((\lambda+E_0)^{\frac{1}{2}}L\right)-i}{\left(\frac{\lambda+E_0}{\lambda}\right)^{\frac{1}{2}} \tan\left((\lambda+E_0)^{\frac{1}{2}}L\right)+i} & 0 \\ 0 & \frac{-\left(\frac{\lambda}{\lambda+E_0}\right)^{\frac{1}{2}} \tan\left((\lambda+E_0)^{\frac{1}{2}}L\right)+i}{\left(\frac{\lambda}{\lambda+E_0}\right)^{\frac{1}{2}} \tan\left((\lambda+E_0)^{\frac{1}{2}}L\right)+i} \end{pmatrix}.$$

Due to the symmetry of the potential V, the expression for S is much nicer when decomposed according to $\mathcal{V}$ rather than $\mathcal{U}$. An interesting point to note is that the poles of $S(\cdot)$ lie on the imaginary axis and correspond precisely to the bound states of H, see [19] for a numerical discussion of the behaviour of such poles.

We note that if $E_0^{\frac{1}{2}}L \neq m\pi$ for any $m \in \mathbb{Z}$ and $E_0^{\frac{1}{2}}L \neq (m + \frac{1}{2})\pi$ for any $m \in \mathbb{Z}$ then we find $\mathrm{Det}(S(0)) = -1$ and we call this the generic case, which corresponds to the non-existence of resonances. See Theorem 4.1.3 for more details.

If there exists $m \in \mathbb{Z}$ such that $E_0^{\frac{1}{2}}L = m\pi$ or $E_0^{\frac{1}{2}}L = (m + \frac{1}{2})\pi$ then $\mathrm{Det}(S(0)) = 1$, which is atypical and corresponds to the existence of resonances. △

Remark 2.5.36. Example 2.5.35 can be extended to higher dimensions in a straightforward manner, decomposing the scattering matrix into spherical harmonics. The explicit terms are however rather difficult to describe, involving ratios of Bessel functions.

We next consider another one dimensional example in which scattering quantities can be computed explicitly, known as the Pöschl-Teller potential.

Example 2.5.37 (Pöschl-Teller potential). For fixed $\alpha \in \mathbb{R}$ and $\beta > 0$ we define the potential

$$V(x) = -\frac{\alpha^2\beta(\beta-1)}{\cosh^2(\alpha x)}.$$

For $k \geq 0$ solutions to the equation $(H_0 + V)\psi = -k^2\psi$ can be determined explicitly in terms of hypergeometric functions (see [49, Equation 9]). Note that if $\beta = 0, 1$ then we have $V = 0$. For $\beta \neq 0, 1$ the scattering matrix can be determined explicitly (see [49, Equations (14) and (15)]) as

$$B^{-1}S(k^2)B = \begin{pmatrix} -\frac{\Gamma(1+ik)\Gamma(\beta-ik)\Gamma(1-\beta-ik)}{\Gamma(1-ik)\Gamma(\beta)\Gamma(1-\beta)} & \frac{\Gamma(\beta-ik)\Gamma(1-\beta-ik)}{\Gamma(1-ik)\Gamma(-ik)} \\ \frac{\Gamma(1+ik)\Gamma(ik)}{\Gamma(1+ik-\beta)\Gamma(ik+\beta)} - \frac{\Gamma(1+ik)\Gamma(ik)\Gamma(\beta-ik)\Gamma(1-\beta-ik)}{\Gamma(\beta)^2\Gamma(1-\beta)^2} & \frac{\Gamma(ik)\Gamma(\beta-ik)\Gamma(1-\beta-ik)}{\Gamma(-ik)\Gamma(1-\beta)\Gamma(\beta)} \end{pmatrix}.$$

One can compute directly that

$$B^{-1}S(0)B = \begin{pmatrix} -1 & 0 \\ 0 & 1, \end{pmatrix}$$

provided that $\beta \notin \mathbb{Z}$. △

The above examples demonstrate that even simple potentials V can result in extremely complicated scattering behaviour and bound state solutions. In fact for most potentials the Schrödinger equation cannot be solved analytically, the list of exactly solveable potentials is short (see [4] and [35] for some limited examples).

Example 2.5.38. Suppose that $\varphi \in C^\infty(\mathbb{R})$ is such that $\varphi(\pm\infty) = c_\pm$ for some $c_\pm \in \mathbb{R}\setminus\{0\}$ with $c_+^2 + c_-^2 = 1$ and $\varphi(x) \neq 0$ for all $x \in \mathbb{R}$. Then we define $V = \frac{\varphi''}{\varphi}$ and compute that

$$(H_0 + V)\varphi = 0,$$

whilst $\varphi \notin L^2(\mathbb{R})$. Such a function will be called a zero energy resonance in Chapter 3. In this case one can show directly (see [56, Remark on p. 46]) that

$$S(0) = \begin{pmatrix} 2c_+c_- & c_+^2 - c_-^2 \\ c_-^2 - c_+^2 & 2c_1c_2 \end{pmatrix}.$$

Direct computation shows that $\mathrm{Det}(S(0)) = 1$. △

Chapter 3

Resolvent expansions and resonances

In this chapter we develop low energy expansions of operators related to the resolvents $R_0(z)$ and $R(z)$. The expansions we consider here follow the technique of Jensen and Nenciu [89] and can be found throughout the literature. In particular, there are no new results in this chapter. In dimension $n \leq 4$, such expansions are complicated by analytic obstructions to invertibility at zero, which give rise to definitions of zero-energy resonances. These resolvent expansions can be used to analyse the behaviour of the scattering matrix at zero-energy and the form of the wave operator in 4.0.1, which allows us to proveide new proofs of Levinson's theorem.

We decompose the potential V into $V = vUv$ where $v(x) = |V(x)|^{\frac{1}{2}}$ and $U(x) = \operatorname{sign}(V)$. Such a factorisation is well-known and was first used in the work of Birman [24] and Schwinger [148]. For $z \in \mathbb{C} \setminus \mathbb{R}$ with $\operatorname{Im}(z^{\frac{1}{2}}) > 0$, we let $k = -iz^{\frac{1}{2}}$. We have the symmetrised resolvent identity

$$\begin{aligned} R(-k^2) - R_0(-k^2) &= -R_0(-k^2)v(U + vR_0(-k^2)v)^{-1}vR_0(-k^2) \\ &=: -R_0(-k^2)vM(k)^{-1}vR_0(-k^2). \end{aligned} \tag{3.1}$$

Thus we see to obtain expansions of the resolvent $R(-k^2)$ it suffices to consider the known expansions of the operators $R_0(-k^2)$ and (the inverse of)

$$M(k) := U + vR_0(-k^2)v. \tag{3.2}$$

The analysis of the inverse of $M(k)$ as $k \to 0$ is sensitive to the fine structure of the spectrum of H near zero. In particular the presence of zero energy resonances will force multiple uses of the Feshbach inversion method of Lemma 3.1.1. We shall find that such obstructions cannot occur for $n \geq 5$. Also the inversion of $M(k)$ is sensitive to the parity of the dimension, due to the fact that the integral kernel of the free resolvent has a logarithmic singularity near $k = 0$ in even dimensions. As such, our analysis is split into six different cases. We begin with the easiest cases of $n \geq 5$ odd to demonstrate the use of Lemma 3.1.1 and end with the most involved cases of dimension $n = 2$ and $n = 1$.

Throughout this chapter we will have to strengthen the decay assumptions on the potential to guarantee that the operators we consider are bounded. The most general assumption we shall need is the following.

Assumption 3.0.1. We suppose that the potential satisfies Assumption 2.2.14 for

1. $\rho > \frac{n+1}{2}$ if $n \geq 11$;
2. $\rho > 7$ if $n = 7, 8, 9, 10$;
3. $\rho > 7$ if $n = 5, 6$;
4. $\rho > 12$ if $n = 4$;
5. $\rho > 5$ if $n = 3$;
6. $\rho > 11$ if $n = 2$; and
7. $\rho > 7$ if $n = 1$.

We do not claim that Assumption 3.0.1 gives the optimal decay required for the existence of the expansions in each case. For ease of exposition, we prefer to give in each dimension only a sufficient value of ρ required for all expansions to exist. More optimal results can be found in the cited references in each section.

The expansions we obtain for the operator $M(k)$ are summarised in the following result.

Theorem 3.0.2. *Suppose that V satisfies Assumption 3.0.1. Then for sufficiently small k and with $\eta = \frac{1}{\ln(k)}$ we have the expansion*

$$M(k)^{-1} = -k^{-2}A + k^{-2}g(k)A_n + k^{-1}h(k)B_n + \tilde{R}(k),$$

where $A_n, B_n = 0$ for $n \geq 5$, $A_n = 0$ for $n = 1, 3$, $g(k), h(k) = O(\eta^{-1})$, A, A_n, B_n are bounded operators and $\tilde{R}(k)$ is uniformly bounded in k.

For ease of exposition, we have used the phrase 'for sufficiently small $k \ldots$' as shorthand for the statement 'there exists $k_0 > 0$ such that for all $0 < |k| < k_0 \ldots$'. The coefficient operators A_n and B_n are related to the presence of analytic obstructions to invertibility, called resonances. Their behaviour is dimension dependent, with a single type of resonance occurring in dimensions $n = 1, 3, 4$ and two distinct types occurring in dimension $n = 2$. Despite the fact that there is only one type, resonances occurring in dimension $n = 4$ behave more similarly to those in dimension $n = 2$ due to the nature of the obstruction and the logarithmic singularity of the free resolvent.

3.1 Algebraic and analytic preliminaries

The starting point for our analysis is the following inversion formulae for particular operator-valued matrices (see [89, Section 2]).

Lemma 3.1.1. *Let A be a closed operator on $\mathcal{H}$, Q a projection and suppose $A+Q$ has a bounded inverse. Then A has a bounded inverse if and only if*

$$B = Q - Q(A+Q)^{-1}Q$$

has a bounded inverse in $Q\mathcal{H}$. In this case A^{-1} is given by

$$C = (A+Q)^{-1} + (A+Q)^{-1}QB^{-1}Q(A+Q)^{-1}. \tag{3.3}$$

Proof. Suppose that B has a bounded inverse and let C be as in Equation (3.3). Then we can check the relations

$$\begin{aligned} AC &= (A+Q-Q)C \\ &= \mathrm{Id} + QB^{-1}Q(A+Q)^{-1} - Q\left((A+Q)^{-1} + (A+Q)^{-1}QB^{-1}Q(A+Q)^{-1}\right) \\ &= \mathrm{Id} + \left(Q - B - Q(A+Q)^{-1}Q\right)B^{-1}Q(A+Q)^{-1} \\ &= \mathrm{Id}. \end{aligned}$$

A similar calculation shows that $CA = \mathrm{Id}$ so that A has a bounded inverse given by $A^{-1} = C$. Next suppose that A has a bounded inverse. Then the operator

$$D = (A+Q)A^{-1}(A+Q) - (A+Q) = Q(\mathrm{Id} + A^{-1})Q$$

defines a bounded operator on $Q\mathcal{H}$. We then compute that

$$\begin{aligned} BD &= \left(Q - Q(A+Q)^{-1}Q\right)Q(\mathrm{Id} + A^{-1})Q \\ &= Q\left(\mathrm{Id} - (A+Q)^{-1} + A^{-1} - (A+Q)^{-1}QA^{-1}\right)Q \\ &= Q\left(\mathrm{Id} - (A+Q)^{-1} + A^{-1} - A^{-1} + (A+Q)^{-1}\right)Q \\ &= Q, \end{aligned}$$

the identity on $Q\mathcal{H}$. A similar calculation shows that $DB = Q$ and thus the operator B has a bounded inverse on $Q\mathcal{H}$ given by $B^{-1} = D$. □

Corollary 3.1.2. *Let $F \subset \mathbb{C}$ have zero as an accumulation point. Let $A(z)$, $z \in F$, be a family of bounded operators of the form*

$$A(z) = A_0 + zA_1(z) \tag{3.4}$$

with $A_1(z)$ uniformly bounded as $z \to 0$ and A_0 self-adjoint. Suppose 0 is an isolated point of the spectrum of A_0, and let Q be the orthogonal projection onto $\mathrm{Ker}(A_0)$. *Then for sufficiently small $z \in F$ the operator $B(z) : Q\mathcal{H} \to Q\mathcal{H}$ defined by*

$$B(z) = z^{-1}(Q - Q(A(z) + Q)^{-1}Q) = \sum_{j=0}^{\infty} (-1)^j z^j Q[A_1(z)(A_0 + Q)^{-1}]^{j+1}Q$$

is uniformly bounded as $z \to 0$. The operator $A(z)$ has a bounded inverse in $\mathcal{H}$ if and only if $B(z)$ has a bounded inverse in $Q\mathcal{H}$. In this case

$$A(z)^{-1} = (A(z) + Q)^{-1} + z^{-1}(A(z) + Q)^{-1}QB(z)^{-1}Q(A(z) + Q)^{-1}$$

Proof. By construction the operator $A_0 + Q$ is invertible. Define $D_0 = (A_0 + Q)^{-1}$. For sufficiently small z the operator $A_1(z)$ satisfies $||zA_1(z)D_0|| < 1$ and so we can compute the Neumann expansion

$$\begin{aligned}(A(z) + Q)^{-1} &= (A_0 + Q + zA_1(z))^{-1} = D_0(\mathrm{Id} + zA_1(z)D_0)^{-1} \\ &= D_0 \sum_{j=0}^{\infty} (-1)^j z^j (A_1(z)D_0)^j.\end{aligned}$$

Since Q is the projection onto $\mathrm{Ker}(A_0)$ and A_0 is self-adjoint, we find $Q = Q(A_0+Q)D_0 = QD_0$ and so by taking adjoints $D_0Q = Q$ also. We can thus compute

$$\begin{aligned}B(z) &= z^{-1}(Q - Q(A(z) + Q)^{-1}Q) = z^{-1}\left(Q - Q\left(D_0 \sum_{j=0}^{\infty} (-1)^j z^j (A_1(z)D_0)^j\right) Q\right) \\ &= z^{-1}\left(Q - QD_0Q - QD_0\left(\sum_{j=1}^{\infty} (-1)^j z^j (A_1(z)D_0)^j\right) Q\right) \\ &= \sum_{j=0}^{\infty} (-1)^j z^j Q[A_1(z)(A_0 + Q)^{-1}]^{j+1}Q.\end{aligned}$$

Since $A_1(z)$ is uniformly bounded as $z \to 0$ we see that $B(z)$ is also. The fact that $A(z)$ has a bounded inverse if and only if $B(z)$ has a bounded inverse given by

$$A(z)^{-1} = (A(z) + Q)^{-1} + z^{-1}(A(z) + Q)^{-1}QB(z)^{-1}Q(A(z) + Q)^{-1}$$

now follows from Lemma 3.1.1. □

The next lemma is a form of what is known as the Feshbach formula.

Lemma 3.1.3. *Let A be an operator-valued matrix on the direct sum of Hilbert spaces*

$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$,

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

with $a_{ij} : \mathcal{H}_j \to \mathcal{H}_i$. *Suppose that* a_{11} *and* a_{22} *are closed and* a_{12} *and* a_{21} *are bounded. Suppose* a_{22} *has a bounded inverse. Then* A *has a bounded inverse if and only if*

$$B = (a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1}$$

exists and is bounded. Furthermore we have

$$A^{-1} = \begin{pmatrix} B & -Ba_{12}a_{22}^{-1} \\ -a_{22}^{-1}a_{21}B & a_{22}^{-1}a_{21}Ba_{12}a_{22}^{-1} + a_{22}^{-1} \end{pmatrix}.$$

Proof. Suppose that B exists and is bounded and let

$$C = \begin{pmatrix} B & -Ba_{12}a_{22}^{-1} \\ -a_{22}^{-1}a_{21}B & a_{22}^{-1}a_{21}Ba_{12}a_{22}^{-1} + a_{22}^{-1} \end{pmatrix}.$$

Then we can compute directly that

$$\begin{aligned} AC &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} B & -Ba_{12}a_{22}^{-1} \\ -a_{22}^{-1}a_{21}B & a_{22}^{-1}a_{21}Ba_{12}a_{22}^{-1} + a_{22}^{-1} \end{pmatrix} \\ &= \begin{pmatrix} a_{11}B - a_{12}a_{22}^{-1}a_{21}B & -a_{11}Ba_{12}a_{22}^{-1} + a_{12}a_{22}^{-1}a_{21}Ba_{12}a_{22}^{-1} + a_{12}a_{22}^{-1} \\ a_{21}B - a_{21}B & -a_{21}Ba_{12}a_{22}^{-1} + a_{21}Ba_{12}a_{22}^{-1} + \mathrm{Id} \end{pmatrix}. \end{aligned}$$

We can then calculate each term individually, finding first

$$(AC)_{11} = a_{11}B - a_{12}a_{22}^{-1}a_{21}B = (a_{11} - a_{12}a_{22}^{-1}a_{21})B = \mathrm{Id}_{\mathcal{H}_1}.$$

Next we have

$$\begin{aligned} (AC)_{12} &= -a_{11}Ba_{12}a_{22}^{-1} + a_{12}a_{22}^{-1}a_{21}Ba_{12}a_{22}^{-1} + a_{12}a_{22}^{-1} \\ &= -a_{11}Ba_{12}a_{22}^{-1} + a_{11}Ba_{12} - (a_{11} - a_{12}a_{22}^{-1}a_{21})Ba_{12}a_{22}^{-1} + a_{12}a_{22}^{-1} \\ &= -a_{11}Ba_{12}a_{22}^{-1} + a_{11}Ba_{12} - a_{12}a_{22}^{-1} + a_{12}a_{22}^{-1} \\ &= 0. \end{aligned}$$

We see immediately that $(AC)_{21} = 0$ and $(AC)_{22} = \mathrm{Id}_{\mathcal{H}_2}$. A similar calculation shows that $CA = \mathrm{Id}_{\mathcal{H}}$ and thus A has a bounded inverse given by C. For the converse, we suppose that A has a bounded inverse given by

$$C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}.$$

We now use the relations $AC = CA = \mathrm{Id}$ to demonstrate the existence of the operator B. The relation $AC = \mathrm{Id}$ gives us the four equations

$$a_{11}c_{11} + a_{12}c_{21} = \mathrm{Id}_{\mathcal{H}_1}, \quad a_{11}c_{12} + a_{12}c_{22} = 0, \tag{3.5}$$

$$a_{21}c_{11} + a_{22}c_{21} = 0,, \quad a_{21}c_{12} + a_{22}c_{22} = \mathrm{Id}_{\mathcal{H}_2}. \tag{3.6}$$

The invertibility of a_{22} and Equation (3.6) then immediately gives us $c_{21} = -a_{22}^{-1}a_{21}c_{11}$. Combining with Equation (3.5) we find

$$\mathrm{Id}_{\mathcal{H}_1} = a_{11}c_{11} + a_{12}c_{21} = a_{11}c_{11} - a_{12}a_{22}^{-1}a_{21}c_{11} = (a_{11} - a_{12}a_{22}^{-1}a_{21})c_{11}$$

so that $a_{11} - a_{12}a_{22}^{-1}a_{21}$ is a left inverse for c_{11}. Similarly the relation $CA = \mathrm{Id}_{\mathcal{H}}$ gives us the four equations

$$c_{11}a_{11} + c_{12}a_{21} = \mathrm{Id}_{\mathcal{H}_1},, \quad c_{21}a_{11} + c_{22}a_{21} = 0, \tag{3.7}$$

$$c_{11}a_{12} + c_{12}a_{22} = 0, \quad c_{21}a_{12} + c_{22}a_{22} = \mathrm{Id}_{\mathcal{H}_2}. \tag{3.8}$$

The invertibility of a_{22} and Equation (3.8) then immediately gives us $c_{12} = -c_{11}a_{12}a_{22}^{-1}$. Combining with Equation (3.7) we find

$$\mathrm{Id}_{\mathcal{H}_1} = c_{11}a_{11} + c_{12}a_{21} = c_{11}a_{11} - c_{11}a_{12}a_{22}^{-1}a_{21} = c_{11}(a_{11} - a_{12}a_{22}^{-1}a_{21}),$$

so that $a_{11} - a_{12}a_{22}^{-1}a_{21}$ is a right inverse of c_{11} also. Thus we have shown $c_{11} = (a_{11} - a_{12}a_{22}^{-1}a_{21})^{-1} = B$ exists and defines a bounded operator. □

We shall now give a broad overview of how the above algebraic results will be used. If the operator $M(k)$ is of the form $M(k) = A_0 + kA_1(k)$ with A_0 self-adjoint and not invertible and $A_1(k)$ uniformly bounded as $k \to 0$, define the orthogonal projection Q_1 onto the kernel of A_0. Then for sufficiently small k we have $||kA_1(k)|| < 1$ and thus we can compute the inverse of $M(k) + Q_1 = A_0 + Q_1 + kA_1(k)$ via a Neumann expansion. Then by Lemma 3.1.1 the operator $M(k)$ is invertible if and only if

$$B_1(k) = Q_1 - Q_1(M(k) + Q_1)^{-1}Q_1$$

is invertible. If $B_1(k)$ can be written as $B_1(k) = A_2 + kA_3(k)$ with A_2 invertible, then for sufficiently small k we can invert $B_1(k)$ via a Neumann expansion and find the inverse of

$M(k)$ as

$$M(k)^{-1} = (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}.$$

If $B_1(k)$ has self-adjoint leading term A_2 which is not invertible, we repeat the procedure by defining Q_2 to be the orthogonal projection onto the kernel of A_2 so that the operator $B_1(k)$ is invertible if and only if

$$B_2(k) = Q_2 - Q_2(B_1(k)+Q_2)^{-1}Q_2$$

is invertible. Write $B_2(k) = A_4 + kA_5(k)$. If the leading term A_4 of $B_2(k)$ is invertible, we can again use (for sufficiently small k, taking a new k_0 if necessary) a Neumann expansion to obtain

$$B_1(k)^{-1} = (B_1(k)+Q_2)^{-1} + (B_1(k)+Q_2)^{-1}Q_2B_2(k)^{-1}Q_2(B_1(k)+Q_2)^{-1}.$$

Substituting back into the formula for $M(k)^{-1}$ we obtain

$$\begin{aligned}M(k)^{-1} &= (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}\\ &+ (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_2B_2(k)^{-1}Q_2(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}.\end{aligned}$$

If the self-adjoint leading term A_4 of $B_2(k)$ is not invertible, we repeat the procedure by defining the orthogonal projection Q_3 onto the kernel of A_4. Due to general resolvent estimates (see [89]), the procedure terminates after a finite number of steps. In fact, we shall show that at most three projections are required (this occurs in the case $n = 2$) and the final inversion formula takes the form

$$\begin{aligned}M(k)^{-1} &= (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}\\ &+ (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_2B_2(k)^{-1}Q_2(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}\\ &+ (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_2(B_2(k)+Q_2)^{-1}Q_2(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}\\ &+ (M(k)+Q_1)^{-1}Q_1(B_1(k)+Q_2)^{-1}Q_2(B_2(k)+Q_2)^{-1}Q_3B_3(k)^{-1}Q_3\\ &\times (B_2(k)+Q_2)^{-1}Q_2(B_1(k)+Q_2)^{-1}Q_1(M(k)+Q_1)^{-1}.\end{aligned}$$

Another key feature to note is that the above is only a heuristic, in some of our applications the leading term is multiplied by a function of k and this is the scenario in which an application of Corollary 3.1.2 is more appropriate. In some cases the leading term is of the form $A + \eta^{-1}B$ and thus it is easier to decompose the Hilbert space into the span of complementary projections. In this case an application of Lemma 3.1.3 is more appropriate. We note also that by construction the projections satisfy $Q_3 \le Q_2 \le Q_1$.

The advantage of the Feshbach method just described is that it allows us to systematically isolate the obstructions to invertibility of the operator $M(k)$ into the range of a finite number of decreasing projections, which can be related to the spectrum of H using analytic methods.

We now note several algebraic identities which will be frequently used in our expansions.

Lemma 3.1.4. *Suppose that A_0 is a bounded self-adjoint operator on a Hilbert space $\mathcal{H}$ and that Q_1 is the orthogonal projection onto* $\mathrm{Ker}(A_0)$ *with zero an isolated point of the spectrum. Then the operator A_0+Q_1 is invertible with inverse $D_0 = (A_0+Q_1)^{-1}$ satisfying the relations*

$$Q_1 = D_0 Q_1 = Q_1 D_0.$$

Proof. Since Q_1 is the projection onto $\mathrm{Ker}(A_0)$ we have the relation $Q_1 A_0 = 0$ and thus we find

$$Q_1 = Q_1(A_0 + Q_1)D = Q_1 D.$$

Taking adjoints gives us $DQ_1 = Q_1$ also, since D_0 is a self-adjoint operator. □

Remark 3.1.5. If $Q \geq Q_1$ is an orthogonal projection and $QA_0 = A_0 Q = A_0$ then we have the additional relations $QD_0 = D_0 Q = D_0$, which follow immediately from the fact that Q is the identity on $Q\mathcal{H}$.

We end this section by describing a result which will allow us to show that the inversion procedure terminates in each dimension. The termination of the Feshbach procedure of Lemma 3.1.1 is guaranteed by more abstract bounds on the resolvent, however the next result also allows us to deduce useful relationships between certain integral operators.

Lemma 3.1.6. *Suppose that $f \in L^1(\mathbb{R}^n) \cap C^1(\mathbb{R}^n)$ satisfies $f(0) = 0$. Then for $n \geq 3$ we have*

$$\lim_{k\to 0} \int_{\mathbb{R}^n} \frac{1}{|\xi|^2(|\xi|^2 + k^2)} |f(\xi)|^2 \, \mathrm{d}\xi = \int_{\mathbb{R}^n} \frac{1}{|\xi|^4} |f(\xi)|^2 \, \mathrm{d}\xi. \tag{3.9}$$

If in addition we have $(x \mapsto |x|^{-2} f(x)) \in L^1(\mathbb{R}^n)$ then Equation (3.9) *holds in dimension $n = 1, 2$ also.*

Proof. Since $f \in L^1(\mathbb{R}^n)$ and $f(0) = 0$ we know that $|f(r)| = O(r)$ as $r \to 0$. We compute for any $R > 0$ that

$$\begin{aligned}\int_{\mathbb{R}^n} \frac{1}{|\xi|^4} |f(\xi)|^2 \, \mathrm{d}\xi &= \int_{\mathbb{S}^{n-1}} \int_0^\infty r^{n-5} |f(r\omega)|^2 \, \mathrm{d}r \, \mathrm{d}\omega \\ &= \int_{\mathbb{S}^{n-1}} \int_0^R r^{n-5} |f(r\omega)|^2 \, \mathrm{d}r \, \mathrm{d}\omega + \int_{\mathbb{S}^{n-1}} \int_R^\infty r^{n-5} |f(r\omega)|^2 \, \mathrm{d}r \, \mathrm{d}\omega.\end{aligned}$$

The integral from R to infinity always converges given the assumptions on f, so we must consider only the integral from 0 to R_0. Since $|f(r)| = O(r)$ as $r \to 0$ we see that the integral over $[0, R]$ converges for all $n \geq 3$. Applying the dominated convergence theorem now gives the equality of Equation (3.9).

If in addition we have that $|x|^{-2}f(x) \in L^1(\mathbb{R}^n)$ then we obtain $|f(r)| = O(r^3)$ as $r \to 0$ and thus the integral over $[0, R]$ converges in dimension $n = 1, 2$ also. An application of the dominated convergence theorem completes the proof. □

3.2 Expansions of the operator $M(k)$

We follow the method outlined in [89]. The expansions we present have been computed in various forms throughout the literature, in particular in dimension $n = 1$ in [89, 116], in dimension $n = 2$ in [63, 89, 166] in dimension $n = 3$ in [64, 88], in dimension $n = 4$ in [62, 87] and in dimension $n \geq 5$ in [71, 72, 85]. The older papers [85, 87, 88, 116] compute a non-symmetrised resolvent expansion whilst the more recent papers use the symmetrised technique outlined in [89].

Due to the dependence of the integral kernel of $R_0(z)$ on the parity of the dimension n our analysis is divided into odd and even dimensions. There are no resonances for $n \geq 5$, the only poles of the resolvent at $z = 0$ arising from the presence of zero energy eigenvalues. As a result the analysis is much simpler in dimension $n \geq 5$ and so we consider this first. As a general rule, the logarithmic behaviour of the integral kernel of $R_0(z)$ makes the analysis more difficult in even dimensions.

As discussed in Corollary 2.2.13 for $z \in \mathbb{C} \setminus [0, \infty)$ with $\mathrm{Im}(z^{\frac{1}{2}}) > 0$ (here we are using the principal branch of the logarithm) the integral kernel of the resolvent $R_0(z)$ is given by

$$R_0(x, y, z) = \frac{i}{4} z^{\frac{n-2}{4}} (2\pi)^{-\frac{n-2}{2}} |x - y|^{-\frac{n-2}{2}} H^{(1)}_{\frac{n-2}{2}}(z^{\frac{1}{2}}|x - y|), \tag{3.10}$$

where $H^{(1)}_\nu$ is the Hankel function of the first kind of order ν. We will use the variable $k = -iz^{\frac{1}{2}}$ so that $z = -k^2$. For $n = 1$ we thus have the expansion

$$R_0(x, y, -k^2) = \frac{1}{2} \sum_{p=0}^{\infty} \frac{(-1)^p}{p!} k^{p-1} |x - y|^p. \tag{3.11}$$

For $n \geq 3$ odd we have the expansion

$$R_0(x, y, -k^2) = |x - y|^{-(n-2)} \sum_{p=0}^{\infty} c_{n,p} k^p |x - y|^p. \tag{3.12}$$

Here the $c_{n,p}$ are numerical coefficients whose value is not needed and can be found in [89, Section 3], although we note that $c_{n,1} = 0$ and in fact $c_{n,p} = 0$ for $p = 1, 3, \ldots, n-4$ by [85, Lemma 3.3] (the argument here is purely combinatorial and uses an expansion of the heat kernel). If n is even we obtain

$$R_0(x, y, -k^2) = k^{n-2} \ln\left(k|x-y|\right) \sum_{p=0}^{\infty} c_{n,p} k^{2p} |x-y|^{2p} + |x-y|^{-(n-2)} \sum_{p=0}^{\infty} d_{n,p} k^{2p} |x-y|^{2p} \tag{3.13}$$

where the $c_{n,p}$ and $d_{n,p}$ are numerical coefficients whose value will be recalled as needed and can be found in [89, Section 3].

The above expansions are only formal and one needs to be more precise in what sense they are valid, truncating after finitely many terms. The expansions of Equation (3.11), (3.12) and (3.13) will be used in conjunction with the definition

$$M(k) = U + vR_0(-k^2)v$$

to determine expansions of $M(k)$ in each dimension.

3.2.1 Dimension $n \geq 5$ odd

In this section we employ the methods of [89] to compute an expansion of $M(k)^{-1}$ for $n \geq 5$ odd. For our purposes only the lowest order term in our expansions will be needed and thus we only compute the first term in the expansion, although we remark that more terms could be computed if necessary. We will refer to [85] for some boundedness properties of the operators involved in our expansions. The symmetrised expansions we present have appeared in [71].

The assumptions we make on the potential depend heavily on the dimension.

Assumption 3.2.1. If $n \geq 5$ is odd we assume that V satisfies Assumption 2.2.14 for

1. $\rho > 7$ if $n = 5$,
2. $\rho > 6$ if $n = 7, 9$ and
3. $\rho > \frac{n+1}{2}$ if $n \geq 11$.

We make the following definition, based the asymptotic expansion of $R_0(-k^2)$ in Equation (3.12).

Definition 3.2.2. Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1. We define for $p \in \mathbb{N}$ the integral operators G_p with integral kernels

$$G_p(x, y) = c_{n,p}|x-y|^{2-n+p}$$

and for $p \geq 1$ define the operators M_p by the integral kernels

$$M_p(x, y) = v(x)G_p(x, y)v(y).$$

For $p = 0$ we define the operator M_0 by the integral kernel

$$(M_0 - U)(x, y) = v(x)G_0(x, y)v(y).$$

Note that we have $M_1 = 0$ by [85, Lemma 3.3]. Thus by the definition of $M(k)$ we have the expansion

$$M(k) = U + vR_0(-k^2)v = M_0 + k^2 M_2 + k^3 \tilde{R}_0(k),$$

where $\tilde{R}_0(k)$ is uniformly bounded in $F = \{k \in \mathbb{C} : \mathrm{Re}(k) \geq 0 \text{ and } |k| \leq 1\}$.

Lemma 3.2.3. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1. Then the operators M_0 and M_2 are bounded and $\tilde{R}_0$ is uniformly bounded in norm for $k \in F$.*

Proof. We have by [85, Lemma 3.4] that $G_0, G_2 \in \mathcal{B}(H^{-1,t}, H^{1,-t})$ for all $t \geq 1$ and $G_2 \in \mathcal{B}(H^{-1,t}, H^{1,-t})$ for $t \geq 2$ and ρ satisfying Assumption 3.2.1. Thus the operators M_0 and M_2 are bounded also. □

Note that M_0 is a compact self-adjoint perturbation of U and so has essential spectrum contained in $\{-1, 1\}$. Thus 0 is an isolated point of the spectrum of M_0 and $\mathrm{DimKer}(M_0) < \infty$. If 0 is an eigenvalue of H then M_0 is not invertible, however we can use the Feshbach inversion method to overcome this and make the following definition.

Definition 3.2.4. If the operator M_0 is invertible then we say that zero is a *regular point* of the spectrum of H. If M_0 is not invertible, we say that zero is an *exceptional point* of the spectrum of H. For an exceptional point we can define the orthogonal projection Q_1 onto the kernel of M_0 and note that $M_0 + Q_1$ is invertible on $\mathcal{H}$, so that we may define the operator

$$D_0 = (M_0 + Q_1)^{-1}.$$

Since M_0 is a compact perturbation of U (an invertible operator), the Fredholm alternative guarantees that Q_1 is a finite rank operator.

We will now apply Lemma 3.1.1 with $A = M(k)$ and the projection Q_1. Thus we need to show that $M(k) + Q_1$ has a bounded inverse on $\mathcal{H}$.

Lemma 3.2.5. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point of the spectrum of H. Define the operator $D_0 = (M_0 + Q_1)^{-1}$.*

Then for sufficiently small k we have that $M(k) + Q_1$ is invertible on $\mathcal{H}$. Furthermore, we have the expansion

$$(M(k) + Q_1)^{-1} = D_0 - k^2 D_0 M_2 D_0 + k^3 \tilde{R}_1(k), \tag{3.14}$$

where $\tilde{R}_1(k)$ is uniformly bounded in k.

Proof. For sufficiently small k we find that

$$\left|\left|k^2 M_2 D_0 + k^3 \tilde{R}_0(k) D_0\right|\right| < 1.$$

We can thus use a Neumann expansion to compute that

$$\begin{aligned}
(M(k) + Q_1)^{-1} &= \left(M_0 + Q_1 + k^2 M_2 + k^3 \tilde{R}_0(k)\right)^{-1} = D_0 \left(\mathrm{Id} + (k^2 M_2 + k^3 \tilde{R}_0(k)) D_0\right)^{-1} \\
&= D_0 \left(\mathrm{Id} + \sum_{j=1}^{\infty} (-1)^j \left((k^2 M_2 + k^3 \tilde{R}_0(k)) D_0\right)^j\right) \\
&= D_0 - k^2 D_0 M_2 D_0 - k^3 D_0 \tilde{R}_0(k) D_0 \\
&\quad + \sum_{j=2}^{\infty} (-1)^j D_0 \left((k^2 M_2 + k^3 \tilde{R}_0(k)) D_0\right)^j D_0.
\end{aligned}$$

Defining the operator

$$\tilde{R}_1(k) = -D_0 \tilde{R}_0(k) D_0 + \sum_{j=2}^{\infty} (-1)^j k^{-3} D_0 \left((k^2 M_2 + k^3 \tilde{R}_0(k)) D_0\right)^j D_0$$

completes the proof. □

Lemma 3.1.1 states that $M(k)$ is invertible if and only if the operator

$$B_1(k) := Q_1 - Q_1 (M(k) + Q_1)^{-1} Q_1,$$

is invertible on $Q_1 \mathcal{H}$ and in this case

$$M(k)^{-1} = (M(k) + Q_1)^{-1} + (M(k) + Q_1)^{-1} Q_1 B_1(k)^{-1} Q_1 (M(k) + Q_1)^{-1}.$$

We thus need to determine an inverse for $B_1(k)$. Using Lemma 3.2.5 and the fact that $Q_1 = Q_1 D_0 Q_1$ (see Lemma 3.1.4) we can first determine an expansion for $B_1(k)$.

Lemma 3.2.6. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point of the spectrum of H. Then for sufficiently small k we have the*

expansion

$$B_1(k) = k^2 Q_1 M_2 Q_1 - k^3 Q_1 \tilde{R}_1(k). \tag{3.15}$$

Proof. We compute that

$$\begin{aligned} B_1(k) &= Q_1 - Q_1(M(k)+Q_1)^{-1}Q_1 = Q_1 - Q_1\left(D_0 - k^2 D_0 M_2 D_0 + k^3 \tilde{R}_1(k)\right) Q_1 \\ &= Q_1 - Q_1 D_0 Q_1 + k^2 Q_1 D_0 M_2 D_0 Q_1 - k^3 Q_1 \tilde{R}_1(k) Q_1 \\ &= k^2 Q_1 M_2 Q_1 - k^3 Q_1 \tilde{R}_1(k), \end{aligned}$$

where we have used the relations $Q_1 D_0 = D_0 Q_1 = Q_1$ of Lemma 3.1.4 several times. □

Hence the invertibility of $B_1(k)$ depends on the invertibility of the operator $Q_1 M_2 Q_1$ on $Q_1\mathcal{H}$.

Lemma 3.2.7. *[71, Lemma 5.3] Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point of the spectrum of H. Then the operator $Q_1 M_2 Q_1$ is invertible on $Q_1\mathcal{H}$. Furthermore, for $f \in Q_1\mathcal{H}$ we have the relation $\langle G_2 v f, v f\rangle = \langle G_0 v f, G_0 v f\rangle$.*

Proof. Take $f \in Q_1\mathcal{H}$, so that $(U + vG_0 v)f = 0$, and suppose $Q_1 M_2 Q_1 f = 0$. We note that the resolvent expansion (3.12) implies the weak operator topology limit

$$\lim_{k\to 0} k^{-2}(R_0(k^2) - G_0) = G_2.$$

Note also that $vf \in L^1(\mathbb{R}^n)$ and $x \mapsto |x|vf \in L^1(\mathbb{R}^n)$, so that $\mathcal{F}(vf) \in L^1(\mathbb{R}^n) \cap C^1(\mathbb{R}^n)$. So we find

$$\begin{aligned} \langle Q_1 v G_2 v Q_1 f, f\rangle &= \langle G_2 v f, v f\rangle = \lim_{k\to 0} \langle k^{-2}(R_0(k^2) - G_0) v f, v f\rangle \\ &= \lim_{k\to 0} k^{-2} \int_{\mathbb{R}^n} \left((|\xi|^2 - k^2)^{-1} - |\xi|^{-2}\right) [\mathcal{F}(vf)](\xi)\overline{[\mathcal{F}(vf)](\xi)} \,\mathrm{d}\xi \\ &= \lim_{k\to 0} \int_{\mathbb{R}^n} \frac{1}{|\xi|^2(|\xi|^2 - \lambda^2)} |[\mathcal{F}(vf)](\xi)|^2 \,\mathrm{d}\xi \\ &= \int_{\mathbb{R}^n} |\xi|^{-4} |[\mathcal{F}(vf)](\xi)|^2 \,\mathrm{d}\xi \\ &= \langle G_0 v f, G_0 v f\rangle, \end{aligned}$$

where we have used Lemma 3.1.6 to bring the limit inside the integral. The relation $\langle G_2 v f, v f\rangle = \langle G_0 v f, G_0 v f\rangle$ follows from the above equalities. Since $Q_1 M_2 Q_1 f = 0$ the final equality implies that $\mathcal{F}(vf) = 0$ which in turn gives $vf = 0$. So we see that $\mathrm{Ker}(Q_1 M_2 Q_1) = \{0\}$ and the claim is proved. □

We now have a well-defined bounded operator $D_1 = (Q_1 M_2 Q_1)^{-1}$ on $Q_1\mathcal{H}$. Noting that $D_1 = Q_1 D_1 Q_1$ we see that D_1 is finite rank.

Lemma 3.2.8. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point of the spectrum of H. Then for sufficiently small k the operator $B_1(k)$ is invertible and we have the expansion*

$$B_1(k)^{-1} = k^{-2}D_1 + k^{-1}D_1 Q_1 \tilde{R}_1(k) Q_1 D_1 + k^2 \tilde{R}_2(k),$$

where $\tilde{R}_2(k)$ is uniformly bounded in k and $D_1 = (Q_1 M_2 Q_1)^{-1}$.

Proof. For sufficiently small k we have the estimate

$$\left|\left|kQ_1\tilde{R}_1(k)Q_1D_1\right|\right| < 1.$$

We thus begin with Equation (3.15) to compute the Neumann expansion

$$\begin{aligned} B_1(k)^{-1} &= \left(k^2 Q_1 M_2 Q_1 - k^3 Q_1 \tilde{R}_1(k)\right)^{-1} = k^{-2}D_1\left(\mathrm{Id} - kQ_1\tilde{R}_1(k)Q_1D_1\right)^{-1} \\ &= k^{-2}D_1\left(\mathrm{Id} + kQ_1\tilde{R}_1(k)Q_1D_1 + \sum_{j=2}^{\infty} k^j(\tilde{R}_1(k)^j Q_1 D_1)^j\right). \end{aligned}$$

Defining $\tilde{R}_2(k) = \sum_{j=2}^{\infty} k^{j-2}(\tilde{R}_1(k)^j Q D_1)^j$ completes the proof. □

We finally have the required tools for our expansion of $M(k)$.

Theorem 3.2.9. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point for the spectrum of H. Then for sufficiently small k we have the expansion*

$$M(k)^{-1} = k^{-2}Q_1 D_1 Q_1 + \tilde{R}_3(k), \tag{3.16}$$

where the operator $\tilde{R}_3(k)$ is uniformly bounded in k.

Proof. We apply Lemma 3.1.1 to $A = M(k)$ and use Lemmas 3.2.5 and 3.2.8 to obtain

$$\begin{aligned} M(k)^{-1} &= (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} \\ &= D_0 - k^2 D_0 M_2 D_0 + k^3\tilde{R}_1(k) + \big(D_0 - k^2 D_0 M_2 D_0 + k^3 \tilde{R}_1(k)\big) \\ &\quad \times Q_1\big(k^{-2}D_1 + k^{-1}D_1Q_1\tilde{R}_1(k)Q_1D_1 + k^2\tilde{R}_2(k)\big)Q_1\big(D_0 - k^2D_0M_2D_0 + k^3\tilde{R}_1(k)\big). \end{aligned}$$

Expanding out the product shows that

$$\begin{aligned} (M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} &= k^{-2}Q_1D_1Q_1 - Q_1D_1Q_1M_2D_0 \\ &\quad + k^{-1}Q_1D_1Q_1\tilde{R}_1(k)Q_1D_1Q_1 + k\tilde{R}_4(k), \end{aligned}$$

where $\tilde{R}_4(k)$ is uniformly bounded for $k \in F$. Thus we find $M(k)^{-1} = k^{-2}Q_1D_1Q_1 + \tilde{R}_3(k)$, where we have defined the operator

$$\begin{aligned}\tilde{R}_3(k) = D_0 - k^2 D_0 M_2 D_0 + k^3 \tilde{R}_1(k) - Q_1 D_1 Q_1 M_2 D_0 \\ + k^{-1} Q_1 D_1 Q_1 \tilde{R}_1(k) Q_1 D_1 Q_1 + k\tilde{R}_4(k),\end{aligned}$$

which is uniformly bounded in k. □

Finally we characterise the zero eigenspace of H in terms of the operators just described. The following result is implicit in [85] and can be found as [71, Lemma 5.5].

Lemma 3.2.10. *[71, Lemma 5.5] Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1 and that zero is an exceptional point of the spectrum of H. Then the projection onto the eigenspace at zero is $P_0 = G_0 v Q_1 D_1 Q_1 v G_0$.*

Proof. Suppose that $\mathrm{Dim}(Q_1\mathcal{H}) = N_0$ and let $(\varphi_j)_{j=1}^{N_0}$ be an orthonormal basis for $Q_1\mathcal{H}$. Then we have

$$0 = M_0\varphi_j = UM_0\varphi_j = U(U\varphi_j + vG_0v\varphi_j) = \varphi_j + UvG_0v\varphi_j.$$

Write $\varphi_j = Uv\psi_j$ for $(\psi_j)_{j=1}^{N_0} \subset \mathcal{H}$ a linearly independent set (see [71, Lemma 5.1]), so that

$$0 = Uv\psi_j + UvG_0vUv\psi_j = Uv(\psi_j + G_0V\psi_j),$$

which implies $\psi_j + G_0V\psi_j = 0$. Thus for any $f \in \mathcal{H}$ we may write

$$\begin{aligned}Q_1vG_0f &= \sum_{j=1}^{N_0} \langle vG_0f, \varphi_j\rangle\varphi_j = \sum_{j=1}^{N_0} \langle f, G_0v\varphi_j\rangle\varphi_j \\ &= \sum_{j=1}^{N_0} \langle f, G_0V\psi_j\rangle\varphi_j = -\sum_{j=1}^{N_0} \langle f, \psi_j\rangle\varphi_j.\end{aligned}$$

We let (A_{ij}) be the matrix representation of $Q_1M_2Q_1$ with respect to $(\varphi_j)_{j=1}^{N_0}$, so that

$$A_{ij} = \langle \varphi_i, Q_1M_2Q_1\varphi_j\rangle = \langle v\varphi_i, G_2v\varphi_j\rangle = \langle G_0v\varphi_i, G_0v\varphi_j\rangle = \langle \varphi_i, \varphi_j\rangle,$$

where we have used the relation $\langle G_2vf, vg\rangle = \langle G_0vf, G_0vg\rangle$ valid for all $f, g \in Q_1\mathcal{H}$ (see

Lemma 3.2.7). Then for $f \in \mathcal{H}$ we may calculate that

$$\begin{aligned} P_0 f &= G_0 v Q D_1 Q v G_0 f = G_0 v Q_1 D_1 \left(- \sum_{j=1}^{N_0} \langle f, \psi_j f \rangle \varphi_j \right) = - \sum_{j=1}^{N_0} G_0 v Q D_1 \varphi_j \langle f, \psi_j \rangle \\ &= - \sum_{j=1}^{N_0} \sum_{p=1}^{N_0} G_0 v Q_1 (A^{-1})_{pj} \varphi_p \langle f, \psi_j \rangle = - \sum_{j=1}^{N_0} \sum_{p=1}^{N_0} G_0 v \varphi_p (A^{-1})_{pj} \langle f, \psi_j \rangle \\ &= \sum_{j=1}^{N_0} \sum_{p=1}^{N_0} (A^{-1})_{pj} \psi_p \langle f, \psi_j \rangle. \end{aligned}$$

In particular for $f = \psi_m$ we find $P_0 \psi_m = \psi_m$ and so the range of P_0 is the span of $(\psi_m)_{m=1}^{N_0}$ and since P_0 is self-adjoint it is the desired projection onto the kernel of H. □

The operator P_0 arises when considering the lowest order term in the expansion of

$$R(-k^2) = R_0(-k^2) - R_0(-k^2) v M(k)^{-1} v R_0(-k^2),$$

as we now demonstrate.

Theorem 3.2.11. *Suppose that $n \geq 5$ is odd and V satisfies Assumption 3.2.1. Then for sufficiently small k we have the expansion*

$$R(-k^2) - R_0(-k^2) = -k^{-2} P_0 + \tilde{R}(k), \tag{3.17}$$

where $\tilde{R}(k)$ is uniformly bounded.

Proof. We note that

$$\begin{aligned} R(-k^2) - R_0(-k^2) &= -R_0(-k^2) v M(k)^{-1} v R_0(-k^2) \\ &= -(G_0 v + \tilde{R}_1(k))(k^{-2} Q_1 D_1 Q_1 + \tilde{R}_3(k))(v G_0 + \tilde{R}_2(k)) \\ &= -k^{-2} G_0 v Q_1 D_1 Q_1 v G_0 + \tilde{R}(k). \end{aligned}$$

An application of Lemma 3.2.10 completes the proof. □

3.2.2 Dimension $n \geq 5$ even

In this section we compute the low energy behaviour of the operator $M(k)$ in even dimensions $n \geq 5$. We use the Feshbach inversion formula as described in [89]. Such expansions have been considered in a different context in [72] and first appeared in a non-symmetrised form in [85], to which we will refer for some boundedness properties of the operators involved in our expansions. The statements and proofs in this section are rather similar to the case $n \geq 5$ odd, however are made more cumbersome by the presence of the logarithmic behaviour of the Hankel function appearing in the integral kernel of $R_0(-k^2)$. We thus introduce the variable $\eta = \ln(k)^{-1}$ (we are using the principal branch of the logarithm).

We require stronger assumptions on the potential than Assumption 2.2.14.

Assumption 3.2.12. If $n \geq 5$ is even we assume that V satisfies Assumption 2.2.14 for

1. $\rho > 7$ if $n = 6$,
2. $\rho > 6$ if $n = 8, 10$ and
3. $\rho > \frac{n+1}{2}$ if $n \geq 12$.

We recall that if n is even we have the expansion

$$R_0(x, y, z) = k^{n-2} \ln(k|x-y|) \sum_{p=0}^{\infty} c_{n,p} k^{2p} |x-y|^{2p} + |x-y|^{-(n-2)} \sum_{p=0}^{\infty} d_{n,p} k^{2p} |x-y|^{2p} \tag{3.18}$$

Considering the terms in the expansion of $R_0(x, y, k^2)$ of Equation (3.18) with logarithmic coefficients leads to the following operator definitions.

Definition 3.2.13. For $0 \leq p \leq \frac{n}{2} - 2$ we define the operators $G_{2p,-1} = 0$ and the integral operators $G_{2p,0}$ with the integral kernels

$$G_{2p,0}(x, y) = d_{n,}|x-y|^{2p+2-n}.$$

For $p \geq \frac{n}{2} - 1$ we define the operators $G_{2p,0}$ and $G_{2p,-1}$ by the integral kernels

$$\begin{aligned} G_{2p,0}(x, y) &= |x-y|^{2p} \left(c_{n,2p} \ln(|x-y|) + d_{n,2p+n-2}\right), \\ G_{2p,-1}(x, y) &= c_{n,p}|x-y|^{2p}. \end{aligned}$$

For $(0, 0) \neq (p, q) \in \mathbb{N} \times \{0, -1\}$ we can further define the operators $M_{0,0} = U + vG_{0,0}v$ and $M_{p,q} = vG_{p,q}v$.

We will only need the first few terms in this expansion, although it is helpful to see how each is defined. We may then write using the definition of $M(k)$ the expansion

$$M(k) = U + vR_0(-k^2)v = M_{0,0} + k^2 M_{2,0} + k^4 \eta^{-1} \tilde{R}_0(k)$$

with $\tilde{R}_0(k)$ uniformly bounded in k. The labelling convention we use is that a pair (i, j) of subscripts refers to an operator with coefficient $k^i \eta^j$. We make the following definition of exceptional points.

Definition 3.2.14. We say that zero is a *regular point* for H if the operator $M_{0,0}$ is invertible. If $M_{0,0}$ is not invertible, we say zero is an *exceptional point* for H and define the operator Q_1 to be the orthogonal projection onto the kernel of $M_{0,0}$. The operator $M_{0,0} + Q_1$ is then invertible and we let $D_0 = (M_{0,0} + Q_1)^{-1}$.

We now proceed as in the odd case to obtain an expansion for $M(k)^{-1}$.

Lemma 3.2.15. *Suppose that $n \geq 5$ is even and V satisfies Assumption 3.2.12 and that zero is an exceptional point for H. Then for sufficiently small k we have the expansion*

$$(M(k) + Q_1)^{-1} = D_0 - k^2 D_0 M_{2,0} D_0 + k^4 \eta^{-1} \tilde{R}_2(k),$$

where $\tilde{R}_2(k)$ is uniformly bounded in k and $D_0 = (M_{0,0} + Q_1)^{-1}$.

Proof. For sufficiently small k we have the estimate

$$\left|\left| k^2 M_{2,0} D_0 + k^4 \eta^{-1} \tilde{R}_0(k) D_0 \right|\right| < 1.$$

We are thus able to compute using a Neumann expansion the expansion

$$\begin{aligned}(M(k) + Q_1)^{-1} &= (M_{0,0} + k^2 M_{2,0} + k^4 \eta^{-1} \tilde{R}_0(k) + Q_1)^{-1} \\ &= D_0(\mathrm{Id} + k^2 M_{2,0} D_0 + k^4 \eta^{-1} \tilde{R}_0(k) D_0)^{-1} \\ &= D_0(\mathrm{Id} - k^2 M_{2,0} D_0 - k^4 \eta^{-1} \tilde{R}_0(k) D_0 + k^4 \eta^{-1} \tilde{R}_1(k)),\end{aligned}$$

where $\tilde{R}_1(k)$ is uniformly bounded in k. The result follows by defining the remainder $\tilde{R}_2(k) = \tilde{R}_0(k) + \tilde{R}_1(k)$. □

We next define the operator $B_1(k)$ by

$$B_1(k) = Q_1 - Q_1(M(k) + Q_1)^{-1} Q_1. \tag{3.19}$$

Lemma 3.2.16. *Suppose that $n \geq 5$ is even and V satisfies Assumption 3.2.12 and that zero is an exceptional point for H. Then for sufficiently small k we have the expansion*

$$B_1(k) = k^2 Q_1 M_{2,0} Q_1 - Q_1 k^4 \tilde{R}_2(k).$$

Proof. We compute using the definition of $B_1(k)$ and Lemma 3.2.15 that

$$\begin{aligned}B_1(k) &= Q_1 - Q_1(M(k) + Q_1)^{-1} Q_1 = Q_1 - Q_1(D_0 - k^2 D_0 M_{2,0} D_0 + k^4 \eta^{-1} \tilde{R}_2(k)) Q_1 \\ &= k^2 Q_1 M_{2,0} Q_1 - k^4 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1,\end{aligned}$$

where we have used the relations $Q_1 D_0 = D_0 Q_1 = Q$ (see Lemma 3.1.4). □

We see that the invertibility of $B_1(k)$ depends on the invertibility of the operator $Q_1 M_{2,0} Q_1$. The following result shows that the Feshbach procedure of Lemma 3.1.1 terminates.

Lemma 3.2.17. *[72, Lemma 5.2] Suppose that $n \geq 5$ is even and V satisfies Assumption 3.2.12. Then the operator $Q_1 M_{2,0} Q_1$ is invertible on $Q_1 \mathcal{H}$.*

Proof. The proof is identical to that of Lemma 3.2.7 with the operator M_2 replaced by $M_{2,0}$, since the integral kernels are scalar multiples of each other. □

We can now determine an expansion for the inverse of the operator $B_1(k)$. We write $D_1 = (Q_1 M_{2,0} Q_1)^{-1}$ on $Q_1 \mathcal{H}$.

Lemma 3.2.18. *Suppose that $n \geq 5$ is even and V satisfies Assumption 3.2.12 and that zero is an exceptional point for H. Then for sufficiently small k we have the expansion*

$$B_1(k)^{-1} = k^{-2} D_1 - k^2 D_1 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1 D_1 + k^2 \eta^{-1} \tilde{R}_3(k),$$

where $\tilde{R}_3(k)$ is uniformly bounded in k and $D_1 = (Q_1 M_{2,0} Q_1)^{-1}$.

Proof. For sufficiently small k we have the estimate

$$\left|\left|k^4 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1 D_1\right|\right| < 1$$

We are thus able to compute using the definition of $B_1(k)$ and Lemma 3.2.17 the Neumann expansion

$$\begin{aligned} B_1(k)^{-1} &= (k^2 Q_1 M_{2,0} Q_1 - k^4 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1)^{-1} = k^{-2} D_1 (\mathrm{Id} - k^4 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1 D_1)^{-1} \\ &= k^{-2} D_1 - k^2 D_1 Q_1 \eta^{-1} \tilde{R}_2(k) Q_1 D_1 + k^2 \eta^{-1} \tilde{R}_3(k), \end{aligned}$$

where $\tilde{R}_3(k)$ is uniformly bounded in k. □

We can now use Lemma 3.1.1 to invert $M(k)$.

Theorem 3.2.19. *Suppose that $n \geq 5$ is even and V satisfies Assumption 3.2.12 and that zero is an exceptional point for H. Then for sufficiently small k we have the expansion*

$$M(k)^{-1} = k^{-2} Q_1 D_1 Q_1 + \eta^{-1} \tilde{R}_6(k),$$

where $\tilde{R}_6(k)$ is uniformly bounded in k.

Proof. We use Lemma 3.2.15 to find

$$\begin{aligned} (M(k) + Q_1)^{-1} Q_1 &= Q_1 - k^2 D_0 M_{2,0} Q_1 + k^4 \eta^{-1} \tilde{R}_2(k) Q_1, \\ Q_1 (M(k) + Q_1)^{-1} &= Q_1 - k^2 Q_1 M_{2,0} D_0 + k^4 Q_1 \eta^{-1} \tilde{R}_2(k). \end{aligned}$$

We can thus use Lemma 3.2.18 to find

$$\begin{aligned}
&(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}\\
&=(Q_1-k^2D_0M_{2,0}Q_1+k^4\eta^{-1}\tilde{R}_2(k)Q_1)(k^{-2}D_1-k^2D_1Q_1\eta^{-1}\tilde{R}_2(k)Q_1D_0+k^2\eta^{-1}\tilde{R}_3(k))\\
&\times(Q_1-k^2Q_1M_{2,0}D_0+k^4Q_1\eta^{-1}\tilde{R}_2(k))\\
&=k^{-2}Q_1D_1Q_1+\eta^{-1}\tilde{R}_5(k),
\end{aligned}$$

where $\tilde{R}_5(k)$ is uniformly bounded in k. Lemma 3.1.1 then gives us the expansion

$$\begin{aligned}
M(k)^{-1}&=(M(k)+Q_1)^{-1}+(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}\\
&=D_0-k^2D_0M_{2,0}D_0+k^4\eta^{-1}\tilde{R}_2(k)+k^{-2}Q_1D_1Q_1+\eta^{-1}\tilde{R}_5(k)\\
&=k^{-2}Q_1D_1Q_1+\eta^{-1}\tilde{R}_6(k),
\end{aligned}$$

where $\tilde{R}_6(k)$ is uniformly bounded in k. □

We observe that despite the logarithmic singularity in the integral kernel of $R_0(-k^2)$, the leading behaviour is identical to that of the case $n\geq 5$ odd. We will demonstrate shortly that this is no longer the case in dimension $n=2,4$ and must be handled with care.

Lemma 3.2.20. *[72, Lemma 5.3] Suppose that $n\geq 5$ is even and V satisfies Assumption 3.2.12. Then the projection P_0 onto the zero eigenspace of H is the operator $G_{0,0}vQ_1D_1Q_1vG_{0,0}$.*

Proof. The proof is identical to that of Lemma 3.2.10, so we omit the details. □

Theorem 3.2.21. *Suppose that $n\geq 5$ is even and V satisfies Assumption 3.2.12. Then for sufficiently small k we have*

$$R(-k^2)-R(-k^2)=-k^{-2}P_0+\tilde{R}(k), \tag{3.20}$$

where $\tilde{R}(k)$ is uniformly bounded.

The proof is identical to the odd dimensional case.

3.2.3 Dimension $n=4$

In this section we demonstrate an expansion for the symmetrised resolvent in dimension $n=4$. Such results have been demonstrated in the unsymmetrised case in [87] and have been used in various contexts, see [62]. We will again employ the Feshbach inversion method of [89] discussed at the beginning of this chapter. The resolvent expansions are similar to those found in the case $n\geq 5$ even, however are sensitive to extra obstructions to the invertibility of the operator $M(k)$ near zero arising from the presence of zero eigenvalues and of another phenomena, called a zero energy resonance. Our inversion procedure will lead to a natural definition of zero energy resonance in dimension $n = 4$.

Throughout this section we make the following assumption on the potential.

Assumption 3.2.22. We assume the potential V satisfies Assumption 2.2.14 for some $\rho > 12$.

Equation (3.13) in dimension $n = 4$ reads

$$R_0(x, y, z) = k^2 \ln(k|x-y|) \sum_{p=0}^{\infty} c_{4,p} k^{2p} |x-y|^{2p} + |x-y|^{-2} \sum_{p=0}^{\infty} d_{4,p} k^{2p} |x-y|^{2p} \tag{3.21}$$

and leads to the following operator definitions.

Definition 3.2.23. Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Define the integral operator $G_{0,0}$ by the kernel

$$G_{0,0}(x, y) = d_{4,0} |x-y|^{-2}$$

and for integers $p \geq 1$ the integral operators $G_{2p,0}$ and $G_{2p,-1}$ by the kernels

$$\begin{aligned} G_{2p,0}(x, y) &= (c_{4,2p} \ln(|x-y|) + d_{4,2p+2}) |x-y|^{2p-2}, \\ G_{2p,-1}(x, y) &= c_{4,2p} |x-y|^{2p-2}. \end{aligned}$$

Further define the operators $M_{0,0} = U + vG_{0,0}v$ and $M_{2p,j} = vG_{2p,j}v$ for $j = 0, -1$ and $p \geq 1$ an integer.

The operator $G_{2p,j}$ is the operator coefficient of the term $k^{2p} \ln(k)^j$ in Equation (3.21). As in the previous section we introduce the variable $\eta = \ln(k)^{-1}$. Then using the definition of $M(k)$ we have the expansions

$$M(k) = U + vR_0(-k^2)v = M_{0,0} + k^2 M_{2,0} + k^2 \eta^{-1} M_{2,-1} + k^4 \eta^{-1} \tilde{R}_0(k) \tag{3.22}$$

and

$$M(k) = M_{0,0} + k^2 M_{2,0} + k^2 \eta^{-1} M_{2,-1} + k^4 M_{4,0} + k^4 \eta^{-1} M_{4,-1} + k^6 \eta^{-1} \tilde{R}_1(k), \tag{3.23}$$

where $\tilde{R}_0(k)$ and $\tilde{R}_1(k)$ are uniformly bounded for $k \in F$. The expansion of Equation (3.22) does not have sufficiently many terms for some of the more involved calculations and in these situations we will consider the expansion of Equation (3.23). We also define the projection $P = ||v||^{-2} \langle \cdot, v \rangle v$ which is by definition a scalar multiple of $M_{2,-1}$.

Definition 3.2.24. Suppose that $n = 4$ and V satisfies Assumption 3.2.22. We say that zero is a *regular point* of the spectrum of H if the operator $M_{0,0}$ is invertible. If zero is not a regular point of the spectrum of H, we define Q_1 to be the orthogonal projection onto the kernel of $M_{0,0}$. Then $M_{0,0} + Q_1$ is invertible and we can define $D_0 = (M_{0,0} + Q_1)^{-1}$. We say there is an *exceptional point of the first kind* if $Q_1 M_{2,-1} Q_1$ is invertible on $Q_1\mathcal{H}$. If $Q_1 M_{2,-1} Q_1$ is not invertible, we define Q_2 to be the orthogonal projection onto the kernel of $Q_1 M_{2,-1} Q_1$ (as an operator on $Q_1\mathcal{H}$). Then $Q_1 M_{2,-1} Q_1 + Q_2$ is invertible on $Q_1\mathcal{H}$. If $Q_1 = Q_2$ we say there is an *exceptional point of the second kind*. Otherwise, we say there is an *exceptional point of the third kind*.

In our definition, $Q_2 \neq 0$ (an exceptional point of the second kind) will be shown to correspond to the existence of an eigenvalue whilst $Q_1 \neq 0$ will lead to a definition of resonance in dimension $n = 4$. Before proceeding to our expansion of $M(k)^{-1}$, we characterise the range of the projections Q_1 and Q_2 in terms of solutions to the equation $H\psi = 0$. We can characterise the image of the projections Q_1 and Q_2 in terms of the spectrum of H.

Lemma 3.2.25. *[62, Lemma 7.1] Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Then $0 \neq f \in Q_1\mathcal{H}$ if and only if $f = Uvg$ for some $g \in H^{0,-t}$ for some $t > 0$ such that $Hg = 0$ in the sense of distributions.*

Proof. Composing with H_0 shows that $Hg = 0$ if and only if $(\mathrm{Id} + G_{0,0}V)g = 0$. So suppose that $f \in Q_1\mathcal{H}$ which gives us $(U + vG_{0,0}v)f = 0$ and upon multiplying by U we obtain

$$f(x) = -U(x)v(x)[G_{0,0}vf](x) = d_{4,0}U(x)v(x)\int_{\mathbb{R}^4} |x-y|^{-2}v(y)f(y)\,\mathrm{d}y.$$

Thus we define the function g by

$$g(x) = d_{4,0}\int_{\mathbb{R}^4} |x-y|^{-2}v(y)f(y)\,\mathrm{d}y = -[G_{0,0}vf](x). \tag{3.24}$$

Since $vf \in H^{0,2}$ we find by [85, Lemma 2.3] that $g \in H^{0,-t}$ for some $t > 0$. By construction we have $f = Uvg$ and we have the relation

$$0 = g + G_{0,0}vf = g + G_{0,0}Vg = (\mathrm{Id} + G_{0,0}V)g,$$

so that g satisfies $Hg = 0$ in the sense of distributions. For the converse, suppose $f = Uvg$ for some non-zero g satisfying $Hg = 0$. Then we have

$$(U + vG_{0,0}v)f = vg + vG_{0,0}Vg = v(\mathrm{Id} + G_{0,0}V)g = 0,$$

so that $f \in Q_1\mathcal{H}$. □

Lemma 3.2.26. *[62, Lemma 7.2] Suppose* $n = 4$ *and* V *satisfies Assumption 3.2.22. Then* $0 \neq f \in Q_2\mathcal{H}$ *if and only if* $f = Uvg$ *for some* $0 \neq g \in \mathcal{H}$ *such that* $Hg = 0$ *in the sense of distributions.*

Proof. Suppose that $f \in Q_2\mathcal{H}$. Since $Q_2 \leq Q_1$ we have by Lemma 3.2.25 that $f = Uvg$ and it suffices to show $g \in \mathcal{H}$. We note that $PQ_2 = 0$ implies

$$\int_{\mathbb{R}^4} v(y)f(y)\,\mathrm{d}y = 0. \tag{3.25}$$

By Lemma 3.2.25 we have that g satisfies Equation (3.24). Equation (3.25) gives

$$(1+|x|^2)^{-1}\int_{\mathbb{R}^4} v(y)f(y)\,\mathrm{d}y = 0$$

and thus

$$g(x) = d_{4,0}\int_{\mathbb{R}^4}\left(|x-y|^{-2} - (1+|x|^2)^{-1}\right)v(y)f(y)\,\mathrm{d}y.$$

For $x \neq y \in \mathbb{R}^n$ we have the estimate (see [87, Equation (2.8)])

$$\left||x-y|^{-2} - (1+|x|^2)^{-1}\right| \leq 5\left(\frac{(1+|y|^2)^{\frac{1}{2}}}{(1+|x|^2)^{\frac{1}{2}}|x-y|^2} + \frac{(1+|y|^2)^{\frac{1}{2}}}{(1+|x|^2)|x-y|^2}\right). \tag{3.26}$$

Both terms on the right hand side of the estimate (3.26) are the integral kernels of Riesz operators (see [153, Chapter V.1]). Define the operators $L_1, L_2 : C_c^\infty(\mathbb{R}^4) \to C_c^\infty(\mathbb{R}^4)$ by the integral kernels

$$L_1(x,y) = \frac{1}{|x-y|^2} \quad \text{and} \quad L_2(x,y) = \frac{1}{|x-y|^2}.$$

By Theorem 2.2.5 we have that for $\alpha \in \mathbb{R}$ the operator q_α of multiplication by the function $q_\alpha = (1+|\cdot|^2)^{\frac{\alpha}{2}}$ maps $H^{s,t} \to H^{s,t-\alpha}$ for any $s,t \in \mathbb{R}$. For $t > 0$ we have by [153, Chapter V.1] $L_1 : H^{0,1+t} \to H^{0,-1}$ and $L_2 : H^{0,1+t} \to H^{0,-2}$. Since $q_1 vf \in H^{0,1+t}$ we find for $j = 1,2$ that $q_{-j}L_j q_1 v : \mathcal{H} \to \mathcal{H}$ and thus $g \in \mathcal{H}$.

For the converse, suppose $f = Uvg$ and use Equations (3.24) and (3.25) to show

$$g(x) = d_{4,0}\int_{\mathbb{R}^4}\left(|x-y|^{-2} - (1+|x|^2)^{-1}\right)v(y)f(y)\,\mathrm{d}y + d_{4,0}(1+|x|^2)^{-1}\int_{\mathbb{R}^4} v(y)f(y)\,\mathrm{d}y. \tag{3.27}$$

Then by assumption $g \in \mathcal{H}$ and the first term in Equation (3.27) is in $\mathcal{H}$ by the estimate

(3.26), which forces the second term in Equation (3.27) to be in $\mathcal{H}$ also. That is

$$\left(\mathbb{R}^4 \ni x \mapsto (1+|x|^2)^{-1} \int_{\mathbb{R}^4} v(y) f(y)\,\mathrm{d}y\right) \in \mathcal{H}.$$

which forces $0 = Pf = Q_1 P Q_1 f$ and so $f \in \mathcal{H}$. □

Corollary 3.2.27. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Then*

$$\operatorname{Rank}(Q_1) \leq \operatorname{Rank}(Q_2) + 1.$$

Proof. Suppose that $0 \neq f_1, f_2 \in Q_1\mathcal{H}$ and let g_1, g_2 be the corresponding distributional solutions of $Hg = 0$. Then we just need to show there exists a constant $c \in \mathbb{C}$ and a function $h \in \mathcal{H}$ such that $g_2 - cg_1 = h$, which follows from Equation (3.27). □

The invertibility of the operator $M(k)$ depends on the nature of the singularity at the point zero, however the following result will be used in each exceptional case.

Lemma 3.2.28. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22, and that zero is not a regular point of the spectrum of H. Then for sufficiently small k we have the expansion*

$$(M(k) + Q_1)^{-1} = D_0 - k^2 D_0 M_{2,0} D_0 - k^2 \eta^{-1} D_0 M_{2,-1} D_0 - k^2 \eta^{-1} \tilde{R}_2(k), \tag{3.28}$$

where $\tilde{R}_2(k)$ is uniformly bounded in k and $D_0 = (M_{0,0} + Q_1)^{-1}$.

Proof. For sufficiently small k we have the estimate

$$||M(k) - M_{0,0} + Q_1||_2 < 1.$$

We are thus able to compute the Neumann expansion

$$\begin{aligned}
(M(k) + Q_1)^{-1} &= (M_{0,0} + Q_1 + k^2 M_{2,0} + k^2\eta^{-1} M_{2,-1} + k^4 M_{4,0} \\
&\quad + k^4 \eta^{-1} M_{4,-1} + k^4 \eta^{-1} \tilde{R}_1(k))^{-1} \\
&= D_0(\mathrm{Id} + k^2 M_{2,0} D_0 + k^2 \eta^{-1} M_{2,-1} D_0 + k^4 M_{4,0} D_0 \\
&\quad + k^4 \eta^{-1} M_{4,-1} D_0 + k^4 \eta^{-1} D_0 \tilde{R}_1(k))^{-1} \\
&= D_0(\mathrm{Id} - k^2 M_{2,0} D_0 - k^2 \eta^{-1} M_{2,-1} D_0 - k^4 M_{4,0} D_0 \\
&\quad - k^4 \eta^{-1} M_{4,-1} D_0 - k^4 \eta^{-1} D_0 \tilde{R}_1(k) + k^4 \eta^{-1} \tilde{R}_4(k)) \\
&= D_0 - k^2 D_0 M_{2,0} D_0 - k^2 \eta^{-1} D_0 M_{2,-1} D_0 + k^2 \eta^{-1} \tilde{R}_2(k),
\end{aligned}$$

as claimed. □

Remark 3.2.29. If we use the extra terms in Equation (3.23) we find

$$\begin{aligned}(M(k)+Q_1)^{-1} = D_0 &- k^2 D_0 M_{2,0} D_0 - k^2\eta^{-1} D_0 M_{2,-1} D_0 - k^4 D_0 M_{4,0} D_0 \\ &- k^4\eta^{-1} D_0 M_{4,-1} D_0 + k^4 D_0 M_{2,0} D_0 M_{2,0} D_0 \\ &+ k^4\eta^{-1}(D_0 M_{2,0} D_0 M_{2,-1} D_0 + D_0 M_{2,-1} D_0 M_{2,0} D_0) \\ &+ k^4\eta^{-2} D_0 M_{2,-1} D_0 M_{2,-1} D_0 - k^6\eta^{-1}\tilde{R}_2'(k),\end{aligned}$$

where $\tilde{R}_2'(k)$ is uniformly bounded in k.

We can now handle the relatively simple case of exceptional points of the first kind, which corresponds to resonances with no eigenvalues. Lemma 3.1.1 tells us that $M(k)$ is invertible if and only if $B_1(k)$ defined by

$$B_1(k) := Q_1 - Q_1\left(M(k)+Q_1\right)^{-1} Q_1$$

is invertible.

Lemma 3.2.30. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22, and that zero is an exceptional point of the first kind. Then for sufficiently small k we have $B_1(k)$ is invertible and there exist $c_1, c_2 \in \mathbb{C}$ and a uniformly bounded function $\tilde{c}_3 : F \to \mathbb{C}$ such that*

$$B_1(k)^{-1} = \left(k^2 c_1 + k^2\eta^{-1} c_2 + k^4\eta^{-1}\tilde{c}_3(k)\right)^{-1} Q_1.$$

Proof. We have (see Lemma 3.1.4) the relations $Q_1 D_0 = D_0 Q_1 = Q_1$ and thus using Lemma 3.2.28 we find

$$\begin{aligned}Q_1\left(M(k)+Q_1\right)^{-1} Q_1 &= Q_1\left(D_0 - k^2 D_0 M_{2,0} D_0 - k^2\eta^{-1} D_0 M_{2,-1} D_0 - k^4\eta^{-1}\tilde{R}_2(k)\right) Q_1 \\ &= Q_1 - k^2 Q_1 M_{2,0} Q_1 - k^2\eta^{-1} Q_1 M_{2,-1} Q_1 - k^4\eta^{-1} Q_1 \tilde{R}_2(k) Q_1.\end{aligned}$$

Since Q_1 is a rank one operator in the case of an exceptional point of the first kind by Corollary 3.2.27, we find that $Q_1 M_{2,0} Q_1 = c_1 Q_1$ for some constant c_1, and similarly we have $Q_1 M_{2,-1} Q_1 = c_2 Q_1$ for some constant c_2. In the same manner we find there exists $\tilde{c}_3 : F \to \mathbb{C}$ such that $Q_1 \tilde{R}_2(k) Q_1 = \tilde{c}_3(k) Q_1$. Then we have

$$\begin{aligned}B_1(k) &= Q_1 - Q_1\left(M(k)+Q_1\right)^{-1} Q_1 \\ &= Q_1 - Q_1\left(D_0 - k^2 D_0 M_{2,0} D_0 - k^2\eta^{-1} D_0 M_{2,-1} D_0 - k^2\eta^{-1}\tilde{R}_2(k)\right) \\ &= k^2 Q_1 M_{2,0} Q_1 + k^2\eta^{-1} Q_1 M_{2,-1} Q_1 + k^2\eta^{-1} Q_1 \tilde{R}_2(k) Q_1 \\ &= (k^2 c_1 + k^2\eta^{-1} c_2 + k^4\eta^{-1}\tilde{c}_3(k)) Q_1.\end{aligned}$$

We compute the inverse as $B_1(k)^{-1} = \left(k^2 c_1 + k^2\eta^{-1} c_2 + k^4\eta^{-1}\tilde{c}_3(k)\right)^{-1} Q_1$, as claimed. ☐

We can now use Lemma 3.1.1 to compute the inverse of $M(k)$. We define a recurring function of k to ease the rather involved calculations,

$$g_1(k) = \left(c_1 + \eta^{-1}c_2 + k^2\eta^{-1}\tilde{c}_3(k)\right)^{-1}.$$

We will use the formula

$$M(k)^{-1} = (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}.$$

Note that the first term in this expansion has already been obtained in Lemma 3.2.28.

Theorem 3.2.31. *Suppose that $n=4$ and V satisfies Assumption 3.2.22, and that zero is an exceptional point of the first kind. Then for sufficiently small k we have the expansion*

$$\begin{aligned} M(k)^{-1} = {} & k^{-2}g_1(k)Q_1 + D_0 - g_1(k)(D_0M_{2,0}Q_1 + Q_1M_{2,0}D_0) \\ & - \eta^{-1}g_1(k)(D_0M_{2,-1}Q_1 + Q_1M_{2,-1}D_0) + k^2\tilde{R}_4(k), \end{aligned}$$

where $\tilde{R}_4(k)$ is uniformly bounded in k and $D_0 = (M_{0,0}+Q_1)^{-1}$.

Proof. Lemma 3.1.1 gives us that

$$\begin{aligned} M(k)^{-1} &= (M(k)+Q_1)^{-1} + (M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} \\ &= (M(k)+Q_1)^{-1} + g(k)(M(k)+Q_1)^{-1}Q_1(M(k)+Q_1)^{-1}. \end{aligned}$$

To handle the second term we make, using Lemma 3.2.28 the computations

$$\begin{aligned} (M(k)+Q_1)^{-1}Q_1 &= \left(D_0 - k^2D_0M_{2,0}D_0 - k^2\eta^{-1}D_0M_{2,-1}D_0 - k^2\eta^{-1}\tilde{R}_2(k)\right)Q_1 \\ &= Q_1 - k^2D_0M_{2,0}Q_1 - k^2\eta^{-1}D_0M_{2,-1}Q_1 - k^2\eta^{-1}\tilde{R}_2(k)Q_1 \end{aligned}$$

and

$$\begin{aligned} Q_1(M(k)+Q_1)^{-1} &= Q_1\left(D_0 - k^2D_0M_{2,0}D_0 - k^2\eta^{-1}D_0M_{2,-1}D_0 - k^2\eta^{-1}\tilde{R}_2(k)\right) \\ &= Q_1 - k^2Q_1M_{2,0}D_0 - k^2\eta^{-1}Q_1M_{2,-1}D_0 - k^2\eta^{-1}Q_1\tilde{R}_2(k). \end{aligned}$$

We thus make the computation

$$\begin{aligned} & g_1(k)(M(k)+Q_1)^{-1}Q_1(M(k)+Q_1)^{-1} \\ &= g_1(k)\left(Q_1 - k^2D_0M_{2,0}Q_1 - k^2\eta^{-1}D_0M_{2,-1}Q_1 - k^2\eta^{-1}\tilde{R}_2(k)Q_1\right) \\ &\quad \times \left(Q_1 - k^2Q_1M_{2,0}D_0 - k^2\eta^{-1}Q_1M_{2,-1}D_0 - k^2\eta^{-1}Q_1\tilde{R}_2(k)\right) \\ &= g_1(k)\big(Q_1 - k^2Q_1M_{2,0}D_0 - k^2D_0M_{2,0}Q_1 - k^2\eta^{-1}(D_0M_{2,-1}Q_1 + Q_1M_{2,-1}D_0) + \tilde{R}_3(k), \end{aligned}$$

where $\tilde{R}_3(k)$ is uniformly bounded in k. So we find the inverse of $M(k)$ as

$$\begin{aligned}
M(k)^{-1} &= (M(k)+Q_1)^{-1} + k^{-2}g_1(k)(M(k)+Q_1)^{-1}Q_1(M(k)+Q_1)^{-1} \\
&= D_0 - k^2 D_0 M_{2,0} D_0 - k^2\eta^{-1} D_0 M_{2,-1} D_0 - k^2\eta^{-1}\tilde{R}_2(k) \\
&\quad + g_1(k)\big(Q_1 - k^2 Q_1 M_{2,0} D_0 - k^2 D_0 M_{2,0} Q_1 - k^2\eta^{-1}\tilde{R}_3(k)\big) \\
&= g_1(k)Q_1 + D_0 - k^2 g_1(k)(Q_1 M_{2,0} D_0 + D_0 M_{2,0} Q_1) + k^2\eta^{-1}\tilde{R}_4(k) \\
&= g_1(k)Q_1 + D_0 - c_2^{-1}(Q_1 M_{2,0} D_0 + D_0 M_{2,0} Q_1) \\
&\quad + k^2\eta^{-1}(D_0 M_{2,-1} Q_1 + Q_1 M_{2,-1} D_0) + k^4\tilde{R}_4(k)
\end{aligned}$$

where $\tilde{R}_4(k)$ is uniformly bounded in k. □

The nature of the singularity in the case of exceptional points of the second and third kind requires a little more care to handle, although is not significantly worse. We will need to use the extra terms in the expansion of $(M(k)+Q_1)^{-1}$ in Remark 3.2.29. If there is an exceptional point of the second kind for H then the operator $Q_1 M_{2,-1} Q_1$ is not invertible on $Q_1\mathcal{H}$ and we define Q_2 to be the orthogonal projection onto the kernel of $Q_1 M_{2,-1} Q_1$. Then the operator $Q_1 M_{2,-1} Q_1 + Q_2$ is invertible on $Q_2\mathcal{H}$.

Lemma 3.2.32. *[62, Lemma 7.4] Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Then the operator $Q_2 M_{2,0} Q_2$ is invertible on $Q_2\mathcal{H}$.*

Proof. Suppose that $f \in Q_2\mathcal{H}$ is such that $Q_2 M_{2,0} Q_2 f = 0$. Then $\langle G_{2,0} vf, vf\rangle = 0$. Note also that $vf \in L^1(\mathbb{R}^n)$ and $x \mapsto |x| vf \in L^1(\mathbb{R}^n)$, so that $\mathcal{F}(vf) \in L^1(\mathbb{R}^n)\cap C^1(\mathbb{R}^n)$. Using that $Pf = 0$ for $f \in Q_2\mathcal{H}$ we have the limits

$$\begin{aligned}
\langle G_{2,0} vf, vf\rangle &= \lim_{k\to 0}\big\langle k^{-2}(R_0(k^2) - G_0)vf, vf\big\rangle = \lim_{k\to 0}\big\langle k^{-2}(R_0(k^2) - G_0)vf, vf\big\rangle \\
&= \lim_{k\to 0}\int_{\mathbb{R}^4}\big(|\xi|^{-2} - (|\xi|^2+k^2)^{-1}\big)\,[\mathcal{F}(vf)](\xi)\overline{[\mathcal{F}(vf)](\xi)}\,\mathrm{d}\xi \\
&= \lim_{k\to 0}\int_{\mathbb{R}^4}\frac{|[\mathcal{F}(vf)](\xi)|^2}{|\xi|^2(|\xi|^2+k^2)}\,\mathrm{d}\xi = \int_{\mathbb{R}^4}|\xi|^{-4}|[\mathcal{F}(vf)](\xi)|^2\,\mathrm{d}\xi \\
&= \langle G_{0,0} vf, G_{0,0} vf\rangle,
\end{aligned}$$

where we have used Lemma 3.1.6 to bring the limit inside the integral. Since f satisfies $Q_2 M_{2,0} Q_2 f = 0$, we find $\langle G_{2,0} vf, vf = 0$. Thus $\mathcal{F}(vf) = 0$ and so $vf = 0$, which implies that $\operatorname{Ker}(Q_2 v G_{2,0} v Q_2) = \{0\}$. □

If zero is an exceptional point of the second kind, we have $Q_1 = Q_2$ and so we can define $D_2 = (Q_1 M_{2,0} Q_1)^{-1}$ as an operator on $Q_1\mathcal{H} = Q_2\mathcal{H}$. The operator D_2 satisfies the relation $D_2 = Q_1 D_2 Q_1$ and is thus Hilbert-Schmidt.

Theorem 3.2.33. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22 and that zero is an exceptional point of the second kind. Then for sufficiently small k we have the*

expansion

$$M(k)^{-1} = k^{-2}Q_1D_2Q_1 - \eta^{-1}Q_1D_2Q_1M_{4,-1}Q_1D_2Q_1 + \tilde{R}_7(k),$$

where $\tilde{R}_7(k)$ *is uniformly bounded in* k *and* K *is bounded and* $D_2 = (Q_1M_{2,0}Q_1)^{-1}$.

Proof. We have the identity $Q_2M_{2,-1} = Q_2P = PQ_2 = M_{2,-1}Q_2 = 0$, since for any $f \in Q_2\mathcal{H}$ we have

$$0 = \langle Q_1PQ_1f, f\rangle = \langle Pf, Pf\rangle = ||Pf||^2 .$$

Then we can compute using the expansion in Remark 3.2.29 the relation

$$\begin{aligned}
&Q_1(M(k) + Q_1)^{-1}Q_1\\
&= Q_1 - k^2Q_1M_{2,0}Q_1 - k^2\eta^{-1}Q_1M_{2,-1}Q_1 - k^4Q_1M_{4,0}Q_1\\
&\quad - k^4\eta^{-1}Q_1M_{4,-1}Q_1 + k^4Q_1M_{2,0}D_0M_{2,0}Q_1\\
&\quad + k^4\eta^{-1}(Q_1M_{2,0}D_0M_{2,-1}Q_1 + Q_1M_{2,-1}D_0M_{2,0}Q_1) + k^4\eta^{-2}Q_1M_{2,-1}Q_1M_{2,-1}Q_1\\
&- k^6\eta^{-1}Q_1\tilde{R}_2'(k)Q_1\\
&= Q_1 - k^2Q_1M_{2,0}Q_1 - k^4Q_1M_{4,0}Q_1 - k^4\eta^{-1}Q_1M_{4,-1}Q_1 + k^4Q_1M_{2,0}D_0M_{2,0}Q_1\\
&\quad - k^6\eta^{-1}Q_1\tilde{R}_2'(k)Q_1.
\end{aligned}$$

Note that we have used several times the relations $Q_1 = Q_2$ and $Q_2P = PQ_2 = 0$. Thus we can write $B_1(k)$ as

$$\begin{aligned}
B_1(k) &= Q_1 - Q_1(M(k) + Q_1)^{-1}Q_1\\
&= k^2Q_1M_{2,0}Q_1 + k^4Q_1M_{4,0}Q_1 + k^4\eta^{-1}Q_1M_{4,-1}Q_1 - k^4Q_1M_{2,0}D_0M_{2,0}Q_1\\
&\quad + k^6\eta^{-1}Q_1\tilde{R}_2'(k)Q_1.
\end{aligned}$$

Since each of the operators involved is bounded, we have for sufficiently small k the estimate

$$\left|\left|k^2Q_1\left(M_{4,0}Q_1D_2 + \eta^{-1}M_{4,-1}Q_1D_2 - M_{2,0}D_0M_{2,0}Q_1D_2 + k^2\eta^{-1}\tilde{R}_2'(k)Q_1D_2\right)\right|\right| < 1.$$

Thus we can use a Neumann expansion to determine the inverse of $B(k)$ as

$$\begin{aligned}B_1(k)^{-1} &= k^{-2}\big(Q_1M_{2,0}Q_1 + k^2Q_1M_{4,0}Q_1 + k^2\eta^{-1}Q_1M_{4,-1}Q_1 - k^2Q_1M_{2,0}D_0M_{2,0}Q_1\\ &\quad + k^4\eta^{-1}Q_1\tilde{R}_2'(k)Q_1\big)^{-1}\\ &= k^{-2}D_2\big(\mathrm{Id} + k^2Q_1M_{4,0}Q_1D_2 + k^2\eta^{-1}Q_1M_{4,-1}Q_1D_2 - k^2Q_1M_{2,0}D_0M_{2,0}Q_1D_2\\ &\quad + k^4\eta^{-1}Q_1\tilde{R}_2'(k)Q_1D_2\big)^{-1}\\ &= k^{-2}D_2\big(\mathrm{Id} - k^2Q_1M_{4,0}Q_1D_2 - k^2\eta^{-1}Q_1M_{4,-1}Q_1D_2 + k^2Q_1M_{2,0}D_0M_{2,0}Q_1D_2\\ &\quad - k^4\eta^{-1}Q_1\tilde{R}_2'(k)Q_1D_2 + k^4\tilde{R}_4(k)\big)^{-1}\\ &= k^{-2}D_2 - D_2Q_1M_{4,0}Q_1D_2 - \eta^{-1}D_2Q_2M_{4,-1}Q_1D_2 + Q_1M_{2,0}D_0M_{2,0}Q_1D_2\\ &\quad - k^2\eta^{-1}\tilde{R}_5(k),\end{aligned}$$

where $\tilde{R}_4(k)$ and $\tilde{R}_5(k)$ are uniformly bounded in k. We can compute using Remark 3.2.29 that

$$\begin{aligned}(M(k)+Q_1)^{-1}Q_1 &= Q_1 - k^2D_0M_{2,0}Q_1 - k^2\eta^{-1}D_0M_{2,-1}Q_1 - k^4D_0M_{4,0}Q_1\\ &\quad - k^4\eta^{-1}D_0M_{4,-1}Q_1 + k^4D_0M_{2,0}D_0M_{2,0}Q_1 + k^4\eta^{-1}(D_0M_{2,0}D_0M_{2,-1}Q_1\\ &\quad + D_0M_{2,-1}D_0M_{2,0}Q_1) + k^4\eta^{-2}D_0M_{2,-1}D_0M_{2,-1}Q_1 - k^6\eta^{-1}\tilde{R}_2'(k)Q_1\\ &= Q_1 - k^2D_0M_{2,0}Q_1 - k^4D_0M_{4,0}Q_1 - k^4\eta^{-1}D_0M_{4,-1}Q_1\\ &\quad + k^4D_0M_{2,0}D_0M_{2,0}Q_1 + k^4\eta^{-1}D_0M_{2,-1}D_0M_{2,0}Q_1 - k^6\eta^{-1}\tilde{R}_2'(k)Q_1\end{aligned}$$

and similarly

$$\begin{aligned}Q_1(M(k)+Q_1)^{-1} &= Q_1 - k^2Q_1M_{2,0}D_0 - k^2\eta^{-1}Q_1M_{2,-1}D_0 - k^4Q_1M_{4,0}D_0\\ &\quad - k^4\eta^{-1}Q_1M_{4,-1}D_0 + k^4Q_1M_{2,0}D_0M_{2,0}D_0 + k^4\eta^{-1}(Q_1M_{2,0}D_0M_{2,-1}D_0\\ &\quad + Q_1M_{2,-1}D_0M_{2,0}D_0) + k^4\eta^{-2}Q_1M_{2,-1}D_0M_{2,-1}D_0 - k^6\eta^{-1}Q_1\tilde{R}_2'(k)\\ &= Q_1 - k^2Q_1M_{2,0}D_0 - k^4Q_1M_{4,0}D_0 - k^4\eta^{-1}Q_1M_{4,-1}D_0\\ &\quad + k^4Q_1M_{2,0}D_0M_{2,0}D_0 + k^4\eta^{-1}Q_1M_{2,0}D_0M_{2,-1}D_0 - k^6\eta^{-1}Q_1\tilde{R}_2'(k).\end{aligned}$$

We can then make the computation

$$\begin{aligned}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} &= k^{-2}Q_1D_2Q_1 - \eta^{-1}Q_1D_2Q_1M_{4,-1}Q_1D_2Q_1\\ - Q_1D_2Q_1M_{4,0}Q_1D_2Q_1 - D_0M_{2,0}Q_1D_2Q_1 - Q_1D_2Q_1M_{2,0}D_1 + k^2\tilde{R}_6(k)\end{aligned}$$

where $\tilde{R}_6(k)$ is uniformly bounded in k. Applying Lemma 3.1.1 then gives

$$M(k)^{-1} = D_0 + k^{-2}Q_1D_2Q_1 - \eta^{-1}Q_1D_2Q_1M_{4,-1}Q_1D_2Q_1 + \tilde{R}_7(k),$$

where $\tilde{R}_7(k)$ is uniformly bounded in k. □

We now proceed to the case of an exceptional point of the third kind, which covers the simultaneous existence of a resonance and a zero eigenvalue for H.

Definition 3.2.34. Suppose that $n = 4$ and V satisfies Assumption 3.2.22. We define the operator $T_1 = Q_1 - Q_2$ acting on $Q_1\mathcal{H}$ and decompose $Q_1\mathcal{H} = T_1\mathcal{H} \oplus Q_2\mathcal{H}$. Let $D_2 = (Q_2 M_{2,0} Q_2)^{-1}$. We further define on $Q_1\mathcal{H}$ the related operator

$$\tilde{T}_1 = \begin{pmatrix} T_1 & -T_1 M_{2,0} D_2 \\ -D_2 M_{2,0} T_1 & D_2 M_{2,0} T_1 M_{2,0} D_2 \end{pmatrix}. \tag{3.29}$$

Lemma 3.2.35. *Suppose that V satisfies Assumption 3.2.22 and that zero is an exceptional point of the third kind for H. Then the operator $\tilde{T}_1$ defined by Equation* (3.29) *is a finite rank operator.*

Proof. Since $Q_1 \geq Q_2$ by Corollary 3.2.27 we have that $Q_1 - Q_2 = T_1$ is a rank one operator, which implies $\tilde{T}_1$ is a finite rank operator. □

Since the operator T_1 is rank one, there exists constants $d_1, d_2, d_3 \in \mathbb{C}$ such that $T_1 M_{4,0} T_1 = d_1 T_1$, $T_1 M_{2,-1} T_1 = d_2 T_1$ and $T_1 M_{2,0} D_2 M_{2,0} T_1 = d_3 T_1$. Then for sufficiently small k we may define the function $h : F \to \mathbb{C}$ by

$$h(k) = (d_1 + \eta^{-1} d_2 - d_3)^{-1}.$$

Lemma 3.2.36. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22 and that zero is an exceptional point of the third kind for H. Then there exist bounded operators A, B, C such that for sufficiently small k and with $\tilde{T}_1$ is as in Definition 3.2.34 we have the expansion*

$$\begin{aligned} B_1(k)^{-1} &= k^{-2} h(k) \tilde{T}_1 + k^{-2} D_2 - h(k) \tilde{T}_1 A \tilde{T}_1 - D_2 A D_2 \\ &\quad - \eta^{-1} h(k) \tilde{T}_1 B \tilde{T}_1 - \eta^{-2} h(k) \tilde{T}_1 C T_1 + k^6 \eta^{-1} \tilde{R}_9(k) \end{aligned}$$

where $D_2 = (Q_2 M_{2,0} Q_2)^{-1}$ and $\tilde{R}_9(k)$ is uniformly bounded in k.

Proof. Note that $Q_2 P = P Q_2 = 0$ so that we can write in the direct sum decomposition the equality

$$\begin{aligned} B_1(k) &= k^2 Q_1 M_{2,0} Q_1 + k^2 \eta^{-1} Q_1 M_{2,-1} Q_1 + k^4 Q_1 M_{4,0} Q_1 + k^4 \eta^{-1} Q_1 M_{4,-1} Q_1 \\ &\quad + k^4 \eta^{-1} Q_1 \tilde{R}_2'(k) Q_1 \\ &= k^2 \begin{pmatrix} T_1 M_{2,0} T_1 + \eta^{-1} T_1 M_{2,-1} T_1 & T_1 M_{2,0} Q_2 \\ Q_2 M_{2,0} T_1 & Q_2 M_{2,0} Q_2 \end{pmatrix} + k^4 A + k^4 \eta^{-1} B + k^4 \eta^{-2} C \\ &\quad + k^6 \eta^{-1} \tilde{R}_8(k) \\ &:= B_0(k) + k^4 A + k^4 \eta^{-1} B + k^4 \eta^{-2} C + k^6 \eta^{-1} \tilde{R}_8(k). \end{aligned}$$

Here we have defined the coefficient operators

$$\begin{aligned}
A &= Q_1 M_{4,0} Q_1 - Q_1 M_{2,0} D_0 M_{2,0} Q_1, \\
B &= Q_1 M_{2,-1} Q_1 - Q_1 M_{2,0} D_0 M_{2,-1} Q_1 - Q_1 M_{2,-1} D_0 M_{2,0} Q_1, \\
C &= -Q_1 M_{2,-1} D_0 M_{2,-1} Q_1.
\end{aligned}$$

Lemma 3.1.3 tells us that the invertibility of $B_0(k)$ depends on the invertibility of the operator $Q_2 M_{2,0} Q_2$ (which is guaranteed by Lemma 3.2.32) and the invertibility of

$$a(k) = T_1 M_{2,0} T_1 + \eta^{-1} T_1 M_{2,-1} T_1 - T_1 M_{2,0} D_2 M_{2,0} T_1 = h(k)^{-1} T_1.$$

Thus we find $a(k)^{-1} = h(k) T_1$ and the inverse of $B_0(k)$ is given by

$$B_0(k)^{-1} = k^{-2} h(k) \begin{pmatrix} T_1 & -T_1 M_{2,0} D_2 \\ -D_2 M_{2,0} T_1 & D_2 M_{2,0} T_1 M_{2,0} D_2 \end{pmatrix} + k^{-2} D_2.$$

Then for sufficiently small k we can thus invert $B_1(k)$ via a Neumann expansion to obtain

$$\begin{aligned}
B_1(k)^{-1} &= (B_0(k) + k^4 A + k^4 \eta^{-1} B + k^4 \eta^{-2} C + k^6 \eta^{-1} \tilde{R}_8(k))^{-1} \\
&= B_0(k)^{-1} (\mathrm{Id} + k^4 A B_0(k)^{-1} + k^4 \eta^{-1} B B_0(k)^{-1} + k^4 \eta^{-2} C B_0(k)^{-1} \\
&\quad + k^6 \eta^{-1} \tilde{R}_8(k) B_0(k)^{-1})^{-1} \\
&= B_0(k)^{-1} - k^4 B_0(k)^{-1} A B_0(k)^{-1} - k^4 \eta^{-1} B_0(k)^{-1} B B_0(k)^{-1} \\
&\quad - k^4 \eta^{-2} B_0(k)^{-1} C B_0(k)^{-1} + k^6 \eta^{-1} \tilde{R}_9(k) \\
&= k^{-2} h(k) \begin{pmatrix} T_1 & -T_1 M_{2,0} D_2 \\ -D_2 M_{2,0} T_1 & D_2 M_{2,0} T_1 M_{2,0} D_2 \end{pmatrix} + k^{-2} D_2 - k^4 B_0(k)^{-1} A B_0(k)^{-1} \\
&\quad - k^4 \eta^{-1} B_0(k)^{-1} B B_0(k)^{-1} - k^4 \eta^{-2} B_0(k)^{-1} C B_0(k)^{-1} + k^6 \eta^{-1} \tilde{R}_9(k) \\
&= k^{-2} h(k) \tilde{T}_1 + k^{-2} D_2 - k^4 B_0(k)^{-1} A B_0(k)^{-1} \\
&\quad - k^4 \eta^{-1} B_0(k)^{-1} B B_0(k)^{-1} - k^4 \eta^{-2} B_0(k)^{-1} C B_0(k)^{-1}) + k^6 \eta^{-1} \tilde{R}_9(k),
\end{aligned}$$

where $\tilde{R}_9(k)$ is uniformly bounded in k. Expanding out the $B_0(k)^{-1}$ terms we obtain

$$\begin{aligned}
B_1(k)^{-1} &= k^{-2} h(k) \tilde{T}_1 + k^{-2} D_2 - h(k) \tilde{T}_1 A \tilde{T}_1 - D_2 A D_2 \\
&\quad - \eta^{-1} h(k) \tilde{T}_1 B \tilde{T}_1 - \eta^{-1} D_2 B D_2 - \eta^{-2} h(k) \tilde{T}_1 C \tilde{T}_1 - \eta^{-2} D_2 C D_2 + k^6 \eta^{-1} \tilde{R}_9(k).
\end{aligned}$$

Noting that $D_2 Q_2 = Q_2 D_2 = D_2$ and $Q_2 M_{2,-1} = M_{2,-1} Q_2 = 0$ we can further simplify to the expression

$$\begin{aligned}
B_1(k)^{-1} &= k^{-2} h(k) \tilde{T}_1 + k^{-2} D_2 - h(k) \tilde{T}_1 A \tilde{T}_1 - D_2 A D_2 \\
&\quad - \eta^{-1} h(k) \tilde{T}_1 B \tilde{T}_1 - \eta^{-2} h(k) \tilde{T}_1 C \tilde{T}_1 + k^6 \eta^{-1} \tilde{R}_9(k),
\end{aligned}$$

as claimed. □

We are now finally ready to invert $M(k)$ in the case of an exceptional point of the third kind.

Theorem 3.2.37. *Suppose that $n = 4$ and V satisfies Assumption 3.2.22 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have*

$$\begin{aligned}M(k)^{-1} &= k^{-2}Q_1D_2Q_1 + k^{-2}h(k)Q_1\tilde{T}_1Q_1 + h(k)(Q_1D_2Q_1M_{2,0}D_0 + D_0M_{2,0}Q_1D_2Q_1)\\ &\quad + \eta^{-1}h(k)(D_0M_{2,-1}Q_1\tilde{T}_1Q_1 + Q_1\tilde{T}_1Q_1M_{2,-1}D_0 + Q_1\tilde{T}_1BT_1Q_1)\\ &\quad + -\eta^{-1}Q_1D_2Q_1M_{4,-1}Q_1D_2Q_1 + \tilde{R}_{10}(k),\end{aligned}$$

where $\tilde{R}_{10}(k)$ is uniformly bounded in k.

Proof. Lemma 3.1.1 shows that

$$M(k)^{-1} = (M(k) + Q_1)^{-1} + (M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1}.$$

Remark 3.2.29 handles the first term $(M(k) + Q_1)^{-1}$. Using Lemma 3.1.4 we find the relations $Q_1D_0 = D_0Q_1 = Q_1$ and so Remark 3.2.29 allows us to show that

$$\begin{aligned}(M(k) + Q_1)^{-1}Q_1 &= Q_1 - k^2D_0M_{2,0}Q_1 - k^2\eta^{-1}D_0M_{2,-1}Q_1 - k^4D_0M_{4,0}Q_1\\ &\quad - k^4\eta^{-1}D_0M_{4,-1}Q_1 + k^4D_0M_{2,0}D_0M_{2,0}Q_1 + k^4\eta^{-1}(D_0M_{2,0}D_0M_{2,-1}Q_1\\ &\quad + D_0M_{2,-1}D_0M_{2,0}Q_1) + k^4\eta^{-2}D_0M_{2,-1}D_0M_{2,-1}Q_1 - k^6\eta^{-1}\tilde{R}_2'(k)Q_1\end{aligned}$$

and similarly

$$\begin{aligned}Q_1(M(k) + Q_1)^{-1} &= Q_1 - k^2Q_1M_{2,0}D_0 - k^2\eta^{-1}Q_1M_{2,-1}D_0 - k^4Q_1M_{4,0}D_0\\ &\quad - k^4\eta^{-1}Q_1M_{4,-1}D_0 + k^4Q_1M_{2,0}D_0M_{2,0}D_0 + k^4\eta^{-1}(Q_1M_{2,0}D_0M_{2,-1}D_0\\ &\quad + Q_1M_{2,-1}D_0M_{2,0}D_0) + k^4\eta^{-2}Q_1M_{2,-1}D_0M_{2,-1}D_0 - k^6\eta^{-1}Q_1\tilde{R}_2'(k).\end{aligned}$$

Note that unlike in Theorem 3.2.33 many terms do not vanish. We use Lemma 3.2.36 to expand out

$$\begin{aligned}&(M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1}\\ &= k^{-2}Q_1D_2Q_1 + k^{-2}h(k)Q_1\tilde{T}_1Q_1 + h(k)(Q_1D_2Q_1M_{2,0}D_0 + D_0M_{2,0}Q_1D_2Q_1)\\ &\quad + \eta^{-1}(D_0M_{2,-1}Q_1D_2Q_1 + Q_1D_2Q_1M_{2,-1}D_0) + \eta^{-1}h(k)(D_0M_{2,-1}Q_1\tilde{T}_1Q_1\\ &\quad + Q_1\tilde{T}_1Q_1M_{2,-1}D_0 + Q_1\tilde{T}_1B\tilde{T}_1Q_1) + \tilde{R}_{10}(k),\end{aligned}$$

where $\tilde{R}_{10}(k)$ is uniformly bounded in k. The relations $D_2Q_1P = D_2Q_2P = 0$ combined with the observation that all terms in the expansion of $(M(k) + Q_1)^{-1}$ are uniformly bounded in k gives the statement of the theorem. □

The above calculations lead us to a natural definition of resonances.

Definition 3.2.38. Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Then if $Q_2 \neq Q_1 \neq 0$ we fix $\varphi \in Q_1\mathcal{H} \ominus Q_2\mathcal{H}$ and note that by Lemma 3.2.25 there exists $\psi \in H^{0,-t}$ (for some $t > 0$) such that $\varphi = Uv\psi$. We say that ψ is a zero energy resonance for H. We define a normalised resonance ψ by the condition

$$||v\psi||_1 = (4\pi)^{-1}.$$

We note that the definition of resonance here differs slightly from that of [87, p. 405], although the two are equivalent. The following characterisation of the zero eigenspace is implicit in [87] and can be found as [62, Lemma 7.5].

Lemma 3.2.39. *[62, Lemma 7.5] Suppose that $n = 4$ and V satisfies Assumption 3.2.22. Then the projection P_0 onto the eigenspace at zero is given by $G_{0,0}vQ_2D_2Q_2vG_{0,0}$.*

Proof. Let $(\varphi_j)_{j=1}^{N_0}$ be an orthonormal basis for $Q_2\mathcal{H}$. Then by the definition of Q_1 and the fact $Q_2 \leq Q_1$ we have

$$0 = U(U + vG_{0,0}v)\varphi_j = (\mathrm{Id} + UvG_{0,0}v)\varphi_j = \psi_j + UvG_{0,0}v\varphi_j.$$

Letting $\psi_j = -G_{0,0}v\varphi_j$ we see that the ψ_j are linearly independent and that $\varphi_j = Uv\psi_j$. Thus for any $f \in \mathcal{H}$ we have

$$Q_2vG_{0,0}f = \sum_{j=1}^{N_0} \langle Q_2vG_{0,0}f, \varphi_j\rangle\varphi_j = \sum_{j=1}^{N_0} \langle f, G_{0,0}v\varphi_j\rangle\varphi_j = -\sum_{j=1}^{N_0} \langle f, \psi_j\rangle\varphi_j.$$

Let (A_{ij}) be the matrix representation of the operator $Q_2M_{4,-1}Q_2$. Then we find

$$A_{ij} = \langle \varphi_i, Q_2M_{4,-1}Q_2\varphi_j\rangle = \langle G_{0,0}v\varphi_i, G_{0,0}v\varphi_j\rangle = \langle G_{0,0}V\psi_i, G_{0,0}V\psi_j\rangle = \langle \psi_i, \psi_j\rangle.$$

Then for $f \in \mathcal{H}$ we have

$$\begin{aligned} G_{0,0}vQ_2D_2Q_2vG_{0,0}f &= -\left(\sum_{j=1}^{N_0} \langle f, \psi_j\rangle G_{0,0}vQ_2D_2Q_2\varphi_j\right) = -\sum_{i,j=1}^{N_0} G_{0,0}vQ_2(A_{ij}^{-1})\varphi_i\langle f, \psi_j\rangle \\ &= -\sum_{i,j=1}^{N_0} G_{0,0}v(A_{ij}^{-1})\varphi_i\langle f, \psi_j\rangle = \sum_{i,j=1}^{N_0} (A_{ij}^{-1})\psi_i\langle f, \psi_j\rangle. \end{aligned}$$

In particular for $f = \psi_m$ we find $G_{0,0}vQ_2D_2Q_2vG_{0,0}\psi_m = \psi_m$. So $G_{0,0}vQ_2D_2Q_2vG_{0,0}$ is the identity on $\mathrm{span}(\psi_j)_{j=1}^{N_0}$ and is the identity on $Q_2\mathcal{H}$ and is thus the projection onto the zero eigenspace of H. □

We conclude this section by determining a low energy expansion of the resolvent $R(-k^2)$.

Theorem 3.2.40. *Suppose $n = 4$ and V satisfies Assumption 3.2.22. Then for sufficiently small k we have*

$$R(-k^2) - R_0(-k^2) = -k^{-2}P_0 - k^{-2}h(k)G_{0,0}vQ_1\tilde{T}_1Q_1vG_{0,0} \\ + \eta^{-1}(G_{0,0}v\eta^{-1}Q_1D_2Q_1M_{4,-1}Q_1D_2Q_1vG_{0,0}) + \tilde{R}(k),$$

where $\tilde{R}(k)$ is uniformly bounded in k.

Proof. We begin with the relation

$$R(-k^2) - R_0(-k^2) = -R_0(-k^2)vM(k)^{-1}vR_0(-k^2).$$

Multiplying the expansion of $R_0(-k^2)$ in Equation (3.21) with the expansion of $M(k)^{-1}$ found in Theorem 3.2.37 yields the result immediately. □

3.2.4 Dimension $n = 3$

In this section we demonstrate the expansion of the operator $M(k)^{-1}$ near $k = 0$ in dimension $n = 3$ and use this to define a zero-energy resonance. The results of this section are a straightforward application of the results of [89]. Such expansions have been considered in a different context in [64] and first appeared in a non-symmetrised form in [88].

The assumption on the potential required in this section is the following.

Assumption 3.2.41. Suppose that $n = 3$. We assume that V satisfies Assumption 2.2.14 for some $\rho > 5$.

In dimension $n = 3$ Equation (3.12) reads

$$R_0(x, y, -k^2) = |x-y|^{-1}\sum_{p=0}^{\infty} c_{3,p}k^p|x-y|^p. \tag{3.30}$$

The above expansion leads to the following operator definitions.

Definition 3.2.42. Suppose that $n = 3$ and V satisfies Assumption 3.2.41. We define for $p \in \mathbb{N}$ the integral operators G_j by the kernels

$$G_p(x, y) = (4\pi p!)^{-1}|x-y|^{p-1}$$

and for $p \geq 1$ the integral operators M_p by the kernels

$$M_p(x, y) = i^p v(x)G_p(x, y)v(y).$$

We also define the operator M_0 by the kernel

$$(M_0 - U)(x, y) = v(x)G_0(x, y)v(y).$$

Then from the definition of $M(k)$ we have

$$M(k) = U + vR_0(-k^2)v = M_0 + kM_1 + k^2M_2 + k^3\tilde{R}_0(k),$$

where $\tilde{R}_0(k)$ is uniformly bounded for $k \in F = \{k \in \mathbb{C} : \mathrm{Re}(k) \geq 0 \text{ and } |k| \leq 1\}$.

Lemma 3.2.43. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41. Then for $k \in F$ the operator $M(k) - M_0$ is Hilbert-Schmidt.*

Proof. The operator $M(k) - M_0$ has the kernel

$$(M(k) - M_0)(x, y) = k^{-1}v(x)(4\pi)^{-1}|x - y|^{-1}(\mathrm{e}^{ik|x-y|} - 1)v(y)$$

and thus we have the estimate

$$|(M(k) - M_0)(x, y)| \leq (4\pi)^{-1}|v(x)||v(y)|.$$

Hence we see that $M(k) - M_0 \in \mathcal{L}^2(\mathcal{H})$ provided $|v(x)| \leq C(1 + |x|)^{-\frac{\rho}{2}}$ for some $\rho > 5$, which is our assumption on V. □

We can further define the projection $P : \mathcal{H} \to \mathcal{H}$ by

$$[Pf](x) = ||v||_2^{-2}\, v(x) \int_{\mathbb{R}^3} v(y)f(y)\, \mathrm{d}y = ||v||_2^{-2}\, \langle v, f\rangle v(x).$$

The projection P is related to M_1 by the formula $M_1 = i(4\pi)^{-1}\, ||v||_2^2\, P$.

Note that M_0 is a compact self-adjoint perturbation of U and thus has essential spectrum $\sigma_{ess}(M_0) \subset \{-1, 1\}$. So 0 is an isolated point of the spectrum of M_0 and $\mathrm{Dim}(\mathrm{Ker}(M_0)) < \infty$. These considerations lead us to the following definition.

Definition 3.2.44. Suppose that $n = 3$ and V satisfies Assumption 3.2.41. We say that zero is a *regular point of the spectrum of H* if the operator M_0 is invertible. If zero is not a regular point of the spectrum of H, we define Q_1 to be the orthogonal projection onto the kernel of M_0. Then $M_0 + Q_1$ is invertible and we can define $D_0 = (M_0 + Q)^{-1}$. We say there is an *exceptional point of the first kind* if $Q_1M_1Q_1$ is invertible on $Q_1\mathcal{H}$. If $Q_1M_1Q_1$ is not invertible, we define Q_2 to be the orthogonal projection onto the kernel of $Q_1M_1Q_1$ (as an operator on $Q_1\mathcal{H}$). Then $Q_1M_1Q_1 + Q_2$ is invertible (with inverse defined to be D_1) on $Q_1\mathcal{H}$. If $Q_1 = Q_2$ we say there is an *exceptional point of the second kind*. Otherwise, we say there is an *exceptional point of the third kind*.

We will show $Q_2 \neq 0$ (an exceptional point of the second kind) corresponds to the existence of an eigenvalue at zero whilst $Q_1 \neq 0$ corresponds to the existence of a resonance in dimension $n = 3$. By definition, the projections Q_1 and Q_2 are finite rank operators and $Q_2 \leq Q_1$. The following expansion will be used in each exceptional case.

Lemma 3.2.45. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is not a regular point of the spectrum of H. Then for sufficiently small k we have the expansion*

$$(M(k) + Q_1)^{-1} = D_0 - kD_0M_1D_0 - k^2D_0M_2D_0 + k^2D_0M_1D_0M_1D_0 + k^3\tilde{R}_1(k)$$

where $\tilde{R}_1(k)$ is uniformly bounded in k and $D_0 = (M_0 + Q_1)^{-1}$.

Proof. For sufficiently small k we have the estimate

$$\left|\left|kM_1D_0 + k^2M_2D_0 + k^3\tilde{R}_0(k)D_0\right|\right| < 1,$$

since each of the operators is bounded. We are thus able to factor and use a Neumann expansion to find

$$\begin{aligned}
&(M(k) + Q_1)^{-1} = \left(M_0 + kM_1 + k^2M_2 + k^3\tilde{R}_0(k) + Q_1\right)^{-1} \\
&= D_0\left(\mathrm{Id} + kM_1D_0 + k^2M_2D_0 + k^3\tilde{R}_0(k)D_0\right)^{-1} \\
&= D_0\left(\mathrm{Id} - kM_1D_0 - k^2M_2D_0 - k^3\tilde{R}_0(k)D_0 + \sum_{j=2}^{\infty}(-1)^j((M(k) - M_0)D_0)^j\right) \\
&= D_0 - kD_0M_1D_0 - k^2D_0M_2D_0 - k^3D_0\tilde{R}_0(k)D_0 + \sum_{j=2}^{\infty}(-1)^jD_0((M(k) - M_0)D_0)^j
\end{aligned}$$

Computing the lowest order term in the sum as $k^2D_0M_1D_0M_1D_0$ and defining

$$\tilde{R}_1(k) = -D_0M_1D_0M_1D_0 - kD_0\tilde{R}_0(k)D_0 + k^{-2}\sum_{j=2}^{\infty}(-1)^jD_0((M(k) - M_0)D_0)^j$$

completes the proof. □

Remark 3.2.46. We can further compute the lowest order terms in $\tilde{R}_1(k)$ to obtain

$$\tilde{R}_1(k) = -D_0M_1D_0M_1D_0 - k(D_0M_3D_0 + D_0M_1D_0M_1D_0M_1D_0) + k^2\tilde{R}(k).$$

Corollary 3.1.2 shows that $M(k)$ is invertible if and only if the operator

$$B_1(k) = k^{-1}\left(Q_1 - Q_1(M(k) + Q_1)^{-1}Q_1\right) \tag{3.31}$$

is invertible on $Q_1\mathcal{H}$ and in this case

$$M(k)^{-1} = (M(k)+Q_1)^{-1} + k^{-1}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}.$$

So we now investigate the invertibility of the operator $B_1(k)$ for sufficiently small k.

Lemma 3.2.47. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the first kind for H. Then for sufficiently small k we have the expansion*

$$B_1(k) = Q_1M_1Q_1 + kQ_1M_2Q_1 - kQ_1M_1D_0M_1Q_1 - k^2Q_1\tilde{R}_1(k)Q_1.$$

Proof. We substitute the result of Lemma 3.2.45 into the definition of $B_1(k)$ in Equation (3.31) to obtain

$$\begin{aligned}
kB_1(k) &= Q_1 - Q_1(M(k)+Q_1)^{-1}Q_1 \\
&= Q_1 - Q_1\left(D_0 - kD_0M_1D_0 - k^2D_0M_2D_0 + k^2D_0M_1D_0M_1D_0 + k^3\tilde{R}_1(k)\right)Q_1 \\
&= Q_1 - Q_1D_0Q_1 + kQ_1D_0M_1D_0Q_1 + k^2Q_1D_0M_2D_0Q_1 \\
&\quad - k^2Q_1M_1D_0M_1Q_1 - k^3Q_1\tilde{R}_1(k)Q_1 \\
&= kQ_1M_1Q_1 + k^2Q_1M_2Q_1 - k^2Q_1M_1D_0M_1Q_1 - k^3Q_1\tilde{R}_1(k)Q_1,
\end{aligned}$$

where we have used Lemma 3.1.4 several times. □

If the term $Q_1M_1Q_1$ is invertible (there is an exceptional point of the first kind) then we can invert $B_1(k)$ for small k using a Neumann series and thus obtain an expansion for $M(k)^{-1}$ also. Since the operator $Q_1M_1Q_1$ has rank one, this can only occur if $\mathrm{Rank}(Q_1) = 1$. In this case we can define the operator $D_1 = (Q_1M_1Q_1)^{-1}$. The result is the following.

Lemma 3.2.48. *Suppose that V satisfies Assumption 3.2.41 and that zero is an exceptional point of the first kind for H. Then for sufficiently small k we have the expansion*

$$B_1(k)^{-1} = D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_2(k),$$

where $\tilde{R}_2(k)$ is uniformly bounded in k and $D_1 = (Q_1M_1Q_1)^{-1}$.

Proof. We compute that

$$
\begin{aligned}
B_1(k)^{-1} &= \Big(Q_1M_1Q_1 + kQ_1M_2Q_1 - kQ_1M_1D_0M_1Q_1 - k^2Q_1\tilde{R}_1(k)Q_1\Big)^{-1} \\
&= D_1\Big(\mathrm{Id} + kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)Q_1D_1\Big)^{-1} \\
&= D_1\Bigg(\mathrm{Id} - kQ_1M_2Q_1D_1 + kQ_1M_1D_0M_1Q_1D_1 + k^2Q_1\tilde{R}_1(k)Q_1D_1 \\
&\quad + \sum_{j=2}^{\infty}(-1)^j\Big(kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)Q_1D_1\Big)^j\Bigg) \\
&= D_1 - kD_1Q_1M_2Q_1D_1 + kQ_1M_1D_0M_1Q_1D_1 + k^2D_1Q_1\tilde{R}_1(k)Q_1D_1 \\
&\quad + \sum_{j=2}^{\infty}(-1)^jD_1\Big(kQ_1M_2Q_1D_1 + kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)Q_1D_1\Big)^j.
\end{aligned}
$$

Defining

$$
\tilde{R}_2(k) = D_1Q_1\tilde{R}_1(k)Q_1D_1 + k^{-2}\sum_{j=2}^{\infty}(-1)^jD_1\Big(kQ_1M_2Q_1D_1 - kQ_1\tilde{R}_1(k)Q_1D_1\Big)^j
$$

completes the proof. □

We now have the following expansion for $M(k)^{-1}$.

Theorem 3.2.49. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the first kind for H. Then for sufficiently small k we have the expansion*

$$
\begin{aligned}
M(k)^{-1} &= k^{-1}Q_1D_1Q_1 - Q_1D_1Q_1M_2Q_1D_1Q_1 + Q_1D_1Q_1M_1D_0M_1Q_1D_1Q_1 \\
&\quad - D_0M_1Q_1D_1Q_1 + D_0 + k\tilde{R}_3(k),
\end{aligned}
$$

where $\tilde{R}_3(k)$ is uniformly bounded in k and $D_1 = (Q_1M_1Q_1)^{-1}$.

Proof. Lemma 3.2.45 shows that $M(k) + Q_1$ is invertible and we can compute that

$$
(M(k)+Q_1)^{-1}Q_1 = Q_1 - kD_0M_1Q_1 + k^2D_0M_2Q_1 - k^2D_0M_1D_0M_1Q_1 + k^3\tilde{R}_1(k)Q_1,
$$

and

$$
Q_1(M(k)+Q_1)^{-1} = Q_1 - kQ_1M_1D_0 + k^2Q_1M_2D_0 - k^2Q_1M_1D_0M_1D_0 + k^3Q_1\tilde{R}_1(k).
$$

Lemma 3.2.48 shows that $B_1(k)$ is invertible on $Q_1\mathcal{H}$ and thus we have by Lemmas 3.1.1

and 3.2.45 the expansion

$$\begin{aligned}
M(k)^{-1} &= (M(k)+Q_1)^{-1} + k^{-1}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} \\
&= D_0 - kD_0M_1D_0 + k^2D_0M_2D_0 - k^2D_0M_1D_0M_1D_0 + k^3\tilde{R}_1(k) \\
&\quad + k^{-1}\Big(Q_1 - kD_0M_1Q_1 + k^2D_0M_2Q_1 - k^2D_0M_1D_0M_1Q_1 + k^3\tilde{R}_1(k)Q_1\Big) \\
&\quad \times (D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_2(k)) \\
&\quad \times \Big(Q_1 - kQ_1M_1D_0 + k^2Q_1M_2D_0 - k^2Q_1M_1D_0M_1D_0 + k^3Q_1\tilde{R}_1(k)\Big).
\end{aligned}$$

Explicitly computing the lowest order terms in the product we obtain the statement of the theorem. □

If $Q_1M_1Q_1$ is not invertible, we define $Q_2 : Q_1\mathcal{H} \to Q_1\mathcal{H}$ to be the orthogonal projection onto the kernel of $Q_1M_1Q_1$. For sufficiently small k we have $B_1(k)+Q_2$ is invertible in $Q_1\mathcal{H}$. We define the operator $D_1 = (Q_1M_1Q_1+Q_2)^{-1}$.

Note also that the fact $Q_2 \leq Q_1$ and the definition of Q_2 imply $0 = Q_1M_1Q_2 = Q_1PQ_2$. Lemma 3.1.1 tells us that $B_1(k)$ is invertible if and only if

$$B_2(k) = (Q_2 - Q_2(B_1(k)+Q_2)^{-1}Q_2) \tag{3.32}$$

is invertible on $Q_2\mathcal{H}$ and in this case we have

$$B_1(k)^{-1} = (B_1(k)+Q_2)^{-1} + k^{-1}(B_1(k)+Q_2)^{-1}Q_2B_2(k)^{-1}Q_2(B_1(k)+Q_2)^{-1}.$$

Lemma 3.2.50. *Suppose that $n=3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have the expansion*

$$(B_1(k)+Q_2)^{-1} = D_1 - kD_1Q_1M_2Q_1D_1 - kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_4(k),$$

where $\tilde{R}_4(k)$ is uniformly bounded in k and $D_1 = (Q_1M_1Q_1+Q_2)^{-1}$.

Proof. Since each of the coefficient operators is bounded, we have for sufficiently small k the estimate

$$\Big|\Big|kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)D_1\Big|\Big| < 1.$$

Thus we make the computation

$$\begin{aligned}(B_1(k)+Q_2)^{-1} &= \Big(Q_1M_1Q_1 + kQ_1M_2Q_1 - kQ_1M_1D_0M_1Q_1 - k^2Q_1\tilde{R}_1(k)Q_1 + Q_2\Big)^{-1} \\ &= D_1\Big(\mathrm{Id} + kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)D_1\Big)^{-1} \\ &= D_1\Bigg(\mathrm{Id} - kQ_1M_2Q_1D_1 + kQ_1M_1D_0M_1Q_1D_1 + k^2Q_1\tilde{R}_1(k)D_1 \\ &\quad + \sum_{j=2}^{\infty}(-1)^j\Big(kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)D_1\Big)^j\Bigg) \\ &= D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2D_1Q_1\tilde{R}_1(k)D_1 \\ &\quad + \sum_{j=2}^{\infty}(-1)^jD_1\Big(kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1D_1 - k^2Q_1\tilde{R}_1(k)D_1\Big)^j\end{aligned}$$

where we have used Lemma 3.2.48 and a Neumann expansion. Defining

$$\begin{aligned}&\tilde{R}_4(k) \\ &= D_1Q_1\tilde{R}_1(k)D_1 + k^{-2}\sum_{j=2}^{\infty}(-1)^jD_1\Big(kQ_1M_2Q_1D_1 - kQ_1M_1D_0M_1Q_1 - k^2Q_1\tilde{R}_1(k)D_1\Big)^j\end{aligned}$$

completes the proof. □

Lemma 3.2.51. *Suppose that $n=3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have the expansion*

$$B_2(k) = Q_2M_2Q_2 - Q_2k\tilde{R}_4(k)Q_2.$$

Proof. We use Lemmas 3.2.50 and 3.1.4 and the definition of $B_2(k)$ to obtain

$$\begin{aligned}B_2(k) &= k^{-1}(Q_2 - Q_2(B_1(k)+Q_2)^{-1}Q_2) \\ &= k^{-1}(Q_2 - Q_2(D_1 - kQ_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_4(k))Q_2) \\ &= k^{-1}(Q_2 - Q_2D_1Q_2 + kQ_2Q_1M_2Q_1Q_2 - kQ_2M_1D_0M_1Q_2 - k^2Q_2\tilde{R}_4(k)Q_2) \\ &= Q_2M_2Q_2 - Q_2M_1D_0M_1Q_2 - Q_2k\tilde{R}_4(k)Q_2,\end{aligned}$$

where we have used the relations $Q_1Q_1 = Q_1Q_2 = Q_2$ and $Q_2D_1Q_2 = Q_2$. Note also that $Q_2M_1 = 0$. To complete the proof we note by [88, Lemma 2.2] that we have $G_2 \in \mathcal{L}^2(H^{0,t}, H^{0,-t})$ for $t > \frac{5}{2}$ and thus we have $Q_2M_2Q_2 \in \mathcal{L}^2(\mathcal{H})$ provided $\rho > 5$ in Assumption 2.2.14. □

We now characterise the range of the projections Q_1 and Q_2. The next two results can be inferred from related results in [88] and can aso be found in [64, Lemmas 5 and 6].

Lemma 3.2.52. *[64, Lemma 5] Suppose that $n = 3$ and V satisfies Assumption 3.2.41. Then $0 \neq f \in Q_1\mathcal{H}$ if and only if there exists $t > \frac{1}{2}$ and $g \in H^{0,-t}$ such that $f = Uvg$ and $Hg = 0$ in the sense of distributions.*

Proof. By [88, Lemma 2.4] we find that $g \in H^{0,-t}$ satisfies $Hg = 0$ if and only if

$$(\mathrm{Id} + G_0 V)g = 0.$$

Fix $0 \neq f \in Q_1\mathcal{H}$ so that

$$0 = [M_0 f](x) = U(x)f(x) + (4\pi)^{-1}v(x)\int_{\mathbb{R}^3} |x-y|^{-1}v(y)f(y)\,\mathrm{d}y.$$

Multiplying by $U(x)$ we obtain

$$f(x) = -(4\pi)^{-1}U(x)v(x)\int_{\mathbb{R}^3} |x-y|^{-1}v(y)f(y)\,\mathrm{d}y.$$

Defining $g \in H^{0,-t}$ by

$$g(x) = -(4\pi)^{-1}\int_{\mathbb{R}^3} |x-y|^{-1}v(y)f(y)\,\mathrm{d}y \tag{3.33}$$

we have $f = Uvg$. To see that $Hg = 0$ holds we compute that

$$\begin{aligned} g(x) &= -(4\pi)^{-1}\int_{\mathbb{R}^3} |x-y|^{-1}v(y)f(y)\,\mathrm{d}y = -(4\pi)^{-1}\int_{\mathbb{R}^3} |x-y|^{-1}V(x)g(y))\,\mathrm{d}y \\ &= -[G_0 V g](x). \end{aligned}$$

Conversely, we suppose that $f = Uvg$ for some $0 \neq g \in H^{0,-t}$ satisfying Equation $Hg = 0$. Then $f \in H^{0,2t}$ and applying M_0 we find

$$\begin{aligned} [M_0 f](x) &= U(x)f(x) + (4\pi)^{-1}v(x)\int_{\mathbb{R}^3} |x-y|^{-1}v(y)f(y)\,\mathrm{d}y \\ &= v(x)\left(g(x) + (4\pi)^{-1}\int_{\mathbb{R}^3} |x-y|^{-1}V(y)g(y)\,\mathrm{d}y\right) \\ &= v(x)[(\mathrm{Id} + G_0 V)g](x) \\ &= 0. \end{aligned}$$

Thus we have $0 \neq f \in Q_1\mathcal{H}$. □

Lemma 3.2.53. *[64, Lemma 6] Suppose that $n = 3$ and V satisfies Assumption 3.2.41. Then $0 \neq f \in Q_2\mathcal{H}$ if and only if there exists $g \in \mathcal{H}$ such that $f = Uvg$ and $Hg = 0$ in the sense of distributions.*

Proof. Suppose $0 \neq f \in Q_2\mathcal{H}$. Since $Q_2 \leq Q_1$ we have that by Lemma 3.2.52 that

$f = Uvg$ for some $g \in H^{0,-t}$ with $t > \frac{1}{2}$ and $Hg = 0$ in the sense of distributions. By the definition of Q_2 we find $Q_1 P f = 0$, which holds if and only if either $Q_1 v = 0$ or $Pf = 0$. In either case we have

$$0 = \int_{\mathbb{R}^3} v(y) f(y) \, \mathrm{d}y. \tag{3.34}$$

Using Equation (3.34) in Equation (3.33) we find that g satisfies

$$g(x) = -(4\pi)^{-1} \int_{\mathbb{R}^3} \left(|x-y|^{-1} - (1+|x|)^{-1} \right) v(y) f(y) \, \mathrm{d}y.$$

Define the operator $L : C_c^\infty(\mathbb{R}^3) \to C_c^\infty(\mathbb{R}^3)$ by the integral kernel $L(x,y) = \frac{1+|y|}{|x-y|(1+|x|)}$. By [88, Lemma 2.5] we have $L : H^{0,t} \to H^{2,t-2}$. Then for $t > \frac{3}{2}$ we have that

$$\left| |x-y|^{-1} - (1+|x|)^{-1} \right| \leq \frac{1+|y|}{|x-y|(1+|x|)} \tag{3.35}$$

which when combined with the fact that $f = Uvg \in H^{0,\frac{\varrho}{2}+t}$ shows that $g \in H^{0,t}$ and thus $g \in H^{2,t-2} \subset \mathcal{H}$. For the converse, we assume $f = wg$ for some $0 \neq g \in \mathcal{H}$ satisfying $Hg = 0$. Then we may write

$$\begin{aligned} g(x) & \\ &= -(4\pi)^{-1} \int_{\mathbb{R}^3} \left(|x-y|^{-1} - (1+|x|)^{-1} \right) v(y) f(y) \, \mathrm{d}y + (4\pi)^{-1} (1+|x|)^{-1} \int_{\mathbb{R}^3} v(y) f(y) \, \mathrm{d}y. \end{aligned}$$

The estimate (3.35) shows that the first term is square integrable and thus we find the function $h : \mathbb{R}^3 \to \mathbb{C}$ defined by

$$h(x) = (4\pi)^{-1} (1+|x|)^{-1} \int_{\mathbb{R}^3} v(y) f(y) \, \mathrm{d}y$$

is square integrable alsosince $(x \mapsto (1+|x|)^{-1} \notin L^2(\mathbb{R}^3)$ we have

$$0 = \int_{\mathbb{R}^3} v(y) f(y) \, \mathrm{d}y. \tag{3.36}$$

As discussed at the beginning of the proof, Equation (3.36) is equivalent to $f \in Q_2 \mathcal{H}$. □

The proof of Lemma 3.2.53 allows us to show that the Feshbach expansion terminates after only two applications and thus invert the operator $B_2(k)$.

Lemma 3.2.54. *[64, Lemma 7] Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then the operator $Q_2 M_2 Q_2$ is invertible in $Q_2 \mathcal{H}$.*

Proof. Suppose that $f \in Q_2\mathcal{H}$ and $Q_2M_2Q_2f = 0$. Then we find

$$0 = \langle Q_2M_2Q_2f, f\rangle = \langle M_2f, f\rangle = \langle G_2vf, vf\rangle.$$

The proof of Lemma 3.2.53 shows that we also have

$$0 = \int_{\mathbb{R}^3} v(y)f(y)\,\mathrm{d}y.$$

Note also that $vf \in L^1(\mathbb{R}^n)$ and $x \mapsto |x|vf \in L^1(\mathbb{R}^n)$, so that $\mathcal{F}(vf) \in L^1(\mathbb{R}^n) \cap C^1(\mathbb{R}^n)$. Thus we may compute the limits

$$\begin{aligned}
\langle G_2vf, vf\rangle &= \lim_{k\to 0} k^{-2}\langle (R_0(k^2) - G_0)vf, vf\rangle \\
&= \lim_{k\to 0} k^{-2}\int_{\mathbb{R}^3} ((|\xi|^2 + k^2)^{-1} - |\xi|^{-2})\overline{[\mathcal{F}(vf)](\xi)}[\mathcal{F}(vf)](\xi)\,\mathrm{d}\xi \\
&= \lim_{k\to 0}\int_{\mathbb{R}^3} (|\xi|^2(|\xi|^2 + k^2))^{-1}|[\mathcal{F}(vf)](\xi)|^2\,\mathrm{d}\xi \\
&= \int_{\mathbb{R}^3} |\xi|^{-4}|[\mathcal{F}(vf)](\xi)|^2\,\mathrm{d}\xi = \langle G_0vf, G_0vf\rangle,
\end{aligned}$$

where we have used Lemma 3.1.6 to bring the limit inside the integral. Since $Q_2M_2Q_2f = 0$ we thus find $\mathcal{F}(vf) = 0$ and so $vf = 0$, which further implies $f = 0$ and so $Q_2M_2Q_2$ is invertible in $Q_2\mathcal{H}$. □

Since the operator $Q_2M_2Q_2$ is invertible in $Q_2\mathcal{H}$ we can define $D_2 = (Q_2M_2Q_2)^{-1}$.

Lemma 3.2.55. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have the expansion*

$$B_2(k)^{-1} = D_2 + kB + k^2\tilde{R}_5(k)$$

where $\tilde{R}_5(k)$ is uniformly bounded and

$$B = -D_2Q_2M_3Q_2D_2 + D_2Q_2M_2Q_1D_1Q_1M_2Q_2D_2.$$

Proof. For sufficiently small k we have the estimate

$$\left|\left|kQ_2\tilde{R}_4(k)Q_2D_2\right|\right| < 1.$$

We thus compute the Neumann expansion

$$\begin{aligned} B_2(k)^{-1} &= \left(Q_2M_2Q_2 - kQ_2\tilde{R}_4(k)Q_2\right)^{-1} = D_2\left(\mathrm{Id} - kQ_2\tilde{R}_4(k)Q_2D_2\right)^{-1} \\ &= D_2\left(\mathrm{Id} + \sum_{j=1}^{\infty} k^j(Q_2\tilde{R}_4(k)Q_2D_2)^j\right) \\ &= D_2 + kD_2Q_2\tilde{R}_4(k)Q_2D_2 + \sum_{j=2}^{\infty} k^jD_2(Q_2\tilde{R}_4(k)Q_2D_2)^j. \end{aligned}$$

The lowest order term in $\tilde{R}_4(k)$ can be computed explicitly (see Remark 3.2.46) as

$$A = -D_0M_3D_0 - D_1Q_1D_0M_1D_0M_1D_0M_1D_0D_1 + D_1(Q_1M_2Q_1D_1 - Q_1M_1D_0M_1Q_1)^2.$$

The relations $Q_2D_1 = D_1Q_2 = Q_2$, $Q_2M_1 = M_1Q_2 = 0$ and $Q_2 \leq Q_1$ then give us

$$D_2Q_2AQ_2D_2 = -D_2Q_2M_3Q_2D_2 + D_2Q_2M_2Q_1D_1Q_1M_2Q_2D_2.$$

Defining $\tilde{R}_5(k) = k^{-2}\sum_{j=2}^{\infty} D_2(Q_2\tilde{R}_4(k)Q_2D_2)^j$ completes the proof. □

Lemma 3.2.56. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have the expansion*

$$B_1(k)^{-1} = -k^{-1}Q_2D_2Q_2 + D_1 + Q_2BQ_2 - Q_2D_2Q_2M_2Q_1D_1 - D_1Q_1M_2Q_2D_2Q_2 + k\tilde{R}_6(k),$$

where $\tilde{R}_6(k)$ is uniformly bounded.

Proof. Combining Lemmas 3.2.50 and 3.2.55 gives

$$\begin{aligned} B_1(k)^{-1} &= (B_1(k) + Q_2)^{-1} + k^{-1}(B_1(k) + Q_2)^{-1}Q_2B_2(k)^{-1}Q_2(B_1(k) + Q_2)^{-1} \\ &= D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_4(k) \\ &\quad + k^{-1}\big(D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_4(k)\big) \\ &\quad \times Q_2(D_2 + kB + k^2\tilde{R}_5(k)) \\ &\quad \times Q_2\big(D_1 - kD_1Q_1M_2Q_1D_1 + kD_1Q_1M_1D_0M_1Q_1D_1 + k^2\tilde{R}_4(k)\big) \end{aligned}$$

Collecting all lower order terms gives the result. □

We can now compute an expansion for $M(k)^{-1}$.

Theorem 3.2.57. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that zero is an exceptional point of the third kind for H. Then for sufficiently small k we have the*

expansion

$$M(k)^{-1} = k^{-2}Q_2D_2Q_2 + k^{-1}C_{-\frac{1}{2}} + \tilde{R}_8(k),$$

where $\tilde{R}_7(k)$ *is uniformly bounded and*

$$C_{-\frac{1}{2}} = D_1 + D_2M_2D_1M_2D_2 + D_2M_3D_2 - Q_1M_2D_2 - D_2M_2Q_1.$$

Proof. We begin with the fact that

$$M(k)^{-1} = (M(k)+Q_1)^{-1} + k^{-1}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} \quad (3.37)$$

So we compute the products

$$(M(k)+Q_1)^{-1}Q_1 = Q_1 - kD_0M_1Q_1 + k^2D_0M_2Q_1 - k^2D_0M_1D_0M_1Q_1 + k^3\tilde{R}_1(k)Q_1, \text{ and}$$
$$Q_1(M(k)+Q_1)^{-1} = Q_1 - kQ_1M_1D_0 + k^2Q_1M_2D_0 - k^2Q_1M_1D_0M_1D_0 + k^3Q_1\tilde{R}_1(k).$$

We are interested only in terms in the product with coefficient k^{-2} or k^{-1}. Expanding out the product we obtain

$$\begin{aligned}
&k^{-1}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}\\
&= k^{-1}\big(Q_1 - kD_0M_1Q_1 + k^2D_0M_2Q_1 - k^2D_0M_1D_0M_1Q_1 + k^3\tilde{R}_1(k)Q_1\big)\\
&\quad \times \big(k^{-1}Q_2D_2Q_2 + Q_2BQ_2 - Q_2D_2Q_2M_2Q_1D_1 - D_1Q_1M_2Q_2D_2Q_2 + k\tilde{R}_6(k)\big)\\
&\quad \times \big(Q_1 - kQ_1M_1D_0 + k^2Q_1M_2D_0 - k^2Q_1M_1D_0M_1D_0 + k^3Q_1\tilde{R}_1(k)\big)\\
&= k^{-2}Q_2D_2Q_2 + k^{-1}\big(D_2M_2D_1M_2D_2 + D_2M_3D_2 - Q_1M_2D_2 - D_2M_2Q_1\big) + \tilde{R}_7(k).
\end{aligned}$$

We thus find

$$\begin{aligned}
&k^{-1}(M(k)+Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}\\
&= k^{-1}D_1 + k^{-2}Q_2D_2Q_2 + k^{-1}\big(D_2M_2D_1M_2D_2 + D_2M_3D_2 - Q_1M_2D_2 - D_2M_2Q_1\big) + \tilde{R}_7(k)
\end{aligned}$$

Using Equation (3.37) and the fact that $(M(k)+Q_1)^{-1}$ is uniformly bounded in k completes the proof. □

We note that in the case $Q_2 = 0$ this reduces to the result of Theorem 3.2.49.

Definition 3.2.58. If $Q_1 \neq 0$ (an exceptional point of the first or third kind) we say there exists a *zero energy resonance* for H. In this case Lemmas 3.2.52 and 3.2.53 show that the set $Q_1\mathcal{H} \ominus Q_2\mathcal{H}$ is one dimensional and for each $\varphi \in Q_1\mathcal{H}/Q_2\mathcal{H}$ there exists a $t > \frac{1}{2}$ and $\psi \in H^{0,-t}$ such that $\varphi = Uv\psi$. We define a normalised zero energy resonance by the condition

$$||V\psi||_1 = ||v\varphi||_1 = (4\pi)^{\frac{1}{2}}.$$

We also use the notation $T_1 = Q_1 - Q_2$ for the projection onto the span of φ.

We now justify the choice of normalisation for our resonance ψ.

Lemma 3.2.59. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and that there exists a zero energy resonance for H. Let ψ be the normalised zero energy resonance of Definition 3.2.58. Then for any $t_1, t_2 > \frac{3}{2}$ we have in $\mathcal{B}(H^{-1,t_1}, H^{1,-t_2})$ the equality*

$$G_0 v T_1 D_1 T_1 v G_0 = \langle \psi, \cdot \rangle \psi,$$

where ψ is the normalised zero energy resonance of Definition 3.2.58.

Proof. Fix $t_1, t_2 > \frac{3}{2}$. Since $T_1\mathcal{H}$ is one dimensional, we choose a non-zero $\varphi \in T_1\mathcal{H}$ (a basis). Since T_1 is a rank one operator, we find there exists $\mu \in \mathbb{C}$ such that $T_1 D_1 T_1 \varphi = \mu\varphi$. By Lemma 3.2.52 there exists $t_3 > \frac{1}{2}$ and $\tilde{\psi} \in H^{0,-t_3}$ such that $\varphi = Uv\tilde{\psi}$ and $\tilde{\psi} = -G_0 V\tilde{\psi}$. By rescaling φ if necessary, we may choose $\tilde{\psi} = \psi$. So we compute that for any $f \in H^{1,-t_1}$ we have

$$T_1 v G_0 f = \langle v G_0 f, \varphi\rangle\varphi = \langle f, G_0 v\varphi\rangle\varphi = \langle f, G_0 V\psi\rangle\varphi = -\langle f, \psi\rangle\varphi.$$

Then we find

$$\begin{aligned} G_0 v T_1 D_1 T_1 v G_0 f &= -\langle f, \psi\rangle G_0 v T_1 D_1 T_1 \varphi = -\mu\langle f, \psi\rangle G_0 v\varphi \\ &= -\mu\langle f, \psi\rangle G_0 V\psi = \mu\langle f, \psi\rangle\psi. \end{aligned}$$

We determine μ as $\mu = \langle \varphi, M_1\varphi\rangle = V\langle \psi, G_1 V\psi\rangle = (4\pi)^{-1}\langle V\psi, 1\rangle^2 = 1$, from which the result follows. □

We can also recognise the projection onto the zero eigenspace for H in terms of the operators we have seen. The following characterisation is implicit in [88] and can be found as [64, Lemma 10].

Lemma 3.2.60. *[64, Lemma 10] Suppose that $n = 3$ and V satisfies Assumption 3.2.41 and let P_0 be the kernel projection of H. Then we have the equality $P_0 = G_0 v Q_2 D_2 Q_2 v G_0$.*

Proof. Let $(\varphi_j)_{j=1}^{N_0}$ be an orthonormal basis for $Q_2\mathcal{H}$. Then by Lemmas 3.2.52 and 3.2.53 we have

$$0 = \varphi_j + Uv G_0 v\varphi_j$$

for $1 \leq j \leq N_0$ and we can write $\varphi_j = Uv\psi_j$ for some $\psi_j \in \mathcal{H}$. Furthermore, we have

$$0 = \int_{\mathbb{R}^3} V(x)\psi_j(x)\,\mathrm{d}x = \int_{\mathbb{R}^3} v(x)\varphi_j(x)\,\mathrm{d}x,$$

the ψ_j are linearly independent and satisfy the relation $0 = \psi_j + G_0V\psi_j$. We thus compute for $f \in \mathcal{H}$ that

$$Q_2vG_0f = \sum_{j=1}^{N_0} \langle vG_0f, \varphi_j\rangle\varphi_j = \sum_{j=1}^{N_0} \langle f, G_0v\varphi_j\rangle\varphi_j = -\sum_{j=1}^{N_0} \langle f, \psi_j\rangle\varphi_j.$$

Let (A_{ij}) be the matrix representation of $Q_2vG_2vQ_2$ (the inverse of D_2) relative to the basis $(\varphi_j)_{j=1}^{N_0}$. Since we have $\int_{\mathbb{R}^3} v(x)\varphi_j(x)\,\mathrm{d}x = 0$ we find

$$A_{ij} = \langle \varphi_i, Q_2vG_2vQ_2\varphi_j\rangle = \langle G_0v\varphi_i, G_0v\varphi_j\rangle = \langle G_0V\psi_i, G_0V\psi_j\rangle = \langle \psi_i, \psi_j\rangle.$$

Then we find for $f \in \mathcal{H}$ that

$$\begin{aligned} G_0vQ_2D_2Q_2vG_0f &= -\sum_{j=1}^{N_0} G_0vQ_2D_2\varphi_j\langle f, \psi_j\rangle = -\sum_{i,j=1}^{N_0} G_0vQ_2\varphi_i(A^{-1})_{ij}\langle f, \psi_j\rangle \\ &= \sum_{i,j=1}^{N_0} (A^{-1})_{ij}\psi_i\langle f, \varphi_j\rangle. \end{aligned}$$

In particular for $f = \psi_m$ we find $G_0vQ_2D_2Q_2vG_0\psi_m = \psi_m$. Thus the range of the operator $G_0vQ_2D_2Q_2vG_0$ is $\mathrm{span}(\psi_j)_{j=1}^{N_0}$ and $G_0vQ_2D_2Q_2vG_0 = \mathrm{Id}$ on $\mathrm{Range}(G_0vQ_2D_2Q_2vG_0)$. Since $G_0vQ_2D_2Q_2vG_0$ is self-adjoint, we find P_0 is the projection onto the zero eigenspace $\mathrm{span}(\psi_j)_{j=1}^{N_0}$ as claimed. □

We thus obtain the following expansion for the difference of resolvents.

Theorem 3.2.61. *Suppose that $n = 3$ and V satisfies Assumption 3.2.41. Then for any $s, t > \frac{3}{2}$ and sufficiently small k we have in $\mathcal{B}(H^{-1,t_1}, H^{1,-t_2})$ the expansion*

$$R(-k^2) - R_0(-k^2) = k^{-1}(-\langle\cdot,\psi\rangle\psi + D_{-\frac{1}{2}}) - k^{-2}P_0 + \tilde{R}(k),$$

where $\tilde{R}(k)$ is uniformly bounded in k and

$$D_{-\frac{1}{2}} = -G_0v(D_2M_2D_1M_2D_2 + D_2M_3D_2 - Q_1M_2D_2 - D_2M_2Q_1)vG_0.$$

Proof. Use the relation

$$R(-k^2) - R_0(-k^2) = -R_0(-k^2)vM(k)^{-1}vR_0(-k^2)$$

in conjunction with Theorem 3.2.57 and Lemmas 3.2.59 and 3.2.60. □

3.2.5 Dimension $n = 2$

In this section we determine a low energy expansion of the resolvent in two dimensions using the symmetrised technique introduced in [89]. Such an expansion has been determined explicitly in [89, Theorem 6.2], however we present some additional details for clarity. Similar expansions have been introduced in different contexts in [26], [63] and [166].

We make the following assumption on the potential.

Assumption 3.2.62. Suppose that $n = 2$. We assume the potential V satisfies Assumption 2.2.14 for some $\rho > 11$.

In dimension $n = 2$ Equation (3.13) reads

$$R_0(x, y, z) = \ln(k|x-y|) \sum_{p=0}^{\infty} c_{2,p} k^{2p} |x-y|^{2p} + \sum_{p=0}^{\infty} d_{2,p} k^{2p} |x-y|^{2p} \tag{3.38}$$

Equation (3.38) leads to the following operator definitions.

Definition 3.2.63. Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then we define the integral kernels

$$G_{2p,0}(x, y) = (c_{2,p} \ln(|x-y|) + d_{2,p}) |x-y|^{2p}, \quad \text{and}$$
$$G_{2p,-1}(x, y) = c_{2,p} |x-y|^{2p}.$$

Then for $(2p, j) \neq (0, 0)$ we define the operators $M_{0,0} = U + vG_{0,0}v$ and $M_{2p,j} = vG_{2p,j}v$.

The operator $G_{2p,j}$ is the operator coefficient of the term $k^{2p} \ln(k)^j$ in Equation (3.38). As in higher even dimensions, we make the definition $\eta = \ln(k)^{-1}$. Then we can use the definition of $M(k)$ to write

$$M(k) = U + vR_0(-k^2)v = \sum_{p=0}^{\infty} \left(M_{2p,0} + \eta^{-1} M_{2p,-1}\right) k^{2p}.$$

We immediately obtain the following result.

Lemma 3.2.64. *[89, Lemma 6.1] Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and let $F = \{k \in \mathbb{C} : \mathrm{Re}(k) \geq 0, |k| \leq 1\}$. Then $M(k) - \eta^{-1} M_{0,-1} - U$ is a uniformly bounded compact operator-valued function on F and for sufficiently small k we have*

$$M(k) = M_{0,0} + \eta^{-1} M_{0,-1} + k^2 M_{2,0} + k^2 \eta^{-1} M_{2,-1} + k^4 \eta^{-1} \tilde{R}_0(k),$$

where $\tilde{R}_0(k)$ is uniformly bounded. For $j = 0,1$ the operators $M_{2j,0}$ are compact and self-adjoint and the operators $M_{2j,-1}$ are finite rank.

In particular, we note that $M_{0,-1} = c_{2,0} \|v\|_2^2 P$, where P is the rank one projection $P = \|v\|_2^{-2} \langle v, \cdot \rangle v$. We denote $Q = \mathrm{Id} - P$ the complementary projection.

We now aim to use the Feshbach formula of Lemma 3.1.1 to invert $M(k)$. To do so we need the following definition.

Definition 3.2.65. Suppose that $n = 2$ and V satisfies Assumption 3.2.62. We say that zero is a *regular point of the spectrum of H* if $QM_{0,0}Q$ is invertible on $Q\mathcal{H}$. If zero is not a regular point of the spectrum of H, we denote by Q_1 the orthogonal projection onto $\mathrm{Ker}(QM_{0,0}Q)$. In this case the operator $QM_{0,0}Q + Q_1$ is invertible and we denote the inverse by D_0.

Lemma 3.2.66. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is not a regular point for the spectrum of H. Denote by $M_0(k) = M(k) - \eta^{-1} M_{0,-1}$. For sufficiently small k, the operator $QM_0(k)Q + Q_1$ is invertible and there exists a function $g(k) = \eta^{-1}\tilde{g}(k)$ with $\tilde{g}$ uniformly bounded such that*

$$(M(k) + Q_1)^{-1} = g(k)^{-1} A + QD_0Q - k^2 D(k) + k^4 \tilde{R}_2(k),$$

with $D(k)$ and $\tilde{R}_2(k)$ uniformly bounded in k and

$$A := P - PM_{0,0}QD_0Q - QD_0QM_{0,0}P + QD_0QM_{0,0}PM_{0,0}QD_0Q.$$

Proof. We decompose $\mathcal{H} = P\mathcal{H} \oplus Q\mathcal{H}$ so that we may write

$$\begin{aligned} M(k) + Q_1 &= \begin{pmatrix} P(M(k) + Q_1)P & P(M(k) + Q_1)Q \\ Q(M(k) + Q_1)P & Q(M(k) + Q_1)Q \end{pmatrix} \\ &= \begin{pmatrix} P(M(k) - \eta^{-1} M_{0,-1} + \eta^{-1} M_{0,-1})P & P(M(k) - \eta^{-1} M_{0,-1} + \eta^{-1} M_{0,-1})Q \\ Q(M(k) - \eta^{-1} M_{0,-1} + \eta^{-1} M_{0,-1})P & Q(M(k) - \eta^{-1} M_{0,-1} + \eta^{-1} M_{0,-1})Q + Q_1 \end{pmatrix}, \end{aligned}$$

where we have used that $QP = PQ = 0$ and $QQ_1 = Q_1Q = Q_1$. Since we have defined $M_0(k) = M(k) - \eta^{-1} M_{0,-1}$ we can use the observation $PM_{0,-1} = M_{0,-1}P = c_{2,0} \|v\|_2^2 P$ to obtain

$$\begin{aligned} M(k) + Q_1 &= \begin{pmatrix} PM_0(k)P + \eta^{-1} c_{2,0} \|v\|_2^2 P & PM_0(k)Q \\ QM_0(k)P & QM_0(k)Q + Q_1 \end{pmatrix} \\ &= \begin{pmatrix} PM_{0,0}P + \eta^{-1} c_{2,0} \|v\|_2^2 P & PM_{0,0}Q \\ QM_{0,0}P & QM_{0,0}Q + Q_1 \end{pmatrix} \\ &\quad + k^2 (M_{2,0} + \eta^{-1} M_{2,-1}) + k^4 \eta^{-1} \tilde{R}_0(k), \end{aligned}$$

where $\tilde{R}_0(k)$ is uniformly bounded. Define the operator

$$A(k) = \begin{pmatrix} PM_{0,0}P + \eta^{-1}c_{2,0}\,||v||_2^2\,P & PM_{0,0}Q \\ QM_{0,0}P & QM_{0,0}Q + Q_1 \end{pmatrix}. \tag{3.39}$$

Then by Lemma 3.1.1 the operator $A(k)$ is invertible if and only if the operator

$$B(k) = (PM_{0,0}P + \eta^{-1}c_{2,0}\,||v||_2^2\,P - PM_{0,0}QD_0QM_{0,0}P)^{-1}$$

exists and is bounded, where $D_0 = (QM_{0,0}Q + Q_1)^{-1}$ as in Definition 3.2.65. Since P is a rank one projection there exists a constant c such that

$$B(k) = (c + \eta^{-1}c_{2,0}\,||v||_2^2)^{-1}P =: g(k)^{-1}P.$$

Thus we use Lemma 3.1.3 to write

$$\begin{aligned}
A(k)^{-1} &= \begin{pmatrix} B(k) & -B(k)PM_{0,0}QD_0 \\ -D_0QM_{0,0}PB(k) & D_0QM_{0,0}PB(k)PM_{0,0}QD_0 + D_0 \end{pmatrix} \\
&= g(k)^{-1}\begin{pmatrix} P & -PM_{0,0}QD_0 \\ -D_0QM_{0,0}P & D_0QM_{0,0}PM_{0,0}QD_0 + g(k)D_0 \end{pmatrix} \\
&= g(k)^{-1}\big(P - PM_{0,0}QD_0Q - QD_0QM_{0,0}P + QD_0QM_{0,0}PM_{0,0}QD_0Q\big) + QD_0Q. \\
&= g(k)^{-1}A + QD_0Q.
\end{aligned}$$

Note that for sufficiently small k we have the estimate

$$\left|\left|k^2(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1} + k^4\eta^{-1}\tilde{R}_0(k)A(k)^{-1}\right|\right| < 1.$$

Then we can compute the inverse of $M(k) + Q_1$ using a Neumann expansion as

$$\begin{aligned}
(M(k) + Q_1)^{-1} &= (A(k) + k^2(M_{2,0} + \eta^{-1}M_{2,-1}) + k^4\eta^{-1}\tilde{R}_0(k))^{-1} \\
&= A(k)^{-1}(\mathrm{Id} + k^2(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1} + k^4\eta^{-1}\tilde{R}_0(k)A(k)^{-1})^{-1} \\
&= A(k)^{-1}(\mathrm{Id} - k^2(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1} - k^4\eta^{-1}\tilde{R}_0(k)A(k)^{-1} \\
&\quad + k^4\tilde{R}_1(k)) \\
&= g(k)^{-1}\big(P - PM_{0,0}QD_0Q - QD_0QM_{0,0}P \\
&\quad + QD_0QM_{0,0}PM_{0,0}QD_0Q\big) + QD_0Q \\
&\quad - A(k)^{-1}(k^2(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1} - k^4\eta^{-1}\tilde{R}_0(k)A(k)^{-1} + k^4\tilde{R}_1(k)) \\
&= g(k)^{-1}A + QD_0Q - k^2A(k)^{-1}(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1} + k^4\tilde{R}_2(k) \\
&= g(k)^{-1}A + QD_0Q - k^2D(k) + k^4\tilde{R}_2(k).
\end{aligned}$$

Here we have defined the term $D(k) = A(k)^{-1}(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1}$. □

Remark 3.2.67. We can determine more terms in $\tilde{R}_2(k)$ as

$$\tilde{R}_2(k) = (A(k)^{-1}(M_{2,0} + \eta^{-1}M_{2,-1}))^2 A(k)^{-1} - A(k)^{-1}(M_{4,0} + \eta^{-1}M_{4,-1})A(k)^{-1} + k^2\tilde{R}_3(k),$$

where $\tilde{R}_3(k)$ is uniformly bounded in k

We next need to determine the inverse of the operator

$$B_1(k) = Q_1 - Q_1(M(k) + Q_1)^{-1}Q_1.$$

Definition 3.2.68. Let $n = 2$ and suppose that V satisfies Assumption 3.2.62 and suppose that zero is not a regular point for H. We say that zero is an *exceptional point of the first kind* if the operator $Q_1M_{0,0}PM_{0,0}Q_1$ is invertible on $Q_1\mathcal{H}$. In this case we write $D_1 = (Q_1M_{0,0}PM_{0,0}Q_1)^{-1}$.

Lemma 3.2.69. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is an exceptional point of the first kind for H. Then for sufficiently small k we have*

$$B_1(k)^{-1} = -g(k)D_1 + k^2\tilde{R}_5(k)$$

where $\tilde{R}_5(k)$ is uniformly bounded.

Proof. We use only the lowest order terms in Lemma 3.2.66, denoting the remainder $\tilde{R}_3(k) = -D(k) + k^2\tilde{R}_2(k)$. We use the relations $Q_1Q = Q_1D_0 = QQ_1 = D_0Q_1 = Q_1$ and $Q_1P = PQ_1 = 0$ to write

$$\begin{aligned} B_1(k) &= Q_1 - g(k)^{-1}Q_1AQ_1 - Q_1 - k^2Q_1\tilde{R}_3(k)Q_1 \\ &= -g(k)^{-1}Q_1M_{0,0}PM_{0,0}Q_1 - k^2Q_1\tilde{R}_3(k)Q_1 \end{aligned}$$

By assumption zero is an exceptional point of the first kind and so the operator $QM_{0,0}PM_{0,0}Q$ is invertible with inverse D_1 and using a Neumann expansion we find

$$\begin{aligned} B_1(k)^{-1} &= (-g(k)^{-1}QM_{0,0}PM_{0,0}Q - k^2Q_1\tilde{R}_3(k)Q_1)^{-1} \\ &= -g(k)D_1(\mathrm{Id} + k^2g(k)Q_1\tilde{R}_3(k)Q_1D_1)^{-1} \\ &= -g(k)D_1(\mathrm{Id} + k^2g(k)Q_1\tilde{R}_3(k)Q_1D_1 + k^4\tilde{R}_4(k)) = -g(k)D_1 + k^2\tilde{R}_5(k)). \end{aligned}$$ □

Remark 3.2.70. We note that if more terms are required in the expansion, we may write

$$\begin{aligned} \tilde{R}_5(k) = {} & g(k)^2D_1Q_1A(k)^{-1}(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1}Q_1D_1 - k^2g(k)^{-1}D_1Q_1R_2(k)Q_1D_1 \\ & - g(k)^3k^2D_1Q_1A(k)^{-1}((M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1}Q_1D_1)^2 + k^4\eta^{-1}\tilde{R}_6(k) \end{aligned}$$

where $\tilde{R}_6(k)$ is uniformly bounded and we have defined the term

$$R_2(k) = A(k)^{-1}((M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1})^2 0 A(k)^{-1}(M_{4,0} + \eta^{-1}M_{4,-1}).$$

Lemma 3.1.1 shows that in the case of an exceptional point of the first kind we can compute $M(k)^{-1}$ via the formula

$$M(k)^{-1} = (M(k) + Q_1)^{-1} + (M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1}. \tag{3.40}$$

Theorem 3.2.71. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is an exceptional point of the first kind for H. Then for sufficiently small k we have*

$$\begin{aligned} M(k)^{-1} = g(k)^{-1}A + QD_0Q - g(k)^{-1}AQ_1D_1Q_1A - AQ_1D_1Q_1 - Q_1D_1Q_1A \\ - g(k)Q_1D_1Q_1 + \tilde{R}_8(k) \end{aligned}$$

where $\tilde{R}_7(k)$ is uniformly bounded.

Proof. By Lemma 3.1.1 we have that $M(k)$ has inverse

$$M(k)^{-1} = (M(k) + Q_1)^{-1} + (M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1}.$$

Combining Lemmas 3.2.66 and 3.2.69 we can compute the expression

$$\begin{aligned} &(M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1} = -(g(k)^{-1}A + QD_0Q + k^2\tilde{R}_3(k))Q_1(g(k)D_1 \\ &\quad + k^2\tilde{R}_5(k)) \times Q_1(g(k)^{-1}A + QD_0Q + k^2\tilde{R}_3(k)) \\ &= -g(k)^{-1}AQ_1D_1Q_1A - AQ_1D_1Q_1 - Q_1D_1Q_1A - g(k)Q_1D_1Q_1 + \tilde{R}_7(k), \end{aligned}$$

where we have used the relations $Q_1QD_0Q = QD_0QQ_1 = Q_1$. Thus we find

$$\begin{aligned} M(k)^{-1} &= (M(k) + Q_1)^{-1} + (M(k) + Q_1)^{-1}Q_1B_1(k)^{-1}Q_1(M(k) + Q_1)^{-1} \\ &= g(k)^{-1}A + QD_0Q - g(k)^{-1}AQ_1D_1Q_1A - AQ_1D_1Q_1 - Q_1D_1Q_1A \\ &\quad - g(k)Q_1D_1Q_1 + \tilde{R}_8(k) \end{aligned}$$

where $\tilde{R}_8(k)$ is uniformly bounded. □

If the leading term of $B_1(k)$ is not invertible we need to apply Lemma 3.1.1 again.

Definition 3.2.72. Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that the operator $Q_1M_{0,0}PM_{0,0}Q_1$ is not invertible. Let Q_2 be the orthogonal projection onto the kernel of $Q_1M_{0,0}PM_{0,0}Q_1$. Then the operator $Q_1M_{0,0}PM_{0,0}Q_1 + Q_2$ is invertible with inverse D_1. We say that zero is an *exceptional point of the second kind* if the operator $Q_2M_{2,-1}Q_2$ is invertible and we denote its inverse by D_2.

By repeating the arguments of Lemma 3.2.69 and keeping track of more terms, we can determine an expansion for $B_1(k)^{-1}$ in the case of an exceptional point of the second kind. First we define the operator $\tilde{B}_1(k) = -g(k)B_1(k)$.

Lemma 3.2.73. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is an exceptional point of the second kind for H. Then for sufficiently small k we have*

$$(\tilde{B}_1(k) + Q_2)^{-1} = D_1 + k^2\tilde{R}_{11}(k),$$

where $\tilde{R}_{11}(k)$ is uniformly bounded.

Proof. We compute the Neumann expansion

$$\begin{aligned}(\tilde{B}_1(k) + Q_2)^{-1} &= (-g(k)B_1(k) + Q_2)^{-1} = (Q_1M_{0,0}PM_{0,0}Q_1 + Q_2 - k^2g(k)Q_1\tilde{R}_3(k)Q_1)^{-1}\\ &= D_1(\mathrm{Id} - k^2g(k)Q_1\tilde{R}_3(k)Q_1D_1)^{-1}\\ &= D_1 - k^2g(k)D_1Q_1\tilde{R}_3(k)Q_1D_1 + k^4\tilde{R}_{10}(k)\\ &= D_1 + k^2\tilde{R}_{11}(k),\end{aligned}$$

as claimed. □

Remark 3.2.74. As before we can compute more terms in this expansion, finding

$$\begin{aligned}\tilde{R}_{11}(k) &= -g(k)D_1Q_1\tilde{R}_3(k)Q_1D_1 + k^2\tilde{R}_{10}(k)\\ &= -g(k)D_1Q_1(-D(k) + k^2\tilde{R}_2(k)Q_1D_1 + k^2\tilde{R}_{10}(k)\\ &= g(k)D_1Q_1D(k)Q_1D_1 + k^2g(k)Q_1D_1\tilde{R}_2(k)D_1Q_1 + k^2\tilde{R}_{10}(k)\\ &= -g(k)D_1Q_1D(k)Q_1D_1 + k^2\tilde{R}_{12}(k),\end{aligned}$$

where $\tilde{R}_{12}(k)$ is uniformly bounded.

To compute inverses, we need to use further terms in the expansion of $(M(k)+Q_1)^{-1}$ and so we first prove the following to simplify some later expressions.

Lemma 3.2.75. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is not a regular point or an exceptional point of the second kind for H. Then*

$$A(k)^{-1}Q_2 = Q_2A(k)^{-1} = Q_2,$$

where $A(k)$ is defined in Equation (3.39)*. Furthermore we have the relations*

$$0 = M_{0,0}Q_2 = Q_2M_{0,0}.$$

Proof. Noting that Q_2 is the projection onto the kernel of $Q_1M_{0,0}Q_1$ we find that for any

$f \in \mathcal{H}$ we have the relation

$$\begin{aligned}\langle PM_{0,0}Q_2 f, PM_{0,0}Q_2 f\rangle &= \langle Q_2 M_{0,0} PM_{0,0} Q_2 f, f\rangle = \langle Q_2(Q_1 M_{0,0} PM_{0,0} Q_1)Q_2 f, f\rangle \\ &= \langle Q_2 M_{0,0} PM_{0,0} Q_2 f, f\rangle = 0\end{aligned}$$

and thus $PM_{0,0}Q_2 = 0$. We then compute using $Q_2 D_0 = D_0 Q_2 = Q_2$, $Q_2 P = 0 = PQ_2$ and the fact that $Q_2 \leq Q$ to find

$$\begin{aligned}Q_2 A(k)^{-1} &= g(k)^{-1} Q_2\big(P - PM_{0,0}D_0 Q - QD_0 QM_{0,0}P + QD_0 QM_{0,0} PQD_0 Q\big) + Q_2 D_0 Q \\ &= g(k)^{-1}\big(Q_2 M_{0,0} P + Q_2 M_{0,0} PQD_0 Q\big) + Q_2 \\ &= Q_2,\end{aligned}$$

where we have used the relation $Q_2 M_{0,0} P = 0$. To prove the final relation, we note that by definition we have $QM_{0,0}QQ_1 = 0$ and thus $PM_{0,0}QQ_1 = M_{0,0}Q_1$. Thus we may compute

$$Q_1 M_{0,0} PM_{0,0} Q_1 = (Q_1 M_{0,0} P)(PM_{0,0} Q_1) = (PM_{0,0}Q_1)^*(PM_{0,0}Q_1) = (M_{0,0}Q_1)^*(M_{0,0}Q_1).$$

Thus we see that $\mathrm{Ker}(Q_1 M_{0,0} PM_{0,0} Q_1) = \mathrm{Ker}(M_{0,0}Q_1)$ and so the definition of Q_2 gives $M_{0,0}Q_1 Q_2 = M_{0,0}Q_2 = 0$. □

Keeping track of the many terms appearing in the following resolvent expansions can be rather cumbersome, so the relations in Lemma 3.2.75 will allow us to simplify some terms without too much computational effort.

Lemma 3.2.76. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is an exceptional point of the second kind for H. Then we have the expansion*

$$\begin{aligned}\tilde{B}_1(k)^{-1} &= D_1 + k^{-2} g(k)^{-1} Q_2 D_2(k) Q_2 - (D_1 Q_1 D(k) Q_2 D_2(k) Q_2 + Q_2 D_2(k) Q_2 D(k) Q_1 D_1) \\ &\quad + k^2 \tilde{R}_{15}(k),\end{aligned}$$

where $\tilde{R}_{15}(k)$ is uniformly bounded.

Proof. We know by Lemma 3.1.1 that the operator $\tilde{B}_1(k)$ is invertible if and only if the operator

$$B_2(k) = Q_2 - Q_2(\tilde{B}_1(k) + Q_2)^{-1} Q_2$$

is invertible on $Q_2\mathcal{H}$. Noting the identity $Q_2 D_1 = D_1 Q_2 = Q_2$ we find

$$\begin{aligned}B_2(k) &= Q_2 - Q_2 D_1 Q_2 + k^2 g(k) Q_2 D(k) Q_2 - k^4 Q_2 \tilde{R}_{12}(k) Q_2 \\ &= k^2 g(k) Q_2 D(k) Q_2 - k^4 Q_2 \tilde{R}_{12}(k) Q_2.\end{aligned}$$

We also recall that $D(k) = A(k)^{-1}(M_{2,0} + \eta^{-1}M_{2,-1})A(k)^{-1}$, so that an application of Lemma 3.2.75 gives

$$Q_2D(k)Q_2 = Q_2(M_{2,0} + \eta^{-1}M_{2,-1})Q_2.$$

Since zero is an exceptional point of the second kind for H, the operator $Q_2M_{2,-1}Q_2$ is invertible with inverse D_2 and thus for sufficiently small k the operator $Q_2D(k)Q_2$ is invertible with inverse $D_2(k)$ and we can then form the Neumann expansion

$$\begin{aligned}
B_2(k)^{-1} &= (g(k)k^2Q_2M_{2,0}Q_2 + k^2\eta^{-1}Q_2M_{2,-1}Q_2 - k^4Q_2\tilde{R}_{12}(k)Q_2)^{-1}\\
&= k^{-2}g(k)^{-1}D_2(k)(\mathrm{Id} - k^2g(k)^{-1}Q_2\tilde{R}_{10}(k)Q_2D_2(k))^{-1}\\
&= k^{-2}g(k)^{-1}D_2(k)(\mathrm{Id} + k^2g(k)^{-1}Q_2\tilde{R}_{10}(k)Q_2D_2(k) + k^4\tilde{R}_{13}(k))\\
&= k^{-2}g(k)^{-1}D_2(k) + \tilde{R}_{14}(k),
\end{aligned}$$

where $\tilde{R}_{14}(k)$ is uniformly bounded. We thus find

$$\begin{aligned}
\tilde{B}_1(k)^{-1} &= (\tilde{B}_1(k) + Q_2)^{-1} + (\tilde{B}_1(k) + Q_2)^{-1}Q_2\tilde{B}_2(k)^{-1}Q_2(\tilde{B}_1(k) + Q_2)^{-1}\\
&= D_1 - k^2g(k)D_1Q_1D(k)Q_1D_1 + k^4\tilde{R}_{12}(k) + (D_1 - k^2g(k)D_1Q_1D(k)Q_1D_1\\
&\quad + k^4\tilde{R}_{12}(k))Q_2(k^{-2}g(k)^{-1}D_2(k) + \tilde{R}_{14}(k))Q_2\\
&\quad \times (D_1 - k^2g(k)D_1Q_1D(k)Q_1D_1 + k^4\tilde{R}_{12}(k))\\
&= D_1 + k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 - (D_1Q_1D(k)Q_2D_2(k)Q_2 + Q_2D_2(k)Q_2D(k)Q_1D_1)\\
&\quad + k^2\tilde{R}_{15}(k),
\end{aligned}$$

where $\tilde{R}_{15}(k)$ is uniformly bounded. □

We are now ready to compute $M(k)^{-1}$ in the case of an exceptional point of the second kind for H. Two applications of Lemma 3.1.1 show that we can use the formula

$$M(k)^{-1} = (M(k) + Q_1)^{-1} - g(k)^{-1}(M(k) + Q_1)^{-1}Q_1\tilde{B}_1(k)^{-1}Q_1(M(k) + Q_1)^{-1}. \quad (3.41)$$

Theorem 3.2.77. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that zero is an exceptional point of the second kind for H. Then for sufficiently small k we have*

$$\begin{aligned}
M(k)^{-1} &= k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 + Q_2 + g(k)^{-1}A - g(k)^{-1}D(k)Q_2D_2(k)Q_2 + k^2\tilde{R}_{18}(k)\\
&\quad - g(k)^{-1}Q_2D_2(k)Q_2D(k) - (Q_2D(k)Q_2D_2(k)Q_2 + Q_2D_2(k)Q_2D(k)Q_2),
\end{aligned}$$

where $\tilde{R}_{18}(k)$ is uniformly bounded.

Proof. We begin by noting that

$$M(k)^{-1} = (M(k)+Q_1)^{-1} - g(k)^{-1}(M(k)+Q_1)^{-1}Q_1\tilde{B}_1(k)^{-1}Q_1(M(k)+Q_1)^{-1}.$$

By Lemma 3.2.75 we have $Q_2A = AQ_2 = 0$. So we make the computations

$$\begin{aligned} Q_2(M(k)+Q_1)^{-1} &= Q_2(g(k)^{-1}A + QD_0Q - k^2D(k) + k^4\tilde{R}_2(k)) \\ &= Q_2 - k^2Q_2D(k) + k^4Q_2\tilde{R}_2(k) \end{aligned}$$

and

$$\begin{aligned} (M(k)+Q_1)^{-1}Q_2 &= (g(k)^{-1}A + QD_0Q - k^2D(k) + k^4\tilde{R}_2(k))Q_2 \\ &= Q_2 - k^2D(k)Q_2 + k^4\tilde{R}_2(k)Q_2. \end{aligned}$$

So noting that $\tilde{B}_1(k)^{-1} = Q_2\tilde{B}_1(k)^{-1}Q_2$, we can expand out the product in the next expression to obtain

$$\begin{aligned} &(M(k)+Q_1)^{-1}Q_1\tilde{B}_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} = (Q_2 - k^2D(k)Q_2 + k^4\tilde{R}_2(k)Q_2) \\ &\quad \times (D_1 + k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 - (D_1Q_1D(k)Q_2D_2(k)Q_2 + Q_2D_2(k)Q_2D(k)Q_1D_1) \\ &\quad + k^2\tilde{R}_{15}(k)) \\ &= k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 + Q_2 - g(k)^{-1}D(k)Q_2D_2(k)Q_2 - g(k)^{-1}Q_2D_2(k)Q_2D(k) - \\ &\quad - g(k)(Q_2D(k)Q_2D_2(k)Q_2 + Q_2D_2(k)Q_2D(k)Q_2) + k^2\tilde{R}_{17}(k), \end{aligned}$$

where $\tilde{R}_{17}(k)$ is uniformly bounded. So we find

$$\begin{aligned} M(k)^{-1} &= (M(k)+Q_1)^{-1} - g(k)^{-1}(M(k)+Q_1)^{-1}Q_1\tilde{B}_1(k)^{-1}Q_1(M(k)+Q_1)^{-1} \\ &= g(k)^{-1}A + QD_0Q - k^2D(k) + k^4\tilde{R}_2(k) + k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 \\ &\quad + Q_2 - g(k)^{-1}D(k)Q_2D_2(k)Q_2 - g(k)^{-1}Q_2D_2(k)Q_2D(k) \\ &\quad - g(k)(Q_2D(k)Q_2D_2(k)Q_2 + Q_2D_2(k)Q_2D(k)Q_2) + k^2\tilde{R}_{17}(k) \\ &= k^{-2}g(k)^{-1}Q_2D_2(k)Q_2 + Q_2 + g(k)^{-1}A - g(k)^{-1}D(k)Q_2D_2(k)Q_2 \\ &\quad - g(k)^{-1}Q_2D_2(k)Q_2D(k) - (Q_2D(k)Q_2D_2(k)Q_2 \\ &\quad + Q_2D_2(k)Q_2D(k)Q_2) + k^2\tilde{R}_{18}(k), \end{aligned}$$

where $\tilde{R}_{18}(k)$ is uniformly bounded. □

Definition 3.2.78. Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and that the operator $Q_1M_{0,0}PM_{0,0}Q_1$ is not invertible. We say that zero is an *exceptional point of the third kind* if the operator $Q_2M_{2,-1}Q_2$ is not invertible. In this case we let Q_3 be the orthogonal projection onto the kernel of $Q_2M_{2,-1}Q_2$. Then the operator $Q_2M_{2,-1}Q_2 + Q_3$

is invertible and we write its inverse as D_2. We also define the projection $T_3 = Q_2 - Q_3$.

We now confirm that the Feshbach expansion procedure of Lemma 3.1.1 terminates.

Lemma 3.2.79. *[63, Lemma 5.4] Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then the operator $Q_3 M_{2,0} Q_3$ is invertible on $Q_3\mathcal{H}$.*

Proof. Suppose that $f \in Q_3\mathcal{H}$ satisfies $Q_3 M_{2,0} Q_3 f = 0$. Then we have

$$\int_{\mathbb{R}^2} v(y) f(y)\,\mathrm{d}y = 0$$

and $Q_2 M_{2,-1} Q_2 f = 0$. Note also that $vf \in L^1(\mathbb{R}^n)$ and $x \mapsto |x| vf \in L^1(\mathbb{R}^n)$, so that $\mathcal{F}(vf) \in L^1(\mathbb{R}^n) \cap C^1(\mathbb{R}^n)$ Thus we find

$$\begin{aligned}
\langle Q_2 M_{2,0} Q_2 f, f\rangle &= \langle M_{2,0} f, f\rangle = \lim_{k\to 0} \langle k^{-2}(R_0(k^2) - G_{0,0}) vf, vf\rangle \\
&= \frac{1}{4\pi^2} \lim_{k\to 0} k^{-2} \int_{\mathbb{R}^2} \left(\frac{1}{|\xi|^2 + k^2} - \frac{1}{|\xi|^2} \right) |[\mathcal{F}(vf)](\xi)|^2 \,\mathrm{d}\xi \\
&= \frac{1}{4\pi^2} \lim_{k\to 0} \int_{\mathbb{R}^2} \frac{1}{|\xi|^2(|\xi|^2 + k^2)} |[\mathcal{F}(vf)](\xi)|^2 \,\mathrm{d}\xi \\
&= \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \frac{|[\mathcal{F}(vf)](\xi)|^2}{|\xi|^4} \,\mathrm{d}\xi,
\end{aligned}$$

where we have used Lemma 3.1.6 to bring the limit inside the integral. Our assumptions on v and f guarantee that $(x \mapsto |x|^{-2} v(x) f(x)) \in L^1(\mathbb{R}^2)$ and thus $\mathcal{F}(vf)$ satisfies the extra decay hypothesis of Lemma 3.1.6. Since $Q_2 M_{2,-1} Q_2 f = 0$, our assumptions on v and f guarantee that $vf \in L^1(\mathbb{R}^2)$ and so we find $vf = 0$. Since $f \in Q_1\mathcal{H}$ gives $f = Uv\psi$ for some $\psi \in \mathcal{H}$ and thus $f = 0$. □

We shall write D_3 for the inverse of $Q_3 M_{2,0} Q_3$.

Remark 3.2.80. We note that the above proof also implies the useful relation

$$\langle G_{0,0} vf, G_{0,0} vf\rangle = \langle M_{2,0} f, f\rangle. \tag{3.42}$$

We can further characterise the obstruction subspaces in terms of resonances and zero energy eigenvalues.

Lemma 3.2.81. *[89, Lemma 6.4] Suppose that $n = 2$ and V satisfies Assumption 3.2.62 and $Q_1 \neq 0$ and fix $\varphi \in Q_1\mathcal{H}$ with $||\varphi|| = 1$. Then there exists $\psi \in L^\infty(\mathbb{R}^2)$ such that $\varphi = Uv\psi$ and $H\psi = 0$ in the sense of distributions. Furthermore, there exists $\tilde{\psi} \in \mathcal{H}$ and $c_0, c_1, c_2 \in \mathbb{R}$ such that*

$$\psi(x) = c_0 + \sum_{j=1}^{2} c_j \frac{x_j}{(1 + |x|^2)} + \tilde{\psi}(x). \tag{3.43}$$

Lemma 3.2.82. *[89, Lemma 6.4] Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Suppose $\psi = c + \psi_1 + \psi_2$ with $c \in \mathbb{C}$, $\psi_1 \in L^q(\mathbb{R}^2)$ for some $q \in (2, \infty)$ and $\psi_2 \in \mathcal{H}$. If $H\psi = 0$ in the sense of distributions then $\varphi = Uv\psi \in Q_1\mathcal{H}$.*

The above characterisation leads naturally to a definition of resonances in two dimensions.

Definition 3.2.83. If $Q_3 \neq 0$ there exists a zero energy bound state, a solution to $H\varphi = 0$ for which $\varphi \in \mathrm{Dom}(H)$. If $T_3 \neq 0$ we say there exists a p-resonance, which corresponds to the existence of a distributional solution to $H\varphi = 0$ which satisfies $\varphi \in L^q(\mathbb{R}^2)$ for some $q \in (2, \infty)$. If $T_2 \neq 0$ we say there exists an s-resonance, which corresponds to the existence of a distributional solution of $H\varphi = 0$ with $\varphi \in L^\infty(\mathbb{R}^2)$.

We now repeat the proof of Theorem 3.2.77 in the case of an exceptional point of the third kind. We use the notation

$$D_2(k) = (Q_2 M_{2,-1} Q_2 + \eta Q_2 M_{2,0} Q_2 + Q_3)^{-1} = D_2 + \eta C_2(k),$$

so that $D_2(0) = D_2$. Note that the second equality is obtained via a Neumann expansion.

Lemma 3.2.84. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then for sufficiently small k the operator $\tilde{B}_2(k) = k^{-2} g(k)^{-1} B_2(k)$ has inverse*

$$\tilde{B}_2(k)^{-1} = \tilde{T}_3(k) - k^2 g(k)^{-1} \tilde{T}_3(k) Q_2 (M_{4,0} + \eta^{-1} M_{4,-1}) Q_2 \tilde{T}_3(k) + k^4 \tilde{R}_{13}(k),$$

where $\tilde{R}_{13}(k)$ is uniformly bounded and

$$\tilde{T}_3(k) := (Q_2 D(k) Q_2)^{-1} = \begin{pmatrix} a & -a T_3 M_{2,0} Q_3 D_3 \\ -D_3 Q_3 M_{2,0} T_3 a & D_3 Q_3 M_{2,0} T_3 a T_3 M_{2,0} Q_3 D_3 + D_3 \end{pmatrix}$$

with $a = (T_3 M_{2,0} T_3 + \eta^{-1} T_3 M_{2,-1} T_3 - T_3 M_{2,0} Q_3 (Q_3 M_{2,0} Q_3)^{-1} Q_3 M_{2,0} T_3)^{-1}$.

Proof. We begin by defining $\tilde{B}_2(k) = k^{-2} g(k)^{-1} B_2(k)$ and consider the decomposition $Q_2\mathcal{H} = T_3\mathcal{H} \oplus Q_3\mathcal{H}$. Then we can determine the expression

$$Q_2 D(k) Q_2 = Q_2 (M_{2,0} + \eta^{-1} M_{2,-1}) Q_2 = \begin{pmatrix} T_3 M_{2,0} T_3 + \eta^{-1} T_3 M_{2,-1} T_3 & T_3 M_{2,0} Q_3 \\ Q_3 M_{2,0} T_3 & Q_3 M_{2,0} Q_3 \end{pmatrix}.$$

Lemma 3.1.3 shows that $Q_2 D_2(k) Q_2$ is invertible provided $Q_3 M_{2,0} Q_3$ is (which is guaranteed by Lemma 3.2.79) and the operator

$$a = (T_3 M_{2,0} T_3 + \eta^{-1} T_3 M_{2,-1} T_3 - T_3 M_{2,0} Q_3 (Q_3 M_{2,0} Q_3)^{-1} Q_3 M_{2,0} T_3)^{-1}$$

exists as a bounded operator (note that the explicit k dependence of a comes from the η term). Letting $D_3 = (Q_3 M_{2,0} Q_3)^{-1}$ we find

$$\tilde{T}_3(k) := (Q_2 D(k) Q_2)^{-1} = \begin{pmatrix} a & -aT_3 M_{2,0} Q_3 D_3 \\ -D_3 Q_3 M_{2,0} T_3 a & D_3 Q_3 M_{2,0} T_3 a T_3 M_{2,0} Q_3 D_3 + D_3 \end{pmatrix}.$$

For sufficiently small k we have the estimate

$$\left|\left| k^2 g(k)^{-1} Q_2 \tilde{R}_{12}(k) Q_2 \tilde{T}_3(k) \right|\right| < 1$$

and thus we can determine the Neumann expansion

$$\begin{aligned}\tilde{B}_2(k)^{-1} &= \left(Q_2 D(k) Q_2 - k^2 g(k)^{-1} Q_2 \tilde{R}_{12}(k) Q_2\right)^{-1} \\ &= \tilde{T}_3(k)\left(\mathrm{Id} - k^2 g(k)^{-1} Q_2 \tilde{R}_{12}(k) Q_2 \tilde{T}_3(k)\right)^{-1} \\ &= \tilde{T}_3(k) - k^2 g(k)^{-1} \tilde{T}_3(k) Q_2 \tilde{R}_{12}(k) Q_2 \tilde{T}_3(k) + k^4 \tilde{R}_{13}(k)\end{aligned}$$

where $\tilde{R}_{13}(k)$ is uniformly bounded. We can determine further terms in $\tilde{R}_{12}(k)$ as

$$\begin{aligned}\tilde{R}_{12}(k) &= g(k) Q_1 D_1 \tilde{R}_2(k) + k^2 \tilde{R}_{10}(k) \\ &= g(k) Q_1 D_1 A(k)^{-1}(M_{4,0} + \eta^{-1} M_{4,-1}) A(k)^{-1} + k^2 \tilde{R}_{19}(k).\end{aligned}$$

Thus we can determine $Q_2 \tilde{R}_{12}(k) Q_2 = g(k) Q_2 (M_{4,0} + \eta^{-1} M_{4,-1}) Q_2 + k^2 Q_2 \tilde{R}_{19}(k)$.

□

We now apply Lemma 3.1.3 to the operator $B_2(k)$ to obtain the expansion for $M(k)^{-1}$.

Theorem 3.2.85. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then for sufficiently small k we have the expansion*

$$M(k)^{-1} = -k^{-2} Q_2 \tilde{T}_3(k) Q_2 + \eta^{-1} \tilde{R}(k),$$

where $\tilde{R}(k)$ is uniformly bounded.

Proof. The most singular term which we have not considered yet is given by

$$\begin{aligned}&- k^{-2}(M(k) + Q_1)^{-1} Q_1 (\tilde{B}_1(k) + Q_2)^{-1} Q_2 \tilde{B}_2(k)^{-1} Q_2 (\tilde{B}_1(k) + Q_2)^{-1} Q_1 (M(k) + Q_1)^{-1} \\ &= -k^{-2} Q_2 \tilde{T}_3(k) Q_2.\end{aligned}$$

□

Remark 3.2.86. Note that we can write explicitly the term

$$\tilde{T}_3(k) = D_3 + (a - aT_3 M_{2,0} D_3 - D_3 M_{2,0} T_3 + D_3 M_{2,0} T_3 a T_3 M_{2,0} D_3.$$

We now characterise the image of the operators T_2 and T_3 to analyse resonant behaviour.

Lemma 3.2.87. *[89, Theorem 6.2] Suppose that* $n = 2$ *and* V *satisfies Assumption 3.2.62. The space* $\mathrm{Range}(T_2)$ *is spanned by the vector* $\Theta_0 := Q_1 M_{0,0} v$. *The space* $\mathrm{Range}(T_3)$ *is spanned by the vectors* $\Theta_j := Q_2 X_j v$, *where* X_j *denotes the multiplication operator by the coordinate* x_j.

Proof. By definition we have

$$\mathrm{Range}(T_2) = Q_1\mathcal{H} \cap \mathrm{Range}(Q_1 M_{0,0} P M_{0,0} Q_1),$$

which by Lemma 3.2.81 and the definition of $M_{0,0}$ is spanned by Θ_0. Similarly we have

$$\mathrm{Range}(T_3) = Q_2\mathcal{H} \cap \mathrm{Range}(Q_2 M_{2,-1} Q_2).$$

Since $PQ_1 = PQ_2 = 0$ we find

$$Q_2 M_{2,-1} Q_2 = c_{2,-1} Q_2 T Q_2 = 2c_{2,-1} Q_2 W Q_2,$$

where T and W are the integral operators with kernels

$$T(x,y) = v(x)|x-y|^2 v(y), \quad \text{and} \quad W(x,y) \qquad = v(x)\langle x, y\rangle v(y).$$

Letting X_j be the operator of multiplication by x_j (for $x = (x_1, x_2)$) we find

$$Q_2 M_{2,-1} Q_2 = 2c_{2,0} \sum_{j=1}^{d} \langle \Theta_j, \cdot \rangle \Theta_j,$$

where we have defined $\Theta_j = Q_2 X_j v$. □

Lemma 3.2.88. *[89, Theorem 6.2] Suppose that* V *satisfies Assumption 3.2.62. Then the zero eigenspace of* H *satisfies* $\mathrm{Ker}(H) \cong \mathrm{Range}(Q_3)$.

Proof. Suppose that $\varphi \in \mathrm{Range}(Q_3)$. Then φ is orthogonal to both $\mathrm{Range}(T_2)$ and $\mathrm{Range}(T_3)$, so that

$$\langle v, M_{0,0}\varphi\rangle = 0 = \langle v, X_j \varphi\rangle \tag{3.44}$$

for $j = 1, 2$. Then Lemma 3.2.81 shows that $\psi = Uv\varphi \in \mathcal{N}$. Conversely, suppose that $\psi \in \mathcal{N}$ and let $\varphi = Uv\psi$. Since $\psi \in \mathcal{H}$, Lemma 3.2.82 shows that $\varphi \in Q_1\mathcal{H}$ and Equation (3.44) holds for φ. Thus $\varphi \in \mathrm{Range}(Q_3)$. Hence we find

$$\mathrm{Dim}(\mathrm{Range}(Q_3)) = \mathrm{Dim}(\mathrm{Ker}(H))$$

and the map $\varphi \mapsto \psi$ is a bijection. $\square$

We can explicitly characterise the projection onto the zero eigenspace in terms of the operators we have seen.

Lemma 3.2.89. *[63, Lemma 5.6] Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then the projection P_0 onto the kernel of H is given by*

$$P_0 = G_{0,0} v Q_3 D_3 Q_3 v G_{0,0}.$$

Proof. Let $(\varphi_j)_{j=1}^{N_0}$ be an orthonormal basis for $\mathrm{Range}(Q_3)$. Then for each $1 \le j \le N_0$ we have $0 = \varphi_j + UvG_{0,0}v\varphi_j$ and $\varphi_j = Uv\psi_j$ for some $\psi_j \in \mathcal{H}$. Since $PQ_3 = 0$ we also find

$$\int_{\mathbb{R}^2} V(x)\psi_j(x)\,\mathrm{d}x = \int_{\mathbb{R}^2} v(x)\varphi_j(x)\,\mathrm{d}x = 0$$

for all j. Since the (φ_j) are linearly independent, so are the (ψ_j) and they satisfy

$$\psi_j + G_{0,0}V\psi_j = 0.$$

Using the fact that the (φ_j) are a basis for $Q_3\mathcal{H}$ we find for any $f \in \mathcal{H}$ that

$$Q_3 v G_{0,0} f = \sum_{j=1}^{N_0} \langle vG_{0,0}f, \varphi_j\rangle \varphi_j = -\sum_{j=1}^{N_0} \langle f, \psi_j\rangle \varphi_j.$$

Let $A = (A_{ij})$ be the matrix representation of $Q_3 v G_{2,-1} v Q_3$ with respect to the orthonormal basis (φ_j). Then using Equation (3.42) we find

$$A_{ij} = \langle \varphi_i, Q_3 v G_{2,-1} v Q_3 \varphi_j\rangle = \langle G_{0,0} v\varphi_i, G_{0,0} v\varphi_j\rangle = \langle G_{0,0} V\psi_i, G_{0,0} V\psi_j\rangle = \langle \psi_i, \psi_j\rangle.$$

Defining $P_0 = G_{0,0} v Q_3 D_3 Q_3 v G_{0,0}$ we find for any $f \in \mathcal{H}$ that

$$P_0 f = -\sum_{j=1}^{N_0} G_{0,0} v Q_3 D_3 \varphi_j \langle f, \psi_j\rangle = -\sum_{i,j=1}^{N_0} G_{0,0} v Q_3 (A^{-1})_{ij} \varphi_i \langle f, \psi_j\rangle = \sum_{i,j=1}^{N_0} \psi_i (A^{-1})_{ij} \langle f, \psi_j\rangle.$$

Thus we see that $P_0\psi_j = \psi_j$, so that the range of P_0 is $\mathrm{span}(\psi_j)$ and P_0 is the identity on its range, which implies P_0 is the projection onto the zero eigenspace by Lemma 3.2.88. $\square$

Theorem 3.2.90. *Suppose that $n = 2$ and V satisfies Assumption 3.2.62. Then for sufficiently small k we have*

$$R(k^2) - R_0(k^2) = -k^{-2}(P_0 - X) + k^{-2}\eta^{-1}\tilde{R}_{20}(k),$$

where $\tilde{R}_{20}(k)$ is uniformly bounded. Here X is given by

$$X = G_{0,0}vYvG_{0,-1} + G_{0,-1}vYvG_{0,0}$$

with $Y = \lim_{k\to 0}\eta^{-1}\tilde{T}_3(k)$.

Proof. The proof follows from Theorem 3.2.85 and the definition

$$R(-k^2) = R_0(-k^2) - R_0(-k^2)vM(k)^{-1}vR_0(-k^2)$$

and a comparison of the coefficients of k^{-2}. □

3.2.6 Dimension $n = 1$

In this section we determine the low energy resolvent expansion in dimension $n = 1$ using the Feshbach inversion method of Lemma 3.1.1 until it terminates. The expansions lead to explicit characterisations of the obstruction subspaces in terms of the kernel of H and zero energy resonances. The method we follow has been described in [89], although more detail has been included here regarding the specific coefficient operators as will be required in later chapters. We note that similar expansions have been introduced in various contexts throughout the literature, see for example [116], [29] and [28].

We first write

$$R_0(x, y, k^2) = (2k)^{-1}\mathrm{e}^{-k|x-y|} = (2k)^{-1} - \frac{1}{2}|x-y| + \frac{k}{4}|x-y|^2 + O(k^2).$$

Definition 3.2.91. We define the operators G_j for $j = -1, 0, 1$ by the integral kernels

$$G_{-1}(x, y) = \frac{1}{2}, \quad G_0(x, y) = -\frac{1}{2}|x-y|, \quad \text{and} \quad G_1(x, y) = \frac{1}{4}|x-y|^2$$

and the operators M_j by $M_0 = U + vG_0v$ and $M_j = vG_jv$. Note that $M_{-1} = \frac{1}{2}||v||_2^2 P$, where $P = ||v||_2^{-2}\langle v, \cdot\rangle v$.

Lemma 3.2.92. *[89, Lemma 5.1] Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$. Then $M - k^{-1}M_{-1} - U$ is a uniformly bounded compact operator valued function on $F = \{k \in \mathbb{C} : \mathrm{Re}(k) \geq 0 \text{ and } |k| \leq 1\}$. Furthermore, we have the expansion*

$$M(k) = k^{-1}M_{-1} + M_0 + kM_1 + k^2\tilde{R}_0(k),$$

where $\tilde{R}_0(k)$ is uniformly bounded in k.

We let $\alpha = ||v||_2^2$ and note that since P is a rank one projection, P is never invertible, Define the projection $Q = \mathrm{Id} - P$. We let $\tilde{M}(k) = 2k\alpha^{-1}M(k)$ and obtain the following.

Lemma 3.2.93. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$. Then for sufficiently small k the operator $\tilde{M}(k) + Q$ is invertible and we have the expansion*

$$(\tilde{M}(k) + Q)^{-1} = \mathrm{Id} - 2k\alpha^{-1}M_0 - 2k^2\alpha^{-1}M_1 + 4\alpha^{-2}k^2M_0^2 + k^3\tilde{R}_1(k),$$

where $\tilde{R}_1(k)$ is uniformly bounded.

Proof. For sufficiently small k we have the estimate

$$\left|\left|2k\alpha^{-1}M_0 + 2k^2\alpha^{-1}M_1 + 2k^3\alpha^{-1}\tilde{R}_0(k)\right|\right| < 1.$$

Note that

$$\tilde{M}(k) = P + 2k\alpha^{-1}M_0 + 2k^2\alpha^{-1}M_1 + 2k^3\alpha^{-1}\tilde{R}_0(k).$$

We thus compute the Neumann expansion

$$\begin{aligned}(\tilde{M}(k) + Q)^{-1} &= (\mathrm{Id} + 2k\alpha^{-1}M_0 + 2k^2\alpha^{-1}M_1 + 2k^3\alpha^{-1}\tilde{R}_0(k))^{-1} \\ &= \mathrm{Id} - 2k\alpha^{-1}M_0 - 2k^2\alpha^{-1}M_1 + 4\alpha^{-2}k^2M_0^2 + k^3\tilde{R}_1(k),\end{aligned}$$

where $\tilde{R}_1(k)$ is uniformly bounded. □

We define the operator

$$\begin{aligned}B_1(k) &= Q - Q(\tilde{M}(k) + Q)^{-1}Q \\ &= 2k\alpha^{-1}QM_0Q + 2k^2\alpha^{-1}QM_1Q - 4\alpha^{-2}k^2QM_0^2Q - k^3Q\tilde{R}_1(k)Q.\end{aligned}$$

We also define the operator $\tilde{B}_1(k) = \frac{\alpha}{2k}B_1(k)$, leading to the following definition.

Definition 3.2.94. Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$. We say that zero is a *regular point for H* if the operator QM_0Q is invertible on $Q\mathcal{H}$. In this case we write $D_1 = (QM_0Q)^{-1}$.

In the case of a regular point for H we can determine the inverse of the operator $M(k)$ using Lemma 3.1.1.

Lemma 3.2.95. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$ and that zero is a regular point for H. Then we have the expansion*

$$M(k)^{-1} = D_1 + 2\alpha^{-1}\mathrm{Id} + \tilde{R}_3(k),$$

where $\tilde{R}_3(k)$ is uniformly bounded.

Proof. For sufficiently small k we have the estimate

$$\left|\left|kQM_1QD_1 - 2\alpha^{-1}kQM_0^2QD_1 - \frac{\alpha}{2}k^2Q\tilde{R}_1(k)QD_1\right|\right| < 1.$$

We can thus compute the Neumann expansion

$$\begin{aligned}\tilde{B}_1(k)^{-1} &= (QM_0Q + kQM_1Q - 2\alpha^{-1}kQM_0^2Q - \frac{\alpha}{2}k^2Q\tilde{R}_1(k)Q)^{-1}\\ &= D_1(\mathrm{Id} + kQM_1QD_1 - 2\alpha^{-1}kQM_0^2QD_1 - \frac{\alpha}{2}k^2Q\tilde{R}_1(k)QD_1)^{-1}\\ &= D_1 - kD_1M_1D_1 + 2\alpha^{-1}kD_1M_0^2D_1 + k^2\tilde{R}_2(k),\end{aligned}$$

where $\tilde{R}_2(k)$ is uniformly bounded. We now use Lemma 3.1.1 to obtain

$$\begin{aligned}M(k)^{-1} &= 2\alpha^{-1}k\tilde{M}(k)^{-1} = 2\alpha^{-1}((\tilde{M}(k)+Q)^{-1} + \frac{\alpha}{2k}(\tilde{M}(k)+Q)^{-1}Q\tilde{B}_1(k)^{-1}(\tilde{M}(k)+Q)^{-1})\\ &= D_1 + 2\alpha^{-1}\mathrm{Id} + k\tilde{R}_3(k),\end{aligned}$$

where $\tilde{R}_3(k)$ is uniformly bounded. □

The definition of the operator $\tilde{B}_1(k)$ also leads to the following definition.

Definition 3.2.96. Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$. If the operator QM_0Q is not invertible on $Q\mathcal{H}$ we say that zero is an *exceptional point* for H. In this case we let Q_1 denote the orthogonal projection onto the kernel of QM_0Q. Then the operator $QM_0Q + Q_1$ is invertible and we denote the inverse by D_1.

In the case of an exceptional point, we cannot simply use a Neumann expansion to invert $\tilde{B}_1(k)$ directly. Instead we require another application of Lemma 3.1.1.

Lemma 3.2.97. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$ and that zero is an exceptional point of the second kind for H. Then for sufficiently small k the operator $\tilde{B}_1(k) + Q_1$ is invertible with inverse*

$$(\tilde{B}_1(k) + Q_1)^{-1} = D_1 - kD_1M_1D_1 + 2\alpha^{-1}kD_1M_0^2D_1 + k^2\tilde{R}_2(k)$$

where $\tilde{R}_2(k)$ is uniformly bounded.

Proof. For sufficiently small k we have the estimate

$$\left|\left|kQM_1QD_1 - 2\alpha^{-1}kQM_0^2QD_1 - \frac{\alpha}{2}k^2Q\tilde{R}_1(k)QD_1\right|\right| < 1.$$

We can thus compute the Neumann expansion

$$\begin{aligned}(\tilde{B}_1(k)+Q_1)^{-1} &= (QM_0Q+Q_1+kQM_1Q-2\alpha^{-1}kQM_0^2Q-\frac{\alpha}{2}k^2Q\tilde{R}_1(k)Q)^{-1} \\ &= D_1(\mathrm{Id}+kQM_1QD_1-2\alpha^{-1}kQM_0^2QD_1-\frac{\alpha}{2}k^2Q\tilde{R}_1(k)QD_1)^{-1} \\ &= D_1-kD_1M_1D_1+2\alpha^{-1}kD_1M_0^2D_1+k^2\tilde{R}_2(k),\end{aligned}$$

where $\tilde{R}_2(k)$ is uniformly bounded. □

We now apply Lemma 3.1.1 to the operator $\tilde{B}_1(k)$, however we first need to know that the Feshbach expansion terminates. To do so we determine the obstruction subspace Q_1 explicitly and show that Q_1 is a rank one operator.

Lemma 3.2.98. *[89, Theorem 5.2] Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$ and that $Q_1 \neq 0$. Then $\varphi \in Q_1\mathcal{H}$ with $||\varphi|| = 1$ if and only if there exists $\psi \in L^\infty(\mathbb{R})$, $\psi \notin \mathcal{H}$ such that $H\psi = 0$ in the sense of distributions and $Uv\psi = \varphi$. Furthermore, the space $Q_1\mathcal{H}$ is at most one dimensional.*

Proof. Suppose $\varphi \in Q_1\mathcal{H}$ with $||\varphi|| = 1$ and define

$$\psi(x) = c_1 + \frac{1}{2}\int_{\mathbb{R}} |x-y|v(y)\varphi(y)\,\mathrm{d}y,$$

where $c_1 = ||v||_2^{-2}\langle v, M_0\varphi\rangle$. Then we find

$$Uv\psi = c_1Uv + U(U-M_0)\varphi = c_1Uv + \varphi - UM_0\varphi = c_1Uv + \varphi - UPM_0\varphi = \varphi.$$

Differentiating in the sense of distributions shows $H\psi = 0$. To see that $\psi \notin \mathcal{H}$, we let

$$c_2 = \frac{1}{2}\int_{\mathbb{R}} yv(y)\varphi(y)\,\mathrm{d}y$$

and note that

$$\psi(x) = c_1 - c_2\mathrm{sign}(x) + \begin{cases} -x\int_x^\infty v(y)\varphi(y)\,\mathrm{d}y & \text{if } x \geq 0, \\ x\int_{-\infty}^x v(y)\varphi(y)\,\mathrm{d}y & \text{if } x \leq 0. \end{cases} \tag{3.45}$$

Suppose that $c_1 = c_2 = 0$. Then Equation (3.45) gives

$$\psi(x) = \int_x^\infty (y-x)V(y)\psi(y)\,\mathrm{d}y,$$

a homogenous Volterra equation. Our decay assumptions on V give that $\psi(x) = 0$ for large $|x|$. Uniqueness properties of the Volterra equation then give $\psi = 0$ for all x and thus $c_1 = c_2 = 0$ if and only if $\psi = 0$. We can determine

$$c_+ := \lim_{x\to\infty} \psi(x) = c_1 + c_2, \quad \text{and} \quad c_- := \lim_{x\to-\infty} \psi(x) = c_1 - c_2 \tag{3.46}$$

and thus $\psi \in L^\infty(\mathbb{R})$ and $\psi \notin \mathcal{H}$. For the converse, suppose $\psi \in L^\infty(\mathbb{R})$ satisfies $H\psi = 0$ in the sense of distributions. Defining $\varphi = Uv\psi$ we have (in the sense of distributions) the equality

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = V(x)\psi(x) = v(x)\varphi(x).$$

Let $\chi \in C_c^\infty(\mathbb{R})$ be such that $\chi(x) = 1$ for $|x| \le 1$ and $\chi(x) = 0$ for $|x| > 2$. Then for any $\delta > 0$ we have the estimate

$$\begin{aligned}\left|\int_{\mathbb{R}} v(x)\varphi(x)\chi(\delta x)\,\mathrm{d}x\right| &= \left|\int_{\mathbb{R}} \left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\right)\chi(\delta x)\,\mathrm{d}x\right| = \left|\int_{\mathbb{R}} \psi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\chi(\delta x)\right)\,\mathrm{d}x\right| \\ &= \delta^2\left|\int_{\mathbb{R}} \psi(x)\chi''(\delta x)\,\mathrm{d}x\right| \le \delta\,||\psi||_\infty \int_{\mathbb{R}} |\chi''(x)|\,\mathrm{d}x.\end{aligned}$$

Taking the limit as $\delta \to 0$ using the dominated convergence theorem gives

$$\int_{\mathbb{R}} v(x)\varphi(x)\,\mathrm{d}x = 0,$$

so that $\varphi \in Q\mathcal{H}$. Define

$$\Theta(x) = \frac{1}{2}\int_{\mathbb{R}} |x-y|v(y)\varphi(y)\,\mathrm{d}y = \frac{1}{2}\int_{\mathbb{R}} |x-y|V(y)\psi(y)\,\mathrm{d}y.$$

Differentiating in the sense of distributions gives the equality

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{\mathrm{d}^2\Theta}{\mathrm{d}x^2},$$

so that $\Theta(x) = a + bx + \psi(x)$ for some $a, b \in \mathbb{C}$. A similar argument to the one leading to Equation (3.45) shows that $\Theta \in L^\infty(\mathbb{R})$. Multiplying Θ by v we obtain the relation $(U - M_0)\varphi = U\varphi + av$, which implies $M_0\varphi = -av$ and thus $QM_0\varphi = 0$ and so $\varphi \in Q_1\mathcal{H}$. By construction we have $||\varphi|| = 1$. To prove that $Q_1\mathcal{H}$ is one-dimensional we suppose that there exist $\varphi, \tilde{\varphi} \in Q_1\mathcal{H}$. Then for $x \ge 0$ we have the corresponding $\psi, \tilde{\psi}$ as

$$\psi(x) = c_1 - c_2 - x\int_x^\infty v(y)\varphi(y)\,\mathrm{d}y, \quad \tilde{\psi}(x) = \tilde{c}_1 - \tilde{c}_2 + \int_x^\infty (y-x)v(y)\tilde{\varphi}(y)\,\mathrm{d}y.$$

There exists $a \in \mathbb{C}$ such that $c_1 - c_2 = a(\tilde{c}_1 - \tilde{c}_2)$ and so we find

$$\psi(x) - a\tilde{\psi}(x) = -x\int_x^\infty v(y)(\varphi(y) - a\tilde{\varphi}(y))\,\mathrm{d}y.$$

Again by uniqueness properties of Volterra type equations, we find $\psi - a\tilde{\psi} = 0$ and so $\varphi - a\tilde{\varphi} = 0$ also. Thus we have $\mathrm{Dim}(Q_1\mathcal{H}) = 1$. □

Definition 3.2.99. Suppose that $Q_1 \neq 0$. Then for any $\varphi \in Q_1\mathcal{H}$ we say that the corresponding ψ with $\varphi = Uv\psi$ from Lemma 3.2.98 is a *zero energy resonance* for H. We choose a normalised zero energy resonance by the condition that $c_+^2 + c_-^2 = 1$.

Lemma 3.2.100. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$ and that zero is an exceptional point for H. Then for sufficiently small k the operator $B_2(k)$ is invertible with inverse*

$$B_2(k)^{-1} = k^{-1}\tilde{c}^{-1}Q_1 - \tilde{c}^{-2}Q_1\tilde{R}_2(k)Q_2 + k\tilde{R}_3(k),$$

where $\tilde{R}_3(k)$ is uniformly bounded in k.

Proof. Lemma 3.1.1 gives that the operator $\tilde{B}_1(k)$ is invertible if and only if the operator

$$B_2(k) = Q_1 - Q_1(\tilde{B}_1(k) + Q_1)^{-1}Q_1$$

is invertible. For sufficiently small k we have

$$\left|\left|kQ_1\tilde{R}_2(k)Q_1\right|\right| < 1.$$

So we compute that $B_2(k) = kQ_1M_1Q_1 - \alpha^{-1}kQ_1M_0^2Q_1 - k^2Q_1\tilde{R}_2(k)$, where we have used the relation $Q_1D_1 = D_1Q_1 = Q_1$. Note that there exists a constant $\tilde{c}$ such that $Q_1M_1Q_1 - \alpha^{-1}Q_1M_0^2Q_1 = \tilde{c}Q_1$. We now use a Neumann expansion to obtain

$$B_2(k)^{-1} = k^{-1}\tilde{c}^{-1}Q_1(\mathrm{Id} - \tilde{c}^{-1}kQ_1\tilde{R}_2(k)Q_1)^{-1} = k^{-1}\tilde{c}^{-1}Q_1 - \tilde{c}^{-2}Q_1\tilde{R}_2(k)Q_2 + k\tilde{R}_3(k),$$

where $\tilde{R}_3(k)$ is uniformly bounded in k. □

We are finally ready to determine the inversion formula for $M(k)$.

Theorem 3.2.101. *[89, Theorem 5.2] Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$ and that zero is an exceptional point of the second kind for H. Then for sufficiently small k we have the expansion*

$$M(k)^{-1} = \tilde{c}^{-1}k^{-1}Q_1 + \tilde{R}_4(k),$$

where $\tilde{R}_4(k)$ is uniformly bounded.

Proof. Lemma 3.1.1 gives that

$$\begin{aligned}
&M(k)^{-1}\\
&= 2\alpha^{-1}k\left((\tilde{M}(k)+Q)^{-1} + \frac{\alpha}{2}k^{-1}(\tilde{M}(k)+Q)^{-1}Q\tilde{B}_1(k)^{-1}Q(\tilde{M}(k)+Q)^{-1}\right)\\
&= 2\alpha^{-1}k\Bigg((\tilde{M}(k)+Q)^{-1} + \frac{\alpha}{2}k^{-1}(\tilde{M}(k)+Q)^{-1}Q(\tilde{B}_1(k)+Q_1)^{-1}Q(\tilde{M}(k)+Q)^{-1}\\
&\quad + \frac{\alpha}{2}k^{-1}(\tilde{M}(k)+Q)^{-1}Q(\tilde{B}_1(k)+Q_1)^{-1}Q_1B_2(k)^{-1}Q_1(\tilde{B}_1(k)+Q_1)^{-1}Q(\tilde{M}(k)+Q)^{-1}\Bigg).
\end{aligned}$$

The first two terms have already been determined in Lemma 3.2.95. So we expand out the lowest order terms in the expression

$$\begin{aligned}
&(\tilde{M}(k)+Q)^{-1}Q(\tilde{B}_1(k)+Q_1)^{-1}Q_1B_2(k)^{-1}Q_1(\tilde{B}_1(k)+Q_1)^{-1}Q(\tilde{M}(k)+Q)^{-1}\\
&= \tilde{c}^{-1}k^{-1}Q_1 + \alpha^{-1}\tilde{c}^{-1}(M_0Q_1+Q_1M_1) + \tilde{c}^{-1}(D_1M_1Q_1+Q_1M_1D_1) - \tilde{c}^{-3}Q_1\tilde{R}_2(k)Q_1\\
&\quad + \tilde{R}_4(k),
\end{aligned}$$

where $\tilde{R}_4(k)$ is uniformly bounded. ☐

Remark 3.2.102. We can further simplify the coefficients in the above expansion. Since Q_1 is a rank one projection we can obtain (see [89, Lemma 5.4(iii)]) that

$$\tilde{c}^{-1} = -\alpha^{-1}(c_1^2+c_2^2) = -\frac{1}{2\alpha}(c_+^2+c_-^2),$$

with $c_1, c_2, c_\pm$ defined in the proof of Lemma 3.2.98.

We conclude this chapter with an expansion for the resolvent difference $R(-k^2) - R_0(-k^2)$. We provide only a reference with no proof, since the details are rather involved (see [116, Section 5]). The important feature to note is that as in higher dimensions, the worst singularity as $k \to 0$ is related to the existence of zero-energy eigenvalues for H and the next worst singularity is related to the existence of resonances.

Theorem 3.2.103 ([116, Section 5])**.** *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 7$. Then for sufficiently small k we have the expansion*

$$R(k-^2) - R_0(-k^2) = -P_0k^{-2} + k^{-1}A + \tilde{R}_{16}(k)$$

where A is a bounded operator depending on the existence of a resonance and $\tilde{R}_{16}(k)$ is uniformly bounded.

Chapter 4

The structure of the wave operator

In this chapter we show that the wave operator W_- satisfies

$$W_- = \mathrm{Id} + \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_n) - i\cosh(\pi D_n)^{-1}\right)(S - \mathrm{Id}) + K, \tag{4.1}$$

where D_n is the generator of dilations on $L^2(\mathbb{R}^n)$, S the scattering matrix and K is a compact operator. We will frequently use the notation $\varphi(x) = \frac{1}{2}(1+\tanh(\pi x)-i\cosh(\pi x)^{-1})$. In Section 4.1 we use the resolvent expansions of Chapter 3 to determine the low energy behaviour of the scattering matrix. In Section 4.2 we give a direct intuitive argument why Equation (4.1) should hold based on the generalised eigenfunctions described in Section 2.4.2. Unfortunately this method is limited by difficulties in showing the remainder is compact and is not sensitive to the fine structure of the spectrum of H exhibited in Chapter 3. In Section 4.3 we give a different approach, which yields the answer less directly, using carefully the resolvent expansions of Chapter 3. The main result of this chapter is the following theorem, whose proof relies on several preparatory results and some additional decay assumptions on the potential, described in Assumption 4.3.1.

Theorem 4.0.1. *Let $n \geq 2$ and suppose that ρ satisfies Assumption 4.3.1, and let V satisfy $|V(x)| \leq C(1+|x|)^{-\rho}$ for almost every $x \in \mathbb{R}^n$. In dimension $n = 2$ we suppose also that there are no p-resonances and in dimension $n = 4$ we suppose there are no resonances. Then in $\mathcal{B}(\mathcal{H})$ we have the equality*

$$W_- = \mathrm{Id} + \varphi(D_n)(S - \mathrm{Id}) + K,$$

where $K \in \mathcal{K}(\mathcal{H})$ and $\varphi(x) = \frac{1}{2}(1+\tanh(\pi x) - i\cosh(\pi x)^{-1})$.

Theorem 4.0.1 has appeared in [5] as joint work with Adam Rennie, with the case $n = 3$ having been proved already in [141].

4.1 The scattering matrix

In this section we present how the low energy behaviour of the scattering matrix in each dimension. The stationary expression for the scattering matrix of Theorem 2.4.32 shows that such low energy expansions depend on the low energy behaviour of the resolvent discussed in Chapter 3 and the trace operator $\Gamma_0(\cdot)$ of Definition 2.4.14.

4.1.1 Low energy expansions of the trace operator

In this subsection we present the low energy behaviour of the operator $\Gamma_0(\cdot)$ of Definition 2.4.14. Such an expansion was considered in dimension $n = 3$ in [88, Section 5] and the results we present here are straightforward generalisations.

For $\lambda > 0$ the trace operator $\gamma(\lambda) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{P}$ is continuous and extends to a bounded operator in $\mathcal{B}(H^{s,t}, \mathcal{P})$ for each $s > \frac{1}{2}$ and $t \in \mathbb{R}$ [106, Theorem 2.4.3]. We need the asymptotic development of $\gamma(\lambda^{\frac{1}{2}})\mathcal{F}$ as $\lambda \to 0$. We can compute for $f \in C_c^\infty(\mathbb{R}^n)$ and $\omega \in \mathbb{S}^{n-1}$ the expansion

$$
\begin{aligned}
[\gamma(\lambda^{\frac{1}{2}})\mathcal{F}f](\omega) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\lambda^{\frac{1}{2}}\langle x,\omega\rangle} f(x)\,\mathrm{d}x \\
&= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \sum_{j=0}^{K} \frac{1}{j!}(i\lambda^{\frac{1}{2}})^j (-\langle x,\omega\rangle)^j f(x)\,\mathrm{d}x + O\left(\lambda^{\frac{K+1}{2}}\right) \\
&:= \sum_{j=0}^{K} (i\lambda^{\frac{1}{2}})^j [\gamma_j f](\omega) + O\left(\lambda^{\frac{K+1}{2}}\right)
\end{aligned}
$$

as $\lambda \to 0$ in $\mathcal{B}(H^{s,t}, \mathcal{P})$ for appropriate s, t. The operators γ_j can be considered as operators in certain weighted Sobolev spaces, with higher terms in the series requiring convergence in Sobolev spaces with higher decay. Jensen [88, Equation 5.4] states the following result in dimension $n = 3$ and the result generalises in a straightforward manner to each dimension.

Lemma 4.1.1. *Fix $j \in \mathbb{N}$. For each $s \geq 0$ and $t > j + \frac{n}{2}$ we have $\gamma_j \in \mathcal{B}(H^{s,t}, \mathcal{P})$.*

Proof. For $t > j + \frac{n}{2}$ and $s = 0$, we can estimate that

$$
\begin{aligned}
||\gamma_j f||_{\mathcal{P}}^2 &= \int_{\mathbb{S}^{n-1}} |[\gamma_j f](\omega)|^2\,\mathrm{d}\omega = \int_{\mathbb{S}^{n-1}} \left|(2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} (-\langle x,\omega\rangle)^j f(x)\,\mathrm{d}x\right|^2 \mathrm{d}\omega \\
&\leq (2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} |\langle \omega, x\rangle|^j\, |f(x)|\,\mathrm{d}x\right)^2 \mathrm{d}\omega \\
&= (2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} |\langle \omega, x\rangle|^j\, (1+|x|^2)^{-\frac{t}{2}}(1+|x|^2)^{\frac{t}{2}}|f(x)|\,\mathrm{d}x\right)^2 \mathrm{d}\omega.
\end{aligned}
$$

We next use the Cauchy-Schwarz inequality to obtain the estimate

$$
\begin{aligned}
&(2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} |\langle \omega, x \rangle|^j \, (1+|x|^2)^{-\frac{t}{2}} (1+|x|^2)^{\frac{t}{2}} |f(x)| \, \mathrm{d}x \right)^2 \mathrm{d}\omega \\
&\leq (2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} |\langle \omega, x \rangle|^{2j} (1+|x|^2)^{-t} \, \mathrm{d}x \right)^2 \left(\int_{\mathbb{R}^n} (1+|y|^2)^t |f(y)|^2 \, \mathrm{d}y \right)^2 \mathrm{d}\omega \\
&= C_j \, ||f||^2_{H^{0,t}} \, .
\end{aligned}
$$

Thus for $t > j + \frac{n}{2}$ we find $\gamma_j \in \mathcal{B}(H^{0,t}, \mathcal{P})$. For $s > 0$ we use the inclusion $H^{s,t} \subset H^{0,t}$. □

For each $\lambda > 0$ the operator $\Gamma_0(\lambda) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{P}$ extends to an element of $\mathcal{B}(H^{s,t}, \mathcal{P})$ for each $s \in \mathbb{R}$ and $t > \frac{1}{2}$, as well as $\lambda \mapsto \Gamma_0(\lambda) \in \mathcal{B}(H^{s,t}, \mathcal{P})$ is continuous. These follow immediately since $\Gamma_0(\lambda) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} \gamma(\lambda^{\frac{1}{2}}) \mathcal{F}$.

Lemma 4.1.2. *For $K \in \mathbb{N}$, $s \geq 0$ and $t > \frac{n}{2} + K$ we have the expansion*

$$
\Gamma_0(\lambda) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} \sum_{j=0}^{K} (i\lambda^{\frac{1}{2}})^j \gamma_j + O\left(\lambda^{\frac{n}{4} + \frac{K}{2}} \right)
$$

as $\lambda \to 0$ in $\mathcal{B}(H^{s,t}, \mathcal{P})$.

Proof. Let $s = 0$ and $t > \frac{n}{2} + K$. Let Q_K be the K-th Taylor polynomial for the exponential function. Note for $y \in \mathbb{R}$ the estimate

$$
\left| \mathrm{e}^{iy} - Q_K(iy) \right| \leq \frac{|y|^{K+1}}{(K+1)!}.
$$

Then we can compute for $f \in H^{0,t}$ and $\lambda \geq 0$ that

$$
\begin{aligned}
&\left|\left| \left(\Gamma_0(\lambda) - 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} \sum_{j=0}^{K} (i\lambda^{\frac{1}{2}})^j \gamma_j \right) f \right|\right|_{\mathcal{P}}^2 \\
&= 2^{-1} \lambda^{\frac{n-2}{2}} \int_{\mathbb{S}^{n-1}} \left([\mathcal{F}f](\lambda^{\frac{1}{2}} \omega) - \sum_{j=0}^{K} (i\lambda^{\frac{1}{2}})^j [\gamma_j f](\omega) \right)^2 \mathrm{d}\omega \\
&\leq 2^{-1} \lambda^{\frac{n-2}{2}} (2\pi)^{-n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} \left| \mathrm{e}^{-i\lambda^{\frac{1}{2}} \langle x, \omega \rangle} - Q_K(i\lambda^{\frac{1}{2}} \langle x, \omega \rangle) \right| |f(x)| \, \mathrm{d}x \right)^2 \mathrm{d}\omega \\
&\leq \frac{\lambda^{\frac{n}{2}+K}}{2(K+1)!(2\pi)^n} \int_{\mathbb{S}^{n-1}} \left(\int_{\mathbb{R}^n} |\langle x, \omega \rangle|^{K+1} |f(x)|^2 \, \mathrm{d}x \right)^2 \mathrm{d}\omega.
\end{aligned}
$$

Using the same trick as Lemma 4.1.1 we write

$$
\begin{aligned}
&\left|\left|\left(\Gamma_0(\lambda) - 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}}\sum_{j=0}^{K}(i\lambda^{\frac{1}{2}})^j\gamma_j\right) f\right|\right|_{\mathcal{P}}^2 \\
&\leq \frac{\lambda^{\frac{n-2}{2}}}{2(K+1)!(2\pi)^n}\int_{\mathbb{S}^{n-1}}\left(\int_{\mathbb{R}^n}|\langle x,\omega\rangle|^{K+1}(1+|x|^2)^{-\frac{t}{2}}(1+|x|^2)^{\frac{t}{2}}|f(x)|^2\,\mathrm{d}x\right)^2\mathrm{d}\omega \\
&\leq \frac{C_K\lambda^{\frac{n}{2}+K}}{2(K+1)!(2\pi)^n}\,||f||_{H^{0,t}}^2\,.
\end{aligned}
$$

This proves the claim for $s = 0$. The inclusion $H^{s,t} \subset H^{0,t}$ for $s > 0$ completes the proof. □

Combining Lemma 4.1.2 with the results of Chapter 3 we can determine the low energy behaviour of the scattering matrix.

4.1.2 Low energy expansions of the scattering matrix

In this section we show how the low energy expansions of the resolvent can be used, in conjunction with Theorem 2.4.32, to determine the low energy behaviour of the scattering matrix. We will show that in odd dimensions the low energy behaviour is sensitive to the presence of resonances, whilst in even dimensions resonances have no effect. In dimensions $n \geq 2$ it is found that generically, we have $S(0) = \mathrm{Id}$.

The low energy behaviour of the scattering matrix has been determined using resolvent expansions in dimension $n = 1$ in [29] (see also [56, Theorem 2.15], [116] and [97, Proposition 9]).

Theorem 4.1.3. *Suppose that $n = 1$ and V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$. Then we have*

$$S(0) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{4.2}$$

if there are no resonances and

$$S(0) = \begin{pmatrix} 2c_+c_- & c_+^2 - c_-^2 \\ c_-^2 - c_+^2 & 2c_+c_- \end{pmatrix} \tag{4.3}$$

where $c_\pm \in \mathbb{R}\setminus\{0\}$ with $c_+^2 + c_-^2 = 1$.

Remark 4.1.4. The $c_\pm$ here denote the asymptotic values of the (normalised) resonance wave function at $\pm\infty$ (see Lemma 3.2.98). Due to the use of a different basis some authors (see [97, Proposition 9]) obtain a slightly different expression for $S(0)$. The relevant bases are described in Section 2.5.5. The essential feature to distinguish resonances is that if there are no resonances then $\mathrm{Det}(S(0)) = -1$ and if there are resonances then $\mathrm{Det}(S(0)) = 1$. Many more details about such calculations can be found also in [30] and [116]. We also deduce from our description the relation $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$, which we will demonstrate in Corollary 4.3.10 holds in all dimensions in $\mathcal{B}(\mathcal{P})$.

We note that the dimension $n = 1$ result is atypical in the sense that for all dimensions $n \geq 2$, if there does not exist a resonance at zero then $S(0) = \mathrm{Id}$. The generic failure of $S(0) = \mathrm{Id}$ means that the index pairing we discuss in Chapter 5 requires some modification to be applicable to dimension $n = 1$.

The low energy behaviour of the scattering matrix in dimension $n = 2$ has been proved in [142, Theorem 1.1] (see also [26, Theorem 4.3]). We note that in contrast to dimension $n = 1$ the behaviour is independent of the presence of resonances.

Theorem 4.1.5. *Let $n = 2$ and suppose V satisfies Assumption 2.2.14 for some $\rho > 11$. Then the scattering matrix satisfies $S(0) = \mathrm{Id}$.*

Proof. For $\lambda > 0$ we begin with Equation (2.73) in the symmetrised form

$$\begin{aligned} S(\lambda) - \mathrm{Id} &= -2\pi i \Gamma_0(\lambda) v (U + vR_0(\lambda + i0)v)^{-1} v \Gamma_0(\lambda)^* = -2\pi i \Gamma_0(\lambda) v M(\lambda^{\frac{1}{2}})^{-1} v \Gamma_0(\lambda)^* \\ &= -\pi i (\gamma_0 - i\lambda^{\frac{1}{2}}\gamma_1 + E(\lambda)) v M(\lambda^{\frac{1}{2}})^{-1} v (\gamma_0^* + i\lambda^{\frac{1}{2}}\gamma_1^* + E(\lambda)^*) \\ &= -\pi i (\gamma_0 - i\lambda^{\frac{1}{2}}\gamma_1 + E(\lambda)) v \Big(-\lambda^{-1} D_3 - \lambda^{-1}\tilde{T}_3(\lambda^{\frac{1}{2}}) + \frac{\lambda}{\ln(\lambda) - \frac{i\pi}{2}} K(\lambda) \Big) \\ &\quad \times v (\gamma_0^* + i\lambda^{\frac{1}{2}}\gamma_1^* + E(\lambda)^*) \end{aligned}$$

Here the operators $E(\lambda)$ are $O(\lambda)$ as $\lambda \to 0$ by Lemma 4.1.2 and the operator $K(\lambda)$ is bounded by Theorem 3.2.85. Thus any term involving $E(\lambda)$ or $E(\lambda)^*$ vanishes as $\lambda \to 0$. Using the relations $PQ_3 = PD_3 = PT_3 = 0$ we obtain also $\gamma_0 v Q_3 = Q_3 v \gamma_0^* = 0 = \gamma_0 v T_3 = T_3 v \gamma_0^*$. Observe also that $Q_3 T_3 = 0$ and thus $Q_3 v \gamma_1^* = \gamma_1 v Q_3 = 0$. Finally we check that

$$\lim_{\lambda\to 0} \frac{\lambda}{\ln(\lambda) - \frac{i\pi}{2}} = 0,$$

so that terms involving $K(\lambda)$ vanish as $\lambda \to 0$ and thus we obtain $S(\lambda) \to \mathrm{Id}$, as claimed. □

As in dimension $n = 1$, the behaviour of the scattering matrix at zero in dimension $n = 3$ is dependent on the existence of resonances and has been determined in [88, Theorems 5.1-5.3], which we state below.

Theorem 4.1.6. *Let $n = 3$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > 5$. Then we have*

$$S(0) = \mathrm{Id} - 2P_s,$$

where $P_s = 0$ if there are no resonances and P_s is the projection onto the spherical harmonic subspace of order 0 if there does exist a resonance (irrespective of whether or not V is spherically symmetric).

Proof. For $\lambda > 0$ we begin with Equation (2.73) in the symmetrised form

$$S(\lambda) = \mathrm{Id} - 2\pi i\Gamma_0(\lambda)v(U + vR_0(\lambda + i0)v)^{-1}v\Gamma_0(\lambda)^* = \mathrm{Id} - 2\pi i\Gamma_0(\lambda)vM(\lambda^{\frac{1}{2}})^{-1}v\Gamma_0(\lambda)^*.$$

Now for $\lambda > 0$ we use the expansion of Theorem 3.2.57 to obtain

$$\begin{aligned} S(\lambda) - \mathrm{Id} &= -2\pi i\Gamma_0(\lambda)vM(\lambda^{\frac{1}{2}})^{-1}v\Gamma_0(\lambda)^* \\ &= -2\pi i\Gamma_0(\lambda)v(\lambda^{-1}Q_2D_2Q_2 - \lambda^{-\frac{1}{2}}C_{-\frac{1}{2}} + \tilde{R}_7(\lambda^{\frac{1}{2}}))v\Gamma_0(\lambda)^* \\ &= -\pi i(2\pi)^{-3}\lambda^{\frac{1}{2}}(\gamma_0 + E(\lambda))v(\lambda^{-1}Q_2D_2Q_2 - \lambda^{-\frac{1}{2}}iC_{-\frac{1}{2}} + \tilde{R}_7(\lambda^{\frac{1}{2}})) \\ &\quad \times v(\gamma_0^* + E(\lambda)^*). \end{aligned}$$

Here we have $E(\lambda) = O(\lambda^{\frac{1}{2}})$ as $\lambda \to 0$ by Lemma 4.1.2. The proof of Lemma 3.2.53 shows that $\gamma_0 vQ_2 = 0$ and thus by duality $Q_2v\gamma_0^* = 0$. So for $\lambda > 0$ we find

$$S(\lambda) - \mathrm{Id} = -\pi(2\pi)^{-3}\gamma_0vC_{-\frac{1}{2}}v\gamma_0^* + O(\lambda^{\frac{1}{2}}) = \pi i\gamma_0vT_1D_1T_1v\gamma_0^* + O(\lambda^{\frac{1}{2}}),$$

since every term containing a γ_0vQ_2 or $Q_2v\gamma_0^*$ vanishes. For $f \in L^2(\mathbb{S}^2)$ and $\omega \in \mathbb{S}^2$ we compute the expression

$$\begin{aligned} [\gamma_0vT_1D_1T_1v\gamma_0^*f](\omega) &= \int_{\mathbb{R}^3} v(x)[T_1D_1T_1v\gamma_0^*f](x)\,\mathrm{d}x = \int_{\mathbb{R}^3} v(x)[T_1v\gamma_0^*f](x)\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} v(x)\varphi(x)\langle v\gamma_0^*f, \varphi\rangle\,\mathrm{d}x \\ &= \left(\int_{\mathbb{R}^3} v(x)\varphi(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^3} \varphi(y)v(y)\,\mathrm{d}y\right)\left(\int_{\mathbb{S}^2} f(\theta)\,\mathrm{d}\theta\right) \\ &= ||v\varphi||_1^2 \int_{\mathbb{S}^2} f(\theta)\,\mathrm{d}\theta. \end{aligned}$$

We can write

$$[\gamma_0 f](\omega) = \int_{\mathbb{S}^2} f(\omega)\,\mathrm{d}\omega = 4\pi[P_sf](\omega).$$

Recall that φ was chosen so that $||v\varphi||_1 = (4\pi)^{\frac{1}{2}}$ (see Definition 3.2.58 and the proof of Lemma 3.2.60) and so $4\pi^2\,||v\varphi||_1^2\,(2\pi)^{-3} = 2$. Any remaining terms containing an $E(\lambda)$ or $E(\lambda)^*$ vanish as $\lambda \to 0$. Hence we obtain $S(\lambda) - \mathrm{Id} = -2P_s$ if there exists a zero energy resonance. □

The notation P_s is to indicate that P_s is the projection onto the zeroth order spherical harmonic subspace, which correspond to s-waves. The next statement was almost certainly known to Jensen based on the comments in [85, p.1], although we have found no statements in the literature.

Theorem 4.1.7. *Suppose that $n \geq 4$ and that V satisfies Assumption 2.2.14 for some $\rho > 12$. Then we have $S(0) = \mathrm{Id}$.*

Proof. For $\lambda > 0$ we begin with Equation (2.73) in the symmetrised form

$$S(\lambda) = \mathrm{Id} - 2\pi i \Gamma_0(\lambda) v (U + vR_0(\lambda + i0)v)^{-1} v \Gamma_0(\lambda)^* = \mathrm{Id} - 2\pi i \Gamma_0(\lambda) v M(\lambda^{\frac{1}{2}})^{-1} v \Gamma_0(\lambda)^*.$$

As $\lambda \to 0$ we can then apply Lemma 4.1.2 to obtain the expansion for $\Gamma_0(\lambda)$ and $\Gamma_0(\lambda)^*$.

For $n \geq 5$ we apply, for $\lambda > 0$, Theorem 3.2.9 if n is odd or Theorem 3.2.19 if n is even, the result is the expansion

$$\begin{aligned} S(\lambda) - \mathrm{Id} &= -2\pi i \Gamma_0 v M(\lambda^{\frac{1}{2}}) v \Gamma_0(\lambda)^* \\ &= -\pi i \lambda^{\frac{n-2}{2}} (\gamma_0 + E(\lambda)) v (\lambda^{-1} D_1 + \tilde{R}(\lambda^{\frac{1}{2}})) v (\gamma_0^* + E(\lambda)^*) \to 0 \end{aligned}$$

as $\lambda \to 0$ since $\frac{n-2}{2} > 1$. Here we have $E(\lambda) = O(\lambda^{\frac{1}{2}})$ as $\lambda \to 0$ by Lemma 4.1.2.

In the case $n = 4$, we use for $\lambda > 0$, Theorem 3.2.37 to obtain the expansion

$$\begin{aligned} S(\lambda) - \mathrm{Id} &= -2\pi i \Gamma_0(\lambda) v (M(\lambda^{\frac{1}{2}}) v \Gamma_0(\lambda)^* \\ &= -2\pi i \lambda \Big(\gamma_0 + E(\lambda)\Big) \Big(\lambda^{-1} h(\lambda^{\frac{1}{2}}) Q_1 \tilde{T}_1 Q_1 + \lambda^{-1} D_2 + h(\lambda^{\frac{1}{2}}) K_1 + \tilde{R}(\lambda^{\frac{1}{2}}))\Big) \\ &\quad \times \Big(\gamma_0^* + E(\lambda)^*\Big) \to 0 \end{aligned}$$

as $\lambda \to 0$, since $\tilde{R}(\lambda^{\frac{1}{2}})$ is uniformly bounded, $h(\lambda^{\frac{1}{2}}) \to 0$ as $\lambda \to 0$, the fact that $\gamma_0 v Q_2 = 0$ by the proof of Lemma 3.2.26, the relation $Q_2 D_2 Q_2 = D_2$ and $E(\lambda) = O(\lambda^{\frac{1}{2}})$ as $\lambda \to 0$. □

4.2 Intuition for the form of the wave operator

Unpacking Equation (2.62) for the generalised plane waves $\psi_\pm$ gives intuition about the form of the wave operator W_-, much like [98] in dimension $n = 3$, although unfortunately does not lead to a complete proof.

Recall from Theorem 2.4.17 that the scattering amplitude a_- is defined to be the sub-leading behaviour of the generalised eigenfunction ψ_- as $|x| \to \infty$; that is,

$$\psi_-(x, \omega, \lambda) = \psi_0(x, \omega, \lambda) + a_-(\hat{x}, \omega, \lambda) w_+(|x|, \lambda) + k(x, \omega, \lambda) \tag{4.4}$$

where k decays as $|x| \to \infty$ and we have used the notation $\hat{x} = |x|^{-1} x$ for $x \neq 0$. The spherical wave is given by

$$w_\pm(r, |x|) = |x|^{-\frac{n-1}{2}} r^{\frac{n-2}{2}} \mathrm{e}^{\pm i r |x|} \mathrm{e}^{\mp i \frac{n-3}{4} \pi}. \tag{4.5}$$

Define the operator $T : C_c^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ by

$$[Tf](x) = c_n|x|^{-\frac{n-1}{2}} \int_{\mathbb{R}^+} \lambda^{\frac{n-3}{4}} \mathrm{e}^{i\lambda^{\frac{1}{2}}|x|}[\mathcal{F}f](\lambda^{\frac{1}{2}}\hat{x})\mathrm{d}\lambda = 2c_n|x|^{-\frac{n-1}{2}} \int_{\mathbb{R}^+} \tau^{\frac{n-1}{2}} \mathrm{e}^{i\tau|x|}[\mathcal{F}f](\tau\hat{x})\,\mathrm{d}\tau, \tag{4.6}$$

where $f \in C_c^\infty(\mathbb{R}^n)$, $x \in \mathbb{R}^n$ and $c_n = -i2^{-1}(2\pi)^{-\frac{1}{2}}\mathrm{e}^{-i\frac{n-3}{4}\pi}$. Define the integral operator $K : C_c^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ by

$$[Kf](x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} k(x, \hat{\xi}, |\xi|^2)[\mathcal{F}f](\xi)\,\mathrm{d}\xi. \tag{4.7}$$

Using the approximation to the generalised eigenfunction ψ_- in Equation (4.4) in the stationary expression for the wave operators of Theorem 2.4.29 combined with the generalised Fourier transforms of Lemma 2.4.31 we obtain the following.

Lemma 4.2.1. *Suppose that $|V(x)| \leq (1+|x|)^{-\rho}$ for some $\rho > \frac{n+1}{2}$. Define operators T and K by Equations* (4.6) *and* (4.7)*. Then the wave operator W_- satisfies*

$$W_- = \mathrm{Id} + T(S - \mathrm{Id}) + K. \tag{4.8}$$

Proof. We recall from Theorem 2.4.29 and Lemma 2.4.31 the action of the wave operator as an integral against generalised eigenfunctions ψ_- for $f \in C_c^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$ as

$$\begin{aligned}
[W_-f](x) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \psi_-(x, \hat{\xi}, |\xi|^2)[\mathcal{F}f](\xi)\,\mathrm{d}\xi \\
&= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \psi_0(x, \hat{\xi}, |\xi|^2)[\mathcal{F}f](\xi)\mathrm{d}\xi + (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} k(x,\xi)[\mathcal{F}f](\xi)\,\mathrm{d}\xi \\
&\quad + (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} a_-(\hat{x}, \hat{\xi}, |\xi|^2) w_+(|x|, |\xi|^2)[\mathcal{F}f](\xi)\,\mathrm{d}\xi \\
&= f(x) + (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} a_-(\hat{x}, \hat{\xi}, |\xi|^2) w_+(|x|, |\xi|^2)[\mathcal{F}f](\xi)\,\mathrm{d}\xi + [Kf](x).
\end{aligned}$$

We have $[(W_- - \mathrm{Id})f](x) = [Zf](x) + [Kf](x)$, where for $x \in \mathbb{R}^n$ we have defined

$$[Zf](x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} a_-(\hat{x}, \hat{\xi}, |\xi|^2) w_+(|x|, |\xi|^2)[\mathcal{F}f](\xi)\,\mathrm{d}\xi.$$

It remains to show that $Z = T(S - \mathrm{Id})$. To see this, we recall that for $\lambda \in \mathbb{R}^+$ and $\omega \in \mathbb{S}^{n-1}$ the scattering operator satisfies $[F_0Sf](\lambda, \omega) = S(\lambda)[F_0f](\lambda, \omega)$, where $S(\lambda) \in \mathcal{B}(L^2(\mathbb{S}^{n-1}))$ is the scattering matrix at energy λ, and by Lemma 2.4.33 we have for

$\theta \in \mathbb{S}^{n-1}$ the expression

$$[(S(\lambda) - \mathrm{Id})g](\theta) = 2\pi i (2\pi)^{-\frac{n+1}{2}} \lambda^{\frac{n-1}{4}} \int_{\mathbb{S}^{n-1}} a_-(\theta, \omega, \lambda) g(\omega) \, \mathrm{d}\omega.$$

Thus, for $\lambda > 0$ and $\theta \in \mathbb{S}^{n-1}$ we have

$$\begin{aligned}[F_0(S - \mathrm{Id})f](\lambda, \theta) &= (S(\lambda) - \mathrm{Id})[F_0 f](\lambda, \theta) \\ &= 2\pi i (2\pi)^{-\frac{n+1}{2}} \lambda^{\frac{n-1}{4}} \int_{\mathbb{S}^{n-1}} a_-(\theta, \omega, \lambda)[F_0 f](\lambda, \omega) \, \mathrm{d}\omega,\end{aligned}$$

so that

$$\int_{\mathbb{S}^{n-1}} a_-(\theta, \omega, \lambda)[F_0 f](\lambda, \omega) \mathrm{d}\omega = \frac{1}{2\pi i} (2\pi)^{\frac{n+1}{2}} \lambda^{-\frac{n-1}{4}} [F_0(S - \mathrm{Id})f](\lambda, \theta). \tag{4.9}$$

Recalling that $[F_0 f](\lambda, \omega) = 2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} [\mathcal{F} f](\lambda^{\frac{1}{2}} \omega)$ we return to the operator Z and decompose into polar coordinates to find for $x \in \mathbb{R}^n$ that

$$\begin{aligned}[Zf](x) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} \int_{\mathbb{S}^{n-1}} r^{n-1} a_-(\hat{x}, \omega, r^2) w_+(|x|, r^2)[\mathcal{F} f](r\omega) \, \mathrm{d}\omega \, \mathrm{d}r \\ &= 2^{-1} (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} \int_{\mathbb{S}^{n-1}} \lambda^{\frac{n-2}{2}} a_-(\hat{x}, \omega, \lambda) w_+(|x|, \lambda)[\mathcal{F} f](\lambda^{\frac{1}{2}} \omega) \, \mathrm{d}\omega \, \mathrm{d}\lambda \\ &= 2^{-\frac{1}{2}} (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} \int_{\mathbb{S}^{n-1}} \lambda^{\frac{n-2}{4}} a_-(\hat{x}, \omega, \lambda) w_+(|x|, \lambda) \left(2^{-\frac{1}{2}} \lambda^{\frac{n-2}{4}} [\mathcal{F} f](\lambda^{\frac{1}{2}} \omega) \right) \mathrm{d}\omega \, \mathrm{d}\lambda \\ &= 2^{-\frac{1}{2}} (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} \int_{\mathbb{S}^{n-1}} \lambda^{\frac{n-2}{4}} a_-(\hat{x}, \omega, \lambda) w_+(|x|, \lambda)[F_0 f](\lambda, \omega) \, \mathrm{d}\omega \, \mathrm{d}\lambda.\end{aligned}$$

Using the relation between a_- and S described in Equation (4.9) we have

$$\begin{aligned}[Zf](x) &= 2^{-\frac{1}{2}} (2\pi i)^{-1} (2\pi)^{\frac{n+1}{2}} (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} \lambda^{\frac{n-2}{4}} \lambda^{-\frac{n-1}{4}} w_+(|x|, \lambda)[F_0(S - \mathrm{Id})f](\lambda, \hat{x}) \, \mathrm{d}\lambda \\ &= 2^{-\frac{1}{2}} (2\pi i)^{-1} (2\pi)^{\frac{1}{2}} \int_{\mathbb{R}^+} \lambda^{\frac{1}{4}} w_+(|x|, \lambda)[F_0(S - \mathrm{Id})f](\lambda, \hat{x}) \, \mathrm{d}\lambda.\end{aligned}$$

Noting that

$$[Tf](x) = \frac{\sqrt{\pi}}{2\pi i} \int_{\mathbb{R}^+} \lambda^{\frac{1}{4}} w_+(|x|, \lambda)[F_0 f](\lambda, \hat{x}) \, \mathrm{d}\lambda, \tag{4.10}$$

we see that $Z = T(S - \mathrm{Id})$ and we are done. □

The operator T satisfies a number of useful properties, summarised in the next theorem.

Theorem 4.2.2. *The operator $T : C_c^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ of Equation (4.6) extends to a bounded operator $T : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ with norm $||T|| \leq 1$. Furthermore,* *the operator T commutes with the dilation group $(U_n(t))$ of Definition 2.2.24 and with all rotations.*

Proof. We first check that T is bounded. Note that $|c_n|^2 = \frac{1}{8\pi}$. For $\tau, \rho \in \mathbb{R}$ we have

$$\int_{\mathbb{R}^+} \mathrm{e}^{-ir(\tau-\rho)}\mathrm{d}r = \frac{i}{\rho-\tau} + \pi\delta(\tau-\rho) \tag{4.11}$$

in the sense of distributions. So for $f \in \mathcal{S}(\mathbb{R}^n)$ we have

$$\begin{aligned}\langle Tf, Tf\rangle &= \int_{\mathbb{R}^n} \overline{[Tf](x)}[Tf](x)\,\mathrm{d}x \\ &= 4|c_n|^2 \int_{\mathbb{R}^n}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+} |x|^{-(n-1)}(\tau\rho)^{\frac{n-1}{2}}\mathrm{e}^{-i|x|(\tau-\rho)}\overline{[\mathcal{F}f](\tau\hat{x})}[\mathcal{F}f](\rho\hat{x})\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}x \\ &= \frac{1}{2\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}(\tau\rho)^{\frac{n-1}{2}}\mathrm{e}^{-ir(\tau-\rho)}\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}r\,\mathrm{d}\omega,\end{aligned}$$

where in the last line we have changed to polar coordinates. Using Equation (4.11) we can compute the r integral and obtain

$$\begin{aligned}\langle Tf, Tf\rangle &= \frac{1}{2\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}(\tau\rho)^{\frac{n-1}{2}}\left(\frac{i}{\rho-\tau}+\pi\delta(\tau-\rho)\right)\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}\omega \\ &= \frac{1}{2}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}(\tau\rho)^{\frac{n-1}{2}}\delta(\tau-\rho)\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}\omega \\ &\quad+ \frac{i}{2\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\frac{(\tau\rho)^{\frac{n-1}{2}}}{\rho-\tau}\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}\omega \\ &:= T_1 + T_2.\end{aligned}$$

Both of these integrals are computable. The first is simply

$$\begin{aligned}T_1 &= \frac{1}{2}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}(\tau\rho)^{\frac{n-1}{2}}\delta(\tau-\rho)\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}\omega \\ &= \frac{1}{2}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\rho^{n-1}|[\mathcal{F}f](\rho\omega)|^2\,\mathrm{d}\rho\,\mathrm{d}\omega = \frac{1}{2}\int_{\mathbb{R}^n}|[\mathcal{F}f](x)|^2\,\mathrm{d}x \\ &= \frac{1}{2}\langle\mathcal{F}f, \mathcal{F}f\rangle.\end{aligned}$$

The second requires a little more care. We make the substitution $\rho = \mathrm{e}^t\tau$, $\mathrm{d}\rho = \mathrm{e}^t\tau\mathrm{d}t$ to obtain

$$\begin{aligned}
T_2 &= \frac{i}{2\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\frac{(\tau\rho)^{\frac{n-1}{2}}}{\rho-\tau}\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\rho\omega)\,\mathrm{d}\rho\,\mathrm{d}\tau\,\mathrm{d}\omega \\
&= \frac{i}{2\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\int_{\mathbb{R}}\frac{\tau^{n-1}\mathrm{e}^{\frac{n-1}{2}t}}{\mathrm{e}^t\tau-\tau}\overline{[\mathcal{F}f](\tau\omega)}[\mathcal{F}f](\mathrm{e}^t\tau\omega)\mathrm{e}^t\tau\,\mathrm{d}t\,\mathrm{d}\tau\,\mathrm{d}\omega \\
&= \frac{i(2\pi)^{\frac{1}{2}}}{4\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\tau^{n-1}\overline{[\mathcal{F}f](\tau\omega)}\left((2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}\frac{2}{\mathrm{e}^{\frac{t}{2}}-\mathrm{e}^{-\frac{t}{2}}}\mathrm{e}^{\frac{nt}{2}}[\mathcal{F}f](\mathrm{e}^t\tau\omega)\,\mathrm{d}t\right)\mathrm{d}\tau\,\mathrm{d}\omega \\
&= \frac{i(2\pi)^{\frac{1}{2}}}{4\pi}\int_{\mathbb{S}^{n-1}}\int_{\mathbb{R}^+}\tau^{n-1}\overline{[\mathcal{F}f](\tau\omega)}\left(-i(2\pi)^{\frac{1}{2}}[\tanh(\pi D_n)\mathcal{F}f](\tau\omega)\right)\mathrm{d}\tau\,\mathrm{d}\omega \\
&= \frac{1}{2}\int_{\mathbb{R}^n}\overline{[\mathcal{F}f](x)}[\tanh(\pi D_n)\mathcal{F}f](x)\,\mathrm{d}x \\
&= \frac{1}{2}\langle\mathcal{F}f,\tanh(\pi D_n)\mathcal{F}f\rangle,
\end{aligned}$$

where we have used the functional calculus for D_n of Lemma 2.2.30. Now note that $0 \leq 1 + \tanh(\pi y) \leq 2$ for all y and thus we find

$$\langle Tf, Tf\rangle = T_1 + T_2 = \frac{1}{2}\langle\mathcal{F}f, (\mathrm{Id} + \tanh(\pi D_n))\mathcal{F}f\rangle \leq \langle\mathcal{F}f, \mathcal{F}f\rangle = \langle f, f\rangle.$$

Since $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$, the operator T extends by continuity to a bounded operator $T : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ with $||T|| \leq 1$. That T commutes with dilations and rotations follows by direct computation. □

Since T commutes with the dilation group U_n, we can consider T as a function of the generator D_n of dilations on $L^2(\mathbb{R}^n)$. Since T commutes with rotations we can decompose $L^2(\mathbb{R}^n)$ into spherical harmonics and compute the action of T on each harmonic component. The spherical harmonic decomposition demonstrated here was proved in dimension three in [98].

Definition 4.2.3. A polynomial P in the variables $x_1, \dots, x_n$ which is homogenous of degree ℓ (so $P(x) = |x|^\ell P(\hat{x})$ for all $x \in \mathbb{R}^n$) which satisfies $\Delta P = 0$ is called a *harmonic polynomial of degree* ℓ. Let V_ℓ be the vector space of harmonic polynomials of degree ℓ in n variables. Define the subspace H_ℓ of *spherical harmonics* by

$$H_\ell = \{f : \mathbb{S}^{n-1} \to \mathbb{C} : f = P|_{\mathbb{S}^{n-1}} \text{ for some } P \in V_\ell\}.$$

Clearly $H_\ell \subset L^2(\mathbb{S}^{n-1})$ and inherits the inner product. The Funcke-Hecke theorem [9, Theorem 9.7.1] allows us to decompose functions on the sphere into spherical harmonics. In particular, the following result shows how to decompose a plane wave into spherical harmonics, which will be particularly useful for decomposing Fourier transforms into spherical harmonic subspaces.

Lemma 4.2.4 ([9, Lemma 9.10.2]). *For any spherical harmonic S_ℓ of degree ℓ in n variables and $\theta \in \mathbb{S}^{n-1}$ we have*

$$\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-it\langle\theta,\omega\rangle} S_\ell(\omega)\,\mathrm{d}\omega = (2\pi)^{\frac{n}{2}} i^{-\ell} S_\ell(\theta) t^{-\frac{n-2}{2}} J_{\ell+\frac{n-2}{2}}(t). \tag{4.12}$$

Thus, for a Schwarz class function $g \in \mathcal{S}(\mathbb{R}^+)$ and $S_\ell \in H_\ell$ we define $f : \mathbb{R}^n \to \mathbb{C}$ by $f(x) = g(|x|)S_\ell(\hat{x})$ and compute for $\xi \in \mathbb{R}^n$ the Fourier transform

$$\begin{aligned}
[\mathcal{F}f](\xi) &= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-i\langle x,\xi\rangle} g(|x|) S_\ell(\hat{x})\,\mathrm{d}x \\
&= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^+} r^{n-1} g(r) \left(\int_{\mathbb{S}^{n-1}} \mathrm{e}^{-ir|\xi|\langle\omega,\hat{\xi}\rangle} S_\ell(\omega)\,\mathrm{d}\omega \right) \mathrm{d}r \\
&= i^{-\ell} S_\ell(\hat{\xi}) \int_{\mathbb{R}^+} (r|\xi|)^{-\frac{n-2}{2}} r^{n-1} g(r) J_{\ell+\frac{n-2}{2}}(r|\xi|)\,\mathrm{d}r.
\end{aligned}$$

The Fourier transform leaves the space $B_\ell = C_c^\infty(\mathbb{R}^+) \otimes H_\ell$ (considered as a subspace of $C_c^\infty(\mathbb{R}^n)$) invariant. Restricting $\mathcal{F}$ to the harmonic subspace B_ℓ defines the operator $\mathcal{F}_\ell : C_c^\infty(\mathbb{R}^+) \subset L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r) \to C_c^\infty(\mathbb{R}^+) \subset L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r)$ for $\eta \in \mathbb{R}^+$ and $g \in L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r)$ by

$$[\mathcal{F}_\ell g](\eta) = i^{-\ell} \int_{\mathbb{R}^+} (r\eta)^{-\frac{n-2}{2}} g(r) J_{\ell+\frac{n-2}{2}}(r\eta)\, r^{n-1}\,\mathrm{d}r. \tag{4.13}$$

The operator $\mathcal{F}_\ell$ is related to the Hankel transform of Definition 2.2.10 and extends to a unitary from $\mathcal{H}_r = L^2(\mathbb{R}^+, r^{n-1}\,\mathrm{d}r)$ to itself, a fact which follows from the Parseval relation for the Hankel transform [113, Theorem I].

Since T commutes with any rotation, T leaves each subspace B_ℓ invariant, so restricts to an operator $T_\ell \otimes \mathrm{Id}$ on each B_ℓ. Recall that T is defined for $f \in C_c^\infty(\mathbb{R}^n)$ by

$$[Tf](x) = 2(2\pi)^{-\frac{n}{2}} c_n |x|^{-\frac{n-1}{2}} \int_{\mathbb{R}^+} \tau^{\frac{n-1}{2}} \mathrm{e}^{i\tau|x|} [\mathcal{F}f](\tau\hat{x})\,\mathrm{d}\tau.$$

Thus we can define an operator $T_\ell : C_c^\infty(\mathbb{R}^+, r^{n-1}\,\mathrm{d}r) \to C_c^\infty(\mathbb{R}^+, r^{n-1}\,\mathrm{d}r)$ for $\eta \in \mathbb{R}^+$ by

$$[T_\ell g](\eta) = 2(2\pi)^{-\frac{n}{2}} c_n \eta^{-\frac{n-1}{2}} \int_{\mathbb{R}^+} \tau^{\frac{n-1}{2}} \mathrm{e}^{i\tau\eta} [\mathcal{F}_\ell g](\tau)\,\mathrm{d}\tau. \tag{4.14}$$

We recall from Lemma 2.2.21 formula for functions of dilation on the half-line,

$$[\varphi(D_+)g](\eta) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\varphi](t) \mathrm{e}^{\frac{t}{2}} g(\mathrm{e}^t\eta)\,\mathrm{d}t,$$

for $g \in C_c^\infty(\mathbb{R}^+)$ and $\eta \in \mathbb{R}^+$. We shall recognise each T_ℓ as a function $\varphi_\ell(D_+)$. The following is a generalisation of [98, Proposition 2].

Proposition 4.2.5. *For each ℓ the operator T_ℓ extends continuously to the bounded oper-*

ator $\varphi_\ell(D_n)$ on $\mathcal{H}_r = L^2(\mathbb{R}^+, r^{n-1}\,\mathrm{d}r)$, where $\varphi_\ell \in C(\mathbb{R})$ has limits at $\pm\infty$ and is defined for $y \in \mathbb{R}^+$ by by

$$\varphi_\ell(y) = i^{-\ell}\mathrm{e}^{-i\frac{n-3}{4}\pi}\frac{1}{2}\frac{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}+iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}-iy\right)\right)}\frac{\Gamma\left(\frac{1}{2}\left(\frac{3}{2}-iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\frac{3}{2}+iy\right)\right)}\left(1+\tanh(\pi y) - i\cosh(\pi y)^{-1}\right). \tag{4.15}$$

Proof. We recall from Equation (4.6) that for $f \in C_c^\infty(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$ the operator T is given by

$$[Tf](x) = k_n|x|^{-\frac{n-1}{2}}\int_{\mathbb{R}^+}\tau^{\frac{n-1}{2}}\mathrm{e}^{i\tau|x|}[\mathcal{F}f](\tau\hat{x})\mathrm{d}\tau,$$

where for convenience we have let $k_n = 2c_n$. On the space $\mathcal{H}_\ell = \{f \in C_c^\infty(\mathbb{R}^n) : f(x) = g(|x|)Y_{\ell m}(\hat{x})$ for some $g \in C_c^\infty(\mathbb{R}^+), Y_{\ell,m} \in P_\ell\}$ we have that $T|_{\mathcal{H}_\ell} = T_\ell \otimes \mathrm{Id}_{P_\ell}$ where $T_\ell : L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r) \to L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r)$ is given for $g \in C_c^\infty(\mathbb{R}^+)$ and $r \in \mathbb{R}^+$ by

$$[T_\ell g](r) = k_n r^{-\frac{n-1}{2}}\int_{\mathbb{R}^+}\tau^{\frac{n-1}{2}}\mathrm{e}^{i\tau r}[\mathcal{F}_\ell g](\tau)\,\mathrm{d}\tau.$$

We recall the Fourier transform restricted to the space $\mathcal{H}_\ell$ has the form $\mathcal{F}|_{\mathcal{H}_\ell} = \mathcal{F}_\ell \otimes \mathrm{Id}_{P_\ell}$, where $\mathcal{F}_\ell : L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r) \to L^2(\mathbb{R}^+, r^{n-1}\mathrm{d}r)$ is given by Equation (4.13). Hence we can write T_ℓ explicitly as

$$\begin{aligned}[T_\ell g](r) &= k_n i^\ell r^{-\frac{n-1}{2}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\tau^{\frac{n-1}{2}}\mathrm{e}^{i\tau r}(\tau\rho)^{-\frac{n-2}{2}}\rho^{n-1}g(\rho)J_{\ell+\frac{n-2}{2}}(\tau\rho)\mathrm{d}\rho\,\mathrm{d}\tau \\ &= k_n i^\ell r^{-\frac{n-1}{2}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\tau^{\frac{1}{2}}\mathrm{e}^{i\tau r}\rho^{\frac{n}{2}}g(\rho)J_{\ell+\frac{n-2}{2}}(\tau\rho)\,\mathrm{d}\rho\,\mathrm{d}\tau.\end{aligned}$$

and so we may use the substitution $\eta = r\mathrm{e}^t$ to write

$$\begin{aligned}[T_\ell g](r) &= k_n i^\ell r^{-\frac{n-1}{2}}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+}\tau^{\frac{1}{2}}\mathrm{e}^{i\tau r}\eta^{\frac{n}{2}}g(\eta)J_{\ell+\frac{n-2}{2}}(\tau\eta)\,\mathrm{d}\eta\,\mathrm{d}\tau \\ &= k_n i^\ell r^{\frac{3}{2}}\int_{\mathbb{R}}\mathrm{e}^{\frac{nt}{2}}g(\mathrm{e}^t r)\mathrm{e}^t\left(\int_{\mathbb{R}^+}\tau^{\frac{1}{2}}\mathrm{e}^{i\tau r}J_{\ell+\frac{n-2}{2}}(\mathrm{e}^t r\tau)\,\mathrm{d}\tau\right)\mathrm{d}t.\end{aligned}$$

Define the distribution ψ_ℓ by

$$\psi_\ell(t) = k_n i^\ell(2\pi)^{\frac{1}{2}}r^{\frac{3}{2}}\mathrm{e}^{-t}\int_{\mathbb{R}^+}\tau^{\frac{1}{2}}\mathrm{e}^{i\tau r}J_{\ell+\frac{n-2}{2}}(\mathrm{e}^{-t}r\tau)\,\mathrm{d}\tau.$$

We now find the Fourier transform $\varphi_\ell = \mathcal{F}\psi_\ell$ and we may write

$$[T_\ell g](r) = (2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}[\mathcal{F}^*\varphi_\ell](-t)\mathrm{e}^{\frac{nt}{2}}g(\mathrm{e}^t r)\,\mathrm{d}t.$$

Thus we compute the Fourier transform as

$$
\begin{aligned}
\varphi_\ell(y) = [\mathcal{F}\psi_\ell](t) &= k_n i^\ell r^{\frac{3}{2}} \int_{\mathbb{R}} \mathrm{e}^{-iyt}\psi(t)\mathrm{d}t \\
&= k_n i^\ell r^{\frac{3}{2}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{-t}\tau^{\frac{1}{2}}\mathrm{e}^{i\tau r} J_{\ell+\frac{n-2}{2}}(\mathrm{e}^{-t}r\tau)\,\mathrm{d}\tau\,\mathrm{d}t \\
&= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell r^{\frac{3}{2}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{-t}\tau^{\frac{1}{2}}(\tau r)^{\frac{1}{2}} K_{\frac{1}{2}}(-i\tau r) J_{\ell+\frac{n-2}{2}}(\mathrm{e}^{-t}r\tau)\,\mathrm{d}\tau\,\mathrm{d}t,
\end{aligned}
$$

where we have used the relation $\mathrm{e}^{-w} = \sqrt{\frac{2}{\pi}}w^{\frac{1}{2}}K_{\frac{1}{2}}(w)$ (here K_ν denotes a modified Bessel function). Making the substitution $v = \mathrm{e}^{-t}r\tau$, $\mathrm{d}\tau = \mathrm{e}^{t}r^{-1}\mathrm{d}v$ we obtain

$$
\begin{aligned}
\varphi_\ell(y) &= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} r^{\frac{3}{2}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{-t}\tau^{\frac{1}{2}}(\tau r)^{\frac{1}{2}} K_{\frac{1}{2}}(-i\tau r) J_{\ell+\frac{n-2}{2}}(\mathrm{e}^{-t}r\tau)\,\mathrm{d}\tau\,\mathrm{d}t \\
&= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} r^{\frac{3}{2}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{-t}v^{\frac{1}{2}}\mathrm{e}^{\frac{t}{2}}r^{-\frac{1}{2}}v^{\frac{1}{2}}\mathrm{e}^{\frac{t}{2}} K_{\frac{1}{2}}(-iv\mathrm{e}^{t}) J_{\ell+\frac{n-2}{2}}(v)\mathrm{e}^{t}r^{-1}\,\mathrm{d}v\,\mathrm{d}t \\
&= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{t}v K_{\frac{1}{2}}(-iv\mathrm{e}^{t}) J_{\ell+\frac{n-2}{2}}(v)\,\mathrm{d}v\,\mathrm{d}t.
\end{aligned}
$$

We now make the substitution $s = v\mathrm{e}^{t}$, $\mathrm{d}t = s^{-1}\mathrm{d}s$ to see that

$$
\begin{aligned}
\varphi_\ell(y) &= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} \int_{\mathbb{R}}\int_{\mathbb{R}^+} \mathrm{e}^{-iyt}\mathrm{e}^{t}v K_{\frac{1}{2}}(-iv\mathrm{e}^{t}) J_{\ell+\frac{n-2}{2}}(v)\,\mathrm{d}v\,\mathrm{d}t \\
&= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} s^{-it}v^{iy}sv^{-1}v K_{\frac{1}{2}}(-is) J_{\ell+\frac{n-2}{2}}(v)s^{-1}\,\mathrm{d}v\,\mathrm{d}s \\
&= \mathrm{e}^{-i\frac{\pi}{4}} k_n i^\ell \sqrt{\frac{2}{\pi}} \left(\int_{\mathbb{R}^+} s^{-iy}K_{\frac{1}{2}}(-is)\mathrm{d}s\right)\left(\int_{\mathbb{R}^+} v^{iy}J_{\ell+\frac{n-2}{2}}(v)\,\mathrm{d}v\right).
\end{aligned}
$$

By [126, p. 10.1] we have

$$
\int_{\mathbb{R}^+} v^{iy}J_{\ell+\frac{n-2}{2}}(v)\mathrm{d}v = 2^{iy}\frac{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}+iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}-iy\right)\right)}.
$$

Using [126, p. 11.1] we find

$$
\int_{\mathbb{R}^+} s^{-iy}K_{\frac{1}{2}}(-is)\mathrm{d}s = 2^{-iy-1}(-i)^{-iy+1}\Gamma\left(\frac{1}{2}\left(\frac{3}{2}-iy\right)\right)\Gamma\left(\frac{1}{2}\left(\frac{1}{2}-iy\right)\right).
$$

Then φ_ℓ is given by

$$
\varphi_\ell(y) = -i\mathrm{e}^{-i\frac{\pi}{4}}\sqrt{\frac{2}{\pi}}k_n i^\ell 2^{-1}\mathrm{e}^{\frac{\pi y}{2}}\frac{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}+iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\ell+\frac{n}{2}-iy\right)\right)}\Gamma\left(\frac{1}{2}\left(\frac{3}{2}-iy\right)\right)\Gamma\left(\frac{1}{2}\left(\frac{1}{2}-iy\right)\right).
$$

A quick calculation shows that

$$\frac{e^{\frac{i\pi}{4}}e^{\frac{\pi y}{2}}}{e^{\frac{\pi i}{4}}e^{\frac{\pi y}{2}} - e^{-\frac{\pi i}{4}}e^{-\frac{\pi y}{2}}} = \frac{e^{\frac{\pi y}{2}}}{e^{\frac{\pi y}{2}} + ie^{-\frac{\pi y}{2}}} = \frac{1}{2}\frac{\cosh(\pi y) + \sinh(\pi y) - i}{\cosh(\pi y)}$$
$$= \frac{1}{2}\left(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}\right).$$

Using the relation $\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}$ with $z = \frac{1}{2}\left(\frac{1}{2} - iy\right)$ we find

$$e^{-\frac{i\pi}{4}}e^{\frac{\pi y}{2}}\Gamma\left(\frac{1}{2}\left(\frac{1}{2} - iy\right)\right) = \frac{\pi}{\Gamma\left(1 - \frac{1}{2}\left(\frac{1}{2} - iy\right)\right)\sin\left(\frac{1}{2}\left(\frac{1}{2} - iy\right)\pi\right)}$$
$$= e^{-\frac{i\pi}{4}}e^{\frac{\pi y}{2}}\frac{2i\pi}{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} + iy\right)\right)\left(e^{\frac{i\pi}{4}}e^{\frac{\pi y}{2}} - e^{-i\frac{\pi}{4}}e^{-\frac{\pi y}{2}}\right)}$$
$$= \frac{i\pi}{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} + iy\right)\right)}\left(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}\right).$$

Thus,

$$\varphi_\ell(y) = \pi k_n i^\ell \sqrt{\frac{2}{\pi}}\frac{1}{2}\frac{\Gamma\left(\frac{1}{2}\left(\ell + \frac{n}{2} + iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\ell + \frac{n}{2} - iy\right)\right)}\frac{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} - iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} + iy\right)\right)}\left(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}\right).$$

Recall that the constant $k_n = 2c_n$ is given by $k_n = -i(2\pi)^{-\frac{1}{2}}e^{-i\frac{n-3}{4}\pi}$ and so we obtain the expression

$$\varphi_\ell(y) = i^{\ell-1}e^{-i\frac{n-3}{4}\pi}\frac{1}{2}\frac{\Gamma\left(\frac{1}{2}\left(\ell + \frac{n}{2} + iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\ell + \frac{n}{2} - iy\right)\right)}\frac{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} - iy\right)\right)}{\Gamma\left(\frac{1}{2}\left(\frac{3}{2} + iy\right)\right)}\left(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}\right).$$

The limits at $\pm\infty$ follow from the asymptotics of the Gamma function (see [1]). □

The result of Proposition 4.2.5 agrees with the result obtained in [98, Proposition 2] in dimension three and that the operator $\varphi_0(D_n) = \frac{1}{2}(\mathrm{Id} + \tanh(\pi D_n) - i\cosh(\pi D_n)^{-1})$ is precisely of the form of the operator of Equation (4.1). To arrive at a simpler formula without the ratio of Gamma functions, we provide a straightforward generalisation of [151, Theorem 4.1] to operator-valued functions.

Lemma 4.2.6. *Suppose that $f \in L^2(\mathbb{R})\cap C(\mathbb{R})$ and $g \in C(\mathbb{R}, \mathcal{K}(\mathcal{P}))$ is such that $g(\pm\infty) = 0$. Let L denote the (densely defined) operator of multiplication by the variable in $L^2(\mathbb{R}^+)$. Then the operator $(f(D_+)\otimes \mathrm{Id})g(\ln(L))$ defines a compact operator on $\mathcal{H}_{spec}$. Similarly if $h \in C(\mathbb{R}^+, \mathcal{K}(\mathcal{P}))$ is such that $h(0) = h(\infty) = 0$, then $(f(D_+)\otimes \mathrm{Id})h(L)$ defines a compact operator on $\mathcal{H}_{spec}$.*

Proof. The algebraic tensor product $C_0(\mathbb{R}) \odot \mathcal{K}(\mathcal{P})$ is dense in $C_0(\mathbb{R}, \mathcal{K}(\mathcal{P}))$ by [133, Theorem 1.15], when $C_0(\mathbb{R}, \mathcal{K}(\mathcal{P}))$ is equipped with the uniform topology. Thus it suffices to prove that for $a \in C_0(\mathbb{R})$ and $b \in \mathcal{K}(\mathcal{P})$ we have

$$(f(D_+) \otimes \mathrm{Id})(a(\ln(L)) \otimes b) = f(D_+)a(\ln(L)) \otimes b$$

is compact. This follows from [151, Theorem 4.1] after a few steps. First we let $u_m \in C_c^\infty(\mathbb{R})$ be an approximate unit for $C_0(\mathbb{R})$. Then $u_m f$ and $u_m a$ are L^2-functions and so

$$(u_m f)(D_+)(u_m a)(\ln(L)) \otimes b$$

is compact by [151, Theorem 4.1], and since D_+ and $\frac{1}{2}\ln(L)$ are canonically conjugate. Now because f and a vanish at $\pm\infty$ we readily see that $(u_m f)(D_+) \to f(D_+)$ in operator norm, and similarly for $(u_m a)(\ln(L))$. As the compacts are norm closed, the limit is compact. The final claim follows by writing $h = g \circ (\ln)$. □

Lemma 4.2.7. *Let $n \geq 4$ and define $\varphi : \mathbb{R} \to \mathbb{C}$ by $\varphi(y) = \frac{1}{2}(1+\tanh(\pi y)-i\cosh(\pi y)^{-1})$. Then $(T - \varphi(D_n))(S - \mathrm{Id})$ is compact.*

Proof. The operator S satisfies $S(0) = \mathrm{Id}$ and the functions φ_ℓ of Proposition 4.2.5 satisfy $\varphi_\ell(\infty) = 1$, $\varphi_\ell(-\infty) = 0$. Thus the difference $T-\varphi(D_n)$ is a function of ℓ and D_n vanishing at $\pm\infty$ of $\sigma(D_n)$ for each ℓ. We also have the limit $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$ in $\mathcal{B}(\mathcal{P})$, a fact which will be proved in Corollary 4.3.10. The operators D_n and $\frac{1}{2}\ln(H_0)$ are canonically conjugate, so by Lemma 4.2.6 the operator $(T - \varphi(D_n))(S - \mathrm{Id})$ is compact. □

The term $\cosh(\pi D_n)^{-1}(S - \mathrm{Id})$ will give rise to a compact operator by an identical argument, however we shall keep it in our formulas for reasons which will become apparent in Section 5.2.3. We also note that Lemma 4.2.7 is not true in dimension $n = 3$ in the presence of resonances, since the scattering operator does not satisfy $S(0) = \mathrm{Id}$.

Whilst the above arguments give the correct formula for the wave operator, it is difficult to prove that the operator K defined by Equation (4.7) is compact directly. To do so would require all the subtleties of the behaviour of the perturbed resolvent $R(z)$ near $z = 0$. Sadly, we have not found a direct proof of the compactness of the operator K defined by Equation (4.7) directly from its definition as the remainder in the construction of generalised plane waves.

In the next section we offer a different proof which starts from the expansion of the resolvent near zero. This method was first used in dimension three in [141], in dimension two in the absence of resonances in [140] and in dimension two with (some) resonances in [142]. By expanding and modifying these arguments we will obtain the formula for the wave function in all cases where $S(0) = \mathrm{Id}$. As a consequence of Theorem 4.0.1, the operator K defined by Equation (4.7) is compact.

Remark 4.2.8. The proof of Proposition 4.2.5 determines the dominant behaviour of T, and one may use the method of stationary phase [56, Theorem 3.38] to obtain a similar expression to Equation (4.1).

4.3 The form of the wave operator

In this section we use the resolvent expansions of Chapter 3 to provide a proof of Theorem 4.0.1. To make use of the results of Chapter 3 we require some additional assumptions on the potential, which we summarise below.

Assumption 4.3.1. In dimension n we fix ρ and t such that

1. if $n = 1$ then $\rho > \frac{5}{2}$;
2. if $n = 2$ then $\rho > 11$;
3. if $n = 3$ then $\rho > 5$ and $t \in (\frac{5}{2}, \rho - \frac{5}{2})$;
4. if $n = 4$ then $\rho > 12$ and $t \in (6, \rho - 6)$; and
5. if $n \geq 5$ then $\rho > \frac{3n+4}{2}$ and $t \in \left(\frac{n}{2}, \rho - \frac{n}{2}\right)$.

We assume that $|V(x)| \leq C(1 + |x|)^{-\rho}$ for almost all $x \in \mathbb{R}^n$.

We separate out dimension $n = 1$ and $n = 2$ from the higher dimensions, since their proofs use different techniques and have appeared in the literature [97, 140, 142]. The case $n = 3$ has also been demonstrated in [141], however the proof technique we use follows closely that of [141] and so this case fits neatly into the narrative with the $n \geq 4$ cases.

4.3.1 Dimension $n = 1$

As we have seen throughout this thesis, dimension $n = 1$ produces atypical behaviour. In [97, Proposition 4] it was shown that in dimension $n = 1$ the operator K defined by Equation (4.7) is compact (Hilbert-Schmidt even) by directly using subtleties related to Jost functions to obtain estimates on the integral kernel, a method which is only available in dimension $n = 1$. The result is the following [97, Proposition 5].

Theorem 4.3.2. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$ and let $A : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be defined by $[Af](x) = f(-x)$. The wave operator W_- is of the form*

$$W_- = \mathrm{Id} + \frac{1}{2} \left(\mathrm{Id} + \tanh\left(\pi D_1\right) + iA \cosh\left(\pi D_1\right)\right) \left(S - \mathrm{Id}\right) + K, \tag{4.16}$$

where K is a compact operator.

The presence of the operator A is an artefact of dimension $n = 1$ only and cannot be removed, however it causes no issues in our later analysis.

4.3.2 Dimension $n = 2$

We first recall the known form of the wave operator in two dimensions in the presence of s-resonances. We then massage the formula from Theorem 4.3.3 to obtain the statement in Theorem 4.0.1. The following is [142, Theorem 1.3].

Theorem 4.3.3. *Let $n = 2$ and V satisfy Assumption* (2.2.14) *for some $\rho > 11$ and suppose that there are no p-resonances. Then there exist two continuous compact operator valued functions $\eta, \tilde{\eta} : \mathbb{R}^+ \to \mathcal{K}(L^2(\mathbb{S}^1))$ vanishing at* 0 *and* ∞ *and satisfying the relation $\eta(H_0) + \tilde{\eta}(H_0) = S - \mathrm{Id}$, and such that the equality*

$$W_- = \mathrm{Id} + \frac{1}{2}\left(\mathrm{Id} + \tanh\left(\frac{\pi D_2}{2}\right)\right)\eta(H_0) + \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_2) - i\cosh(\pi D_2)^{-1}\right)\tilde{\eta}(H_0)$$

holds modulo compacts.

With the help of a technical result, we can show rather simply that Theorem 4.0.1 holds in dimension $n = 2$.

Lemma 4.3.4. *Let $n = 2$ and V satisfy Assumption* (2.2.14) *for some $\rho > 11$ and suppose that there are no p-resonances. Then W_- satisfies Equation* (4.1).

Proof. Consider the difference

$$\begin{aligned} X &= F_0\left(\frac{1}{2}\left(\mathrm{Id} + \tanh\left(\frac{\pi D_2}{2}\right)\right)\eta(H_0) - \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_2) - i\cosh(\pi D_2)^{-1}\right)\eta(H_0)\right)F_0^* \\ &= \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_+) - \mathrm{Id} - \tanh(2\pi D_+) + i\cosh(2\pi D_+)^{-1}\right)\eta(L) \\ &=: Y(D_+)\eta(L). \end{aligned}$$

The function η vanishes at 0 and ∞ and the function Y is continuous and square integrable. Thus an application of Lemma 4.2.6 shows X is compact. Hence W_- has the form given in Equation (4.1). □

4.3.3 Dimension $n \geq 3$

4.3.3.1 Setting up the proof

We will now provide a number of preparatory results before proceeding to the proof of Theorem 4.0.1 for $n \geq 3$. We note that the case $n = 3$ has been proved in [141], however fits neatly into this section.

The proof is broken up into a number of steps, whose ultimate goal is to factorise (in the spectral representation) the wave operator into the composition of several operators, whose mapping properties as operators between various weighted Sobolev spaces can be analysed. The properties of these factor operators depend heavily on their low energy behaviour and we use the resolvent expansions of Chapter 3 to determine this behaviour.

Definition 4.3.5. Define, for $\varepsilon > 0$ and $\lambda \in \mathbb{R}$, the operator $\varphi_\varepsilon(H_0 - \lambda)$ on $\mathcal{H}$ by $\varphi_\varepsilon(H_0 - \lambda) = \frac{\varepsilon}{\pi} R_0(\lambda \mp i\varepsilon) R_0(\lambda \pm i\varepsilon)$. Similarly for $M = F_0 H_0 F_0^*$, the operator of multiplication by the spectral variable, set $\varphi_\varepsilon(M - \lambda) = \frac{\varepsilon}{\pi}(M - (\lambda \mp i\varepsilon))^{-1}(M - (\lambda \pm i\varepsilon))^{-1}$.

By [165, Section 1.4], the limits $\lim_{\varepsilon\to 0} \langle \varphi_\varepsilon(H_0 - \lambda) f, g\rangle$ exist for almost every $\lambda \in \mathbb{R}$ and $f, g \in L^2(\mathbb{R}^n)$. Moreover the limit satisfies Stone's formula (see Corollary 2.1.13)

$$\langle f, g\rangle = \int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \langle \varphi_\varepsilon(H_0 - \lambda) f, g\rangle\right) \mathrm{d}\lambda.$$

Using the symmetrised resolvent identity and the stationary formula for the wave operator in Equation (2.69) we can then show that

$$\langle (W_\pm - \mathrm{Id}) f, g\rangle = -\int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \langle \varphi_\varepsilon(H_0 - \lambda) f, v(U + vR_0(\lambda \mp i\varepsilon)v)^{-1} v R_0(\lambda \pm i\varepsilon) g\rangle\right) \mathrm{d}\lambda.$$

We now derive formulas for the wave operators in the spectral representation of H_0, that is, $F_0(W_- - \mathrm{Id})F_0^*$. Let $M = F_0 H_0 F_0^*$ be the operator of multiplication by the spectral variable. For suitable $f, g \in \mathcal{H}_{spec}$ we compute that

$$\begin{aligned}
&-\langle F_0(W_\pm - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}} \\
&= \int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \langle v(U + vR_0(\lambda \mp i\varepsilon)v)^{-1} v F_0^* \varphi_\varepsilon(M - \lambda) f, F_0^*(M - \lambda \mp i\varepsilon)^{-1} g\rangle_{\mathcal{H}}\right) \mathrm{d}\lambda \\
&= \int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \int_0^\infty \left\langle \left[F_0 v(U + vR_0(\lambda \mp i\varepsilon)v)^{-1} v F_0^* \varphi_\varepsilon(M - \lambda) f\right](\mu, \cdot), \frac{g(\mu, \cdot)}{\mu - \lambda \mp i\varepsilon}\right\rangle_{\mathcal{P}} \mathrm{d}\mu\right) \mathrm{d}\lambda.
\end{aligned}$$

With $M(k) = U + vR_0(z)v$ for $z \in \mathbb{C}\backslash\mathbb{R}$ and $M_\varepsilon(\lambda) = U + vR_0(\lambda \mp i\varepsilon)v$ we have

$$\begin{aligned}
&\langle F_0(W_\pm - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}} \\
&= -\int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \int_0^\infty \left\langle \left[F_0 M_\varepsilon(\lambda)^{-1} F_0^* \varphi_\varepsilon(M - \lambda) f\right](\mu, \cdot), (\mu - \lambda \mp i\varepsilon)^{-1} g(\mu, \cdot)\right\rangle_{\mathcal{P}} \mathrm{d}\mu\right) \mathrm{d}\lambda.
\end{aligned} \tag{4.17}$$

To interchange the limit as $\varepsilon \to 0$ and the integral over μ in Equation (4.17), which we do in subsection 4.3.3.3, we first analyse $F_0 v M_\varepsilon(\lambda)^{-1} v F_0^*$.

4.3.3.2 Analysing the diagonalisation maps

Recall that the trace operator (see Section 2.4) extends to an element of $\mathcal{B}(H^{s,t}, \mathcal{P})$ for each $s > \frac{1}{2}$ and $t \in \mathbb{R}$, and that $\lambda \mapsto \gamma(\lambda) \in \mathcal{B}(H^{s,t}, \mathcal{P})$ is continuous [86, Section 3]. As a consequence the operator $\Gamma_0(\lambda) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{P}$ extends to an element of $\mathcal{B}(H^{s,t}, \mathcal{P})$ for each $s \in \mathbb{R}$ and $t > \frac{1}{2}$, as well as $\lambda \mapsto \Gamma_0(\lambda) \in \mathcal{B}(H^{s,t}, \mathcal{P})$ is continuous.

We need stronger continuity and boundedness results for Γ_0.

Lemma 4.3.6. *Let $n \geq 3$, $s \geq 0$ and $t > \frac{n}{2}$. Then $G_\pm : (0,\infty) \to \mathcal{B}(H^{s,t}, \mathcal{P})$ defined by $G_\pm(\lambda) = \lambda^{\pm\frac{1}{4}}\Gamma_0(\lambda)$ are continuous and bounded.*

Proof. Continuity is immediate from the previous paragraph. For boundedness, it is sufficient to check boundedness of G_- in a neighbourhood of 0 and G_+ in a neighbourhood of ∞.

For the first bound, we analyse the asymptotic development of $\gamma(\lambda^{\frac{1}{2}})$ as $\lambda \to 0$. Recall that for $f \in C_c^\infty(\mathbb{R}^n)$ and $\omega \in \mathbb{S}^{n-1}$ we have

$$[\gamma(\lambda^{\frac{1}{2}})\mathcal{F}f](\omega) = \sum_{j=0}^{K} (i\lambda^{\frac{1}{2}})^j [\gamma_j f](\omega) + O\left(\lambda^{\frac{K+1}{2}}\right).$$

By Lemma 4.1.1 we have $\gamma_j \in \mathcal{B}(H^{0,t}, \mathcal{P})$ for $t > j + \frac{n}{2}$. From this expansion we see that for $t > j + \frac{n}{2}$ and for any $\alpha \leq \frac{n-2}{4}$ we have

$$\lambda^{-\alpha} \left|\left|\Gamma_0(\lambda)\right|\right| = \lambda^{\frac{n-2}{4}-\alpha} 2^{-\frac{1}{2}} \left|\left|\gamma(\lambda^{\frac{1}{2}})\right|\right| \tag{4.18}$$

is bounded in a neighbourhood of zero. Since $n \geq 3$, taking $\alpha = \frac{1}{4}$ gives immediately the statement for G_-.

For the second statement, we refer to [164, Theorem 1.1.4] for the estimate

$$r^{n-1} \int_{\mathbb{S}^{n-1}} |u(r\omega)|^2 \, \mathrm{d}\omega \leq C \left|\left|u\right|\right|^2_{H^{t,0}}, \tag{4.19}$$

valid for $t > \frac{1}{2}$, from which we obtain (with $r = \lambda^{\frac{1}{2}}$ and $u = \mathcal{F}f$) that

$$\begin{aligned} \left|\left|\Gamma_0(\lambda)f\right|\right|^2_{\mathcal{P}} &= \int_{\mathbb{S}^{n-1}} 2^{-1}\lambda^{\frac{n-2}{2}} |[\mathcal{F}f](\lambda^{\frac{1}{2}}\omega)|^2 \, \mathrm{d}\omega = 2^{-1}\lambda^{-\frac{1}{2}} \int_{\mathbb{S}^{n-1}} \lambda^{\frac{n-1}{2}} |[\mathcal{F}f](\lambda^{\frac{1}{2}}\omega)|^2 \, \mathrm{d}\omega \\ &\leq 2^{-1}\lambda^{-\frac{1}{2}} C \left|\left|\mathcal{F}f\right|\right|^2_{H^{t,0}} = 2^{-1}\lambda^{-\frac{1}{2}} C \left|\left|f\right|\right|^2_{H^{0,t}}. \end{aligned} \tag{4.20}$$

This gives us the estimate $\lambda^{\frac{1}{4}} \left|\left|\Gamma_0(\lambda)f\right|\right| \leq \tilde{C} \left|\left|f\right|\right|_{H^{0,t}}$, so that G_+ is bounded as $\lambda \to \infty$. For $s \geq 0$, we use the inclusion $H^{s,t} \subset H^{0,t}$ for any $s \geq 0$. □

From the arguments above we immediately obtain that $\lambda \mapsto \left|\left|\Gamma_0(\lambda)\right|\right|_{\mathcal{B}(H^{s,t},\mathcal{P})}$ is continuous and bounded for $s \geq 0$ and $t > \frac{1}{2}$. We can strengthen Lemma 4.3.6 for G_-.

Lemma 4.3.7. *Let $s \geq 0$ and $t > \frac{n}{2}$. Then $\Gamma_0(\lambda) \in \mathcal{K}(H^{s,t}, \mathcal{P})$ for any $\lambda \in \mathbb{R}^+$ and the function $G_- : \mathbb{R}^+ \to \mathcal{K}(H^{s,t}, \mathcal{P})$ is continuous and vanishes as $\lambda \to \infty$ and as $\lambda \to 0$.*

Proof. The compactness statement follows from the compact embedding $H^{s,t} \subset H^{q,r}$ for any $q < s$, $r < t$. See [8, Proposition 4.1.5].

For continuity, the same argument as the previous lemma works. That G_- vanishes as $\lambda \to 0$ follows from Equation (4.18) and the fact that $\gamma(\lambda^{\frac{1}{2}})\mathcal{F} \to \gamma_0\mathcal{F}$ in the norm of $\mathcal{B}(H^{s,t}, \mathcal{P})$ as $\lambda \to 0$. It remains to check the limit as $\lambda \to \infty$, which follows from the inclusion $H^{s,t} \hookrightarrow H^{0,t}$ for any $s \geq 0$ and the estimate (4.20).

□

We now consider the multiplication operator $G_- : C_c(\mathbb{R}^+, H^{s,t}) \to \mathcal{H}_{spec}$ given by

$$[G_- f](\lambda, \omega) := [G_-(\lambda)f](\lambda, \omega) = \lambda^{-\frac{1}{4}}[\Gamma_0(\lambda)f](\lambda, \omega). \tag{4.21}$$

Lemmas 4.3.6 and 4.3.7 show that the operator G_- extends, for $s \geq 0$ and $t > \frac{1}{2}$, to an element of $\mathcal{B}(L^2(\mathbb{R}^+, H^{s,t}), \mathcal{H}_{spec})$. The next step is to deal with the limit as $\varepsilon \to 0$ of $\varphi_\varepsilon(M - \lambda)$. The following statement and its proof are simple generalisations of [141, Lemma 2.3] to all $n \geq 2$.

Lemma 4.3.8. *Take $s \geq 0$ and $t > \frac{n}{2}$. For $\lambda \in \mathbb{R}^+$ and $f \in C_c(\mathbb{R}^+, \mathcal{P})$ we have*

$$\lim_{\varepsilon \to 0} ||F_0^* \varphi_\varepsilon(M - \lambda)f - \Gamma_0(\lambda)^* f(\lambda)||_{H^{-s,-t}} = 0.$$

Proof. Fix $f \in C_c(\mathbb{R}^+, \mathcal{P})$, $\lambda \in \mathbb{R}^+$ and $\varepsilon > 0$. We use the duality relation of $H^{s,t}$ with $H^{-s,-t}$ to compute that

$$\begin{aligned}
&||F_0^* \varphi_\varepsilon(M - \lambda)f - \Gamma_0(\lambda)^* f(\lambda)||_{H^{-s,-t}} \\
&= \sup_{g \in \mathcal{S}(\mathbb{R}^n), ||g||_{H^{s,t}} = 1} |\langle g, F_0^* \varphi_\varepsilon(M - \lambda)f - \Gamma_0(\lambda)^* f(\lambda)\rangle_{H^{s,t}, H^{-s,-t}}| \\
&= \sup_{g \in \mathcal{S}(\mathbb{R}^n), ||g||_{H^{s,t}} = 1} \left| \frac{1}{\pi} \int_0^\infty \left\langle \Gamma_0(\mu)g, \frac{\varepsilon}{(\mu - \lambda)^2 + \varepsilon^2} f(\mu) \right\rangle_{\mathcal{P}} \mathrm{d}\mu - \langle \Gamma_0(\lambda)g, f(\lambda)\rangle_{\mathcal{P}} \right|.
\end{aligned}$$

For fixed $g \in \mathbb{S}(\mathbb{R}^n)$ with $||g||_{H^{s,t}} = 1$ define the continuous and bounded function $h : \mathbb{R}^+ \to \mathbb{C}$ by

$$h(\mu) = \langle \Gamma_0(\mu)g, f(\mu)\rangle_{\mathcal{P}}.$$

By an application of the Plemelj formula (see also [161, Theorem 9.8]) we have that

$$\lim_{\varepsilon \to 0} \frac{1}{\pi} \int_0^\infty \frac{\varepsilon}{(\mu - \lambda)^2 + \varepsilon^2} h(\mu)\, \mathrm{d}\mu = h(\lambda). \tag{4.22}$$

Since $||f(\cdot)||_{\mathcal{P}}$ and $||\Gamma_0(\cdot)||_{\mathcal{B}(H^{s,t}, \mathcal{P})}$ are bounded, we have that h is bounded by a constant independent of g. So an application of Equation (4.22) gives

$$\begin{aligned}
&\lim_{\varepsilon\to 0} ||F_0^*\varphi_\varepsilon(M-\lambda)f - \Gamma_0(\lambda)^* f(\lambda)||_{H^{-s,-t}} \\
&= \lim_{\varepsilon\to 0} \sup_{g\in\mathcal{S}(\mathbb{R}^n),||g||_{H^{s,t}}=1} \left| \frac{1}{\pi}\int_0^\infty \left\langle \Gamma_0(\mu)g, \frac{\varepsilon}{(\mu-\lambda)^2+\varepsilon^2} f(\mu)\right\rangle_{\mathcal{P}} \mathrm{d}\mu - \langle \Gamma_0(\lambda)g, f(\lambda)\rangle_{\mathcal{P}} \right| \\
&= 0,
\end{aligned}$$

as claimed. □

From now on we only consider the operator W_- since our resolvent results have only been in the upper-half-plane. Similar results could be derived in the lower-half-plane, however the operator W_+ can be obtained in a much simpler manner from the relation $W_+ = W_- S^*$ at a later stage.

Lemma 4.3.9. *Suppose that $n \geq 3$ ρ, t and V satisfy Assumption 4.3.1, and that there are no resonances for $n = 4$. Then the function $B : \mathbb{R}^+ \to \mathcal{B}(\mathcal{P}, H^{0,\rho-t})$ defined by $B(\lambda) = \lambda^{\frac{1}{4}} vM_0(\lambda)^{-1} v\Gamma_0(\lambda)^*$ is continuous and bounded, and $B : C_c(\mathbb{R}^+, \mathcal{P}) \to L^2(\mathbb{R}^+, H^{0,\rho-t})$ defined by $[Bf](\lambda) = B(\lambda)f(\lambda)$ extends to an element of $\mathcal{B}(\mathcal{H}_{spec}, L^2(\mathbb{R}^+, H^{0,\rho-t}))$.*

Proof. The continuity of B follows from the limiting absorption principle (Theorem 2.4.8). For boundedness, it is sufficient to show that the map $\lambda \mapsto ||B(\lambda)||_{\mathcal{B}(\mathcal{P},H^{0,\rho-t})}$ is bounded in a neighbourhood of 0 and in a neighbourhood of ∞. For $\lambda \geq 1$, a symmetrised analogue of Lemma 2.4.10 shows that the function $\lambda \mapsto ||vM_0(\lambda)^{-1}v||_{\mathcal{B}(H^{0,-t},H^{0,\rho-t})}$ is bounded provided $\rho > \frac{n+1}{2}$, which is guaranteed by our assumptions. We also know from Lemma 4.3.6 that the function $\mathbb{R}^+ \ni \lambda \mapsto \lambda^{\frac{1}{4}} ||\Gamma_0(\lambda)^*||_{\mathcal{B}(\mathcal{P},H^{0,-t})}$ is bounded. This shows that $\lambda \mapsto ||B(\lambda)||_{\mathcal{B}(\mathcal{P},H^{0,\rho-t})}$ is bounded in a neighbourhood of ∞.

For λ in a neighbourhood of 0, we use asymptotic developments for $M_0(\lambda)$ in Chapter 3 and $\Gamma_0(\lambda)^*$ in Section 4.1.1. The asymptotics of $\Gamma_0(\lambda)$ are discussed in Lemma 4.1.2. By taking adjoints in Lemma 4.1.2, we see that for each $s \geq 0$ we have the expansion

$$\Gamma_0(\lambda)^* = 2^{-\frac{1}{2}}\lambda^{\frac{n-2}{4}}(\gamma_0^* - i\lambda^{\frac{1}{2}}\gamma_1^* + O(\lambda)^{\frac{1}{2}})$$

in $\mathcal{B}(\mathcal{P}, H^{s,-t})$ as $\lambda \to 0$.

The form of the asymptotic development of $M_0(\lambda)^{-1}$ as $\lambda \to 0$ depends heavily on the (non)existence of zero energy eigenvalues and resonances as seen in Chapter 3. For $n \geq 5$ the behaviour as $\lambda \to 0$ of $M_0(\lambda)$ is described explicitly in Theorem 3.2.9 (for n odd) and Theorem 3.2.19 (for n even) as

$$M_0(\lambda)^{-1} = \lambda^{-1}D_1 + \tilde{R}(\lambda^{\frac{1}{2}}),$$

in $\mathcal{B}(\mathcal{H})$ as $\lambda \to 0$ where $\tilde{R}$ is uniformly bounded. So the lowest order power of λ in the expansion of $\lambda^{\frac{1}{4}} vM_0(\lambda)^{-1} v\Gamma_0(\lambda)^*$ is the term $\lambda^{\frac{n-5}{4}} vD_1 v\gamma_0^*$. So we see that $\lambda^{\frac{1}{4}} vM_0(\lambda)^{-1} v\Gamma_0(\lambda)^*$

is bounded in $\mathcal{B}(\mathcal{P}, H^{0,\rho-t})$ as $\lambda \to 0$ for $n \geq 5$.

We now consider $n = 4$. For the asymptotic development of $M_0(\lambda)^{-1}$, we appeal to Theorem 3.2.37. We obtain (with φ a normalised vector in $T_1\mathcal{H}$) the expansion

$$M_0(\lambda)^{-1} = \lambda^{-1} D_2 + \lambda^{-1} h(-i\lambda^{\frac{1}{2}}) \langle \varphi, \cdot \rangle \varphi - \ln(\lambda) C_1 + \tilde{R}(\lambda^{\frac{1}{2}})$$

as $\lambda \to 0$ in $\mathcal{B}(H^{1,-t}, H^{0,t})$, where $\tilde{R}$ is uniformly bounded. Hence, we find as $\lambda \to 0$ that

$$\begin{aligned}\lambda^{\frac{1}{4}} v M_0(\lambda)^{-1} v \Gamma_0(\lambda)^* &= 2^{-\frac{1}{2}} \lambda^{\frac{3}{4}} v \left(\lambda^{-1} D_2 + \lambda^{-1} h(-i\lambda^{\frac{1}{2}}) \langle v\varphi, \cdot \rangle v\varphi - \ln(\lambda) C_1 + \tilde{R}(\lambda^{\frac{1}{2}})) \right) \\ &\quad \times v \left(\gamma_0^* - i\lambda^{\frac{1}{2}} \gamma_1^* + o(\lambda^{\frac{1}{2}}) \right) \\ &= 2^{-\frac{1}{2}} \left(\lambda^{-\frac{1}{4}} D_2 \gamma_0^* + \lambda^{-\frac{1}{4}} h(-i\lambda^{\frac{1}{2}}) \langle v\varphi, \cdot \rangle v\varphi + o(\lambda^{\frac{1}{4}} \ln(\lambda)) \right).\end{aligned}$$

There are two terms of concern here as $\lambda \to 0$. The first is the term $\lambda^{-\frac{1}{4}} v D_2 v \gamma_0^*$, which vanishes by the fact $Q_2 P = 0$. The second is the term containing φ, which blows up as $\lambda \to 0$. Thus, we make the assumption $\varphi = 0$, namely there are no resonances in dimension $n = 4$.

Finally we consider $n = 3$. For the asymptotic development of $M_0(\lambda)^{-1}$, we appeal to Theorem 3.2.57. We obtain the expansion

$$M_0(\lambda)^{-1} = \lambda^{-1} D_2 + \lambda^{-\frac{1}{2}} C_{-\frac{1}{2}} + \tilde{R}(\lambda),$$

where $\tilde{R}$ is uniformly bounded. Then as $\lambda \to 0$,

$$\begin{aligned}\lambda^{\frac{1}{4}} v M_0(\lambda)^{-1} v \Gamma_0(\lambda)^* &= 2^{-\frac{1}{2}} \lambda^{\frac{1}{2}} v (\lambda^{-1} D_2 + \lambda^{-\frac{1}{2}} C_{-\frac{1}{2}} + \tilde{R}(\lambda)) v \left(\gamma_0^* - i\lambda^{\frac{1}{2}} \gamma_1^* + o(\lambda^{\frac{1}{2}}) \right) \\ &= 2^{-\frac{1}{2}} \lambda^{-\frac{1}{2}} v D_2 v \gamma_0^* + C_{-\frac{1}{2}} + o(\lambda^{\frac{1}{2}}).\end{aligned}$$

The only term of concern here is $v D_2 v \gamma_0^*$ which vanishes since $Q_2 P = 0$. □

We note that in dimension $n = 3$ a nonsymmetrised proof of Lemma 4.3.9 can be found as [141, Lemma 2.4]. The case $n = 2$ has been resolved in [140] in the non-resonant case and [142] in the case of s-resonances but not p-resonances. The presence of certain resonances in dimensions $n = 2$ and $n = 4$ is well-known to produce complicated behaviour in scattering theory, see for instance [73, Theorem III.3], [29, Theorem 6.3] and the analysis of Chapter 3, and so it is not surprising that we must exclude them in our analysis for dimension $n = 4$, as is done in [142] for dimension $n = 2$. Despite the differing behaviour of resonances in dimensions $n = 2$ and $n = 4$, the analysis required to handle the resonant contributions is similar and is work in progress. We also note the following essential corollary of Lemmas 4.3.7 and 4.3.9.

Corollary 4.3.10. *Suppose that V, ρ and t satisfy Assumption 4.3.1. Then for $n \geq 2$*

we have the equality $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$ *in the norm of* $\mathcal{B}(\mathcal{P})$.

Proof. For dimension $n \geq 3$, $G_-(\lambda)$ and $B(\lambda)$ satisfy $G_-(\lambda)B(\lambda) = S(\lambda) - \mathrm{Id}$. Since G_- vanishes as $\lambda \to \infty$ and B is bounded we have the desired result. In dimension $n = 2$, the statement is an immediate corollary of [142, Theorem 1.3]. □

Remark 4.3.11. The convergence of $S(\lambda) \to \mathrm{Id}$ as $\lambda \to \infty$ in Corollary 4.3.10 is in $\mathcal{B}(\mathcal{P})$. When comparing with the equality $\mathrm{Det}(S(\lambda)) = \mathrm{e}^{-2\pi i\xi(\lambda)}$ we must be careful to note that when this equality holds it is a priori only valid in the trace norm. In fact as a further corollary we note that in dimensions $n = 2, 3$, $S(\lambda)$ cannot converge as $\lambda \to \infty$ in trace norm, except possibly when $[\mathcal{F}V](0) = 0$.

4.3.3.3 Interchanging limits

In this subsection we interchange the integral over λ and the limit as $\varepsilon \to 0$ in Equation (4.17). For fixed $\varepsilon, \lambda > 0$ and $s \in \mathbb{R}$ we define for $f, g \in C_c^\infty(\mathbb{R}^+, \mathcal{P})$ the following functions

$$\begin{aligned} h_\varepsilon(\lambda) &:= \lambda^{\frac{1}{4}} v M_\varepsilon(\lambda)^{-1} v F_0^* \varphi_\varepsilon(M - \lambda) f \in H^{0,s}, \quad \text{and} \\ p(\lambda) &:= \lambda^{-\frac{1}{4}} \Gamma_0(\lambda)^* g(\lambda) \in H^{0,-s}. \end{aligned} \tag{4.23}$$

We also denote by

$$q_\lambda(\nu) = \begin{cases} \left(\frac{\nu+\lambda}{\lambda}\right)^{\frac{1}{4}} p(\nu+\lambda) & \nu > -\lambda \\ 0 & \nu \leq -\lambda \end{cases} \tag{4.24}$$

the extension by zero of the function $(-\lambda, \infty) \ni \nu \mapsto \left(\frac{\nu+\lambda}{\lambda}\right)^{\frac{1}{4}} p(\nu+\lambda) \in H^{0,-s}$ to all of $\mathbb{R}$.

Lemma 4.3.12. *Let* $n \geq 4$ *and suppose that* ρ, t *satisfy Assumption 4.3.1, and that there are no resonances for* $n = 4$. *If* $|V(x)| \leq C(1+|x|)^{-\rho}$ *then*

$$\langle F_0(W_- - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}} = -i \int_{\mathbb{R}^+} \int_0^\infty \left\langle h_0(\lambda), \int_0^\infty \mathrm{e}^{i\nu z} q_\lambda(\nu)\, \mathrm{d}\nu \right\rangle_{H^{0,s}, H^{0,-s}} \mathrm{d}z\, \mathrm{d}\lambda.$$

Proof. Take $f \in C_c(\mathbb{R}^+, \mathcal{P})$ and $g \in C_c^\infty(\mathbb{R}^+) \odot C(\mathbb{S}^{n-1})$, and set $m = \rho - t$. We may then write the expression (4.17), using the functions h_ε and p defined in Equation (4.23), as

$$\begin{aligned} &\langle F_0(W_- - \mathrm{Id})F_0^* f, g\rangle \\ &= -\int_{\mathbb{R}} \left(\lim_{\varepsilon\to 0} \int_0^\infty \langle v M_\varepsilon(\lambda) v F_0^* \varphi_\varepsilon(M-\lambda) f, (\mu - \lambda + i\varepsilon)^{-1} \Gamma_0(\mu)^* g(\mu) \rangle_{H^{0,m}, H^{0,-m}}\, \mathrm{d}\mu \right) \mathrm{d}\lambda \\ &= -\int_{\mathbb{R}^+} \left(\lim_{\varepsilon\to 0} \int_{\mathbb{R}^+} \left\langle h_\varepsilon(\lambda), \frac{\lambda^{-\frac{1}{4}} \mu^{\frac{1}{4}}}{\mu - \lambda + i\varepsilon} p(\mu) \right\rangle_{H^{0,m}, H^{0,-m}} \mathrm{d}\mu \right) \mathrm{d}\lambda. \end{aligned}$$

Now we make the estimate

$$\int_{\mathbb{R}^+}\left|\left\langle h_\varepsilon(\lambda), \frac{\lambda^{-\frac14}\mu^{\frac14}}{\mu-\lambda+i\varepsilon}p(\mu)\right\rangle_{H^{0,m},H^{0,-m}}\right|\mathrm{d}\mu$$
$$\le ||h_\varepsilon(\lambda)||_{H^{0,m}}\,\lambda^{-\frac14}\int_{\mathbb{R}^+}\mu^{\frac14}((\mu-\lambda)^2+\varepsilon^2)^{-\frac12}\,||p(\mu)||_{H^{0,-m}}\,\mathrm{d}\mu<\infty, \tag{4.25}$$

since p is defined in terms of g, which is compactly supported. Use the formula

$$(\mu-\lambda+i\varepsilon)^{-1}=-i\int_0^\infty \mathrm{e}^{i(\mu-\lambda)z}\mathrm{e}^{-\varepsilon z}\,\mathrm{d}z$$

and Fubini's theorem (valid by the estimate (4.25)) to obtain

$$\lim_{\varepsilon\to0}\int_0^\infty\left\langle h_\varepsilon(\lambda), \frac{\lambda^{-\frac14}\mu^{\frac14}}{\mu-\lambda+i\varepsilon}p(\mu)\right\rangle_{H^{0,m},H^{0,-m}}\mathrm{d}\mu$$
$$=-i\lim_{\varepsilon\to0}\int_0^\infty \mathrm{e}^{-\varepsilon z}\left(\left\langle h_\varepsilon(\lambda),\int_0^\infty \mathrm{e}^{i(\mu-\lambda)z}\lambda^{-\frac14}\mu^{\frac14}p(\mu)\,\mathrm{d}\mu\right\rangle_{H^{0,m},H^{0,-m}}\right)\mathrm{d}z$$
$$=-i\lim_{\varepsilon\to0}\int_0^\infty \mathrm{e}^{-\varepsilon z}\left(\left\langle h_\varepsilon(\lambda),\int_{-\lambda}^\infty \mathrm{e}^{i\nu z}\left(\frac{\nu+\lambda}{\lambda}\right)^{\frac14}p(\nu+\lambda)\,\mathrm{d}\nu\right\rangle_{H^{0,m},H^{0,-m}}\right)\mathrm{d}z, \tag{4.26}$$

where in the last line we have made a change of variables to recognise a Fourier transform. The z-integrand of (4.26) can be bounded independently of $\varepsilon\in(0,1)$ explicitly with

$$\left|\mathrm{e}^{-\varepsilon z}\left\langle h_\varepsilon(\lambda),\int_{-\lambda}^\infty \mathrm{e}^{i\nu z}\left(\frac{\nu+\lambda}{\lambda}\right)^{\frac14}p(\nu+\lambda)\,\mathrm{d}\nu\right\rangle_{H^{0,m},H^{0,-m}}\right|$$
$$\le ||h_\varepsilon(\lambda)||_{H^{0,m}}\left|\left|\int_{-\lambda}^\infty \mathrm{e}^{i\nu z}\left(\frac{\nu+\lambda}{\lambda}\right)^{\frac14}p(\nu+\lambda)\,\mathrm{d}\nu\right|\right|_{H^{0,-m}}:=||h_\varepsilon(\lambda)||_{H^{0,m}}\,j_\lambda(z), \tag{4.27}$$

where we have used $\mathrm{e}^{-\varepsilon z}\le 1$. We also know from Lemma 4.3.8 that as $\varepsilon\to0$, $h_\varepsilon(\lambda)$ converges to $\lambda^{\frac14}vM_0(\lambda)^{-1}v\Gamma_0(\lambda)^*f(\lambda)$ in $H^{0,m}$. Therefore the family $||h_\varepsilon(\lambda)||_{H^{0,m}}$ (and thus the entire expression (4.27)) is bounded by a constant independent of $\varepsilon\in(0,1)$.

In order to exchange the integral over z and the limit as $\varepsilon\to0$ in Equation (4.26), it remains to show that the function j_λ of (4.27) is in $L^1(\mathbb{R}^+,\mathrm{d}z)$. Recall q_λ from Equation (4.24). Note that j_λ in (4.27) can be rewritten as $j_\lambda(z)=(2\pi)^{\frac12}\,||[\mathcal{F}^*q_\lambda](z)||_{H^{0,-m}}$ (here the Fourier transform is one-dimensional).

To estimate j_λ, we denote by $D=-i\frac{\partial}{\partial\nu}$ the self-adjoint operator acting (densely) on $L^2(\mathbb{R})$ and by $Y=(\mathrm{Id}+D^2)$. Then,

$$||[\mathcal{F}^*q_\lambda](z)||_{H^{0,-m}}=(1+z^2)^{-1}\,||[\mathcal{F}^*Yq_\lambda](z)||_{H^{0,-m}}\,. \tag{4.28}$$

The function $z \mapsto (1+z^2)^{-1}$ is in $L^1(\mathbb{R}^+, \mathrm{d}z)$ and so it suffices to show $||[\mathcal{F}^* Y q_\lambda](z)||_{H^{0,-m}}$ is bounded independently of z. Suppose that $g = \eta \otimes \xi \in C_c^\infty(\mathbb{R}^+) \otimes C(\mathcal{P})$ is a simple tensor, so that

$$\left(\frac{\nu+\lambda}{\lambda}\right)^{\frac{1}{4}} [p(\nu+\lambda)](x) = 2^{-\frac{1}{2}}(2\pi)^{-\frac{n}{2}}\lambda^{-\frac{1}{4}}(\nu+\lambda)^{\frac{n-2}{4}}\eta(\nu+\lambda)\int_{\mathbb{S}^{n-1}} \mathrm{e}^{i(\nu+\lambda)^{\frac{1}{2}}\langle x,\omega\rangle}\xi(\omega)\,\mathrm{d}\omega.$$

Differentiating with respect to ν twice shows that there are $\eta_{j,\lambda} \in C_c^\infty(\mathbb{R}^+)$ such that for $x \in \mathbb{R}^n$ we have

$$\begin{aligned}[Y q_\lambda](\nu)(x) = \eta_{1,\lambda}(\nu)\int_{\mathbb{S}^{n-1}} \mathrm{e}^{i(\nu+\lambda)^{\frac{1}{2}}\langle x,\omega\rangle}\xi(\omega)\,\mathrm{d}\omega + \eta_{2,\lambda}(\nu)\int_{\mathbb{S}^{n-1}} \langle x,\omega\rangle \mathrm{e}^{i(\nu+\lambda)^{\frac{1}{2}}\langle x,\omega\rangle}\xi(\omega)\,\mathrm{d}\omega \\ + \eta_{3,\lambda}(\nu)\int_{\mathbb{S}^{n-1}} (\langle x,\omega\rangle)^2 \mathrm{e}^{i(\nu+\lambda)^{\frac{1}{2}}\langle x,\omega\rangle}\xi(\omega)\,\mathrm{d}\omega.\end{aligned}$$

Estimating each term individually we obtain $C_1, C_2, C_3, C > 0$ such that

$$|[\mathcal{F}^* Y q_\lambda](z)(x)| \le C_1 + C_2|x| + C_3|x|^2 \le C(1+|x|^2),$$

which gives

$$||[[\mathcal{F}^* Y q_\lambda](z)](x)| \le C(1+|x|^2).$$

For $\tau(x) = (1+|x|^2)$, we compute

$$||\tau||^2_{H^{0,-m}} = \int_{\mathbb{R}^n} (1+|x|^2)^{-\frac{m}{2}}(1+|x|^2)\,\mathrm{d}x = \mathrm{Vol}(\mathbb{S}^{n-1})\int_0^\infty r^{n-1}(1+r^2)^{1-\frac{m}{2}}\,\mathrm{d}r,$$

which is finite for $n-m-1 < -1$, or $m > n+2$. So $\tau \in H^{0,-m}$ for $m > n+2$.

We note in passing that the condition on $m = \rho - t$ requires $\rho > n+t+2$, which is guaranteed by Assumption 4.3.1.

By linearity, for each $g \in C_c^\infty(\mathbb{R}^+) \odot C(\mathbb{S}^{n-1})$ we find that $||[\mathcal{F}^* Y q_\lambda](z)||_{H^{0,-m}}$ is bounded independently of z. So using Equation (4.28) we have $||[\mathcal{F}^* q_\lambda](z)||_{H^{0,-m}} \le \tilde{C}(1+z^2)^{-1}$, and so $||[\mathcal{F}^* q_\lambda](z)||_{H^{0,-m}} \in L^1(\mathbb{R}^+)$.

As a consequence, we can apply Lebesgue's dominated convergence theorem to exchange the limit as $\varepsilon \to 0$ with the integral over z in Equation (4.26) and obtain

$$\begin{aligned}&-i\lim_{\varepsilon\to 0}\int_0^\infty \mathrm{e}^{-\varepsilon z}\left(\left\langle h_\varepsilon(\lambda), \int_{-\lambda}^\infty \mathrm{e}^{i\nu z}\left(\frac{\nu+\lambda}{\lambda}\right)^{\frac{1}{4}} p(\nu+\lambda)\,\mathrm{d}\nu\right\rangle_{H^{0,m},H^{0,-m}}\right)\mathrm{d}z \\ &= -i\left\langle h_0(\lambda), \int_0^\infty\int_{\mathbb{R}} \mathrm{e}^{i\nu z} q_\lambda(\nu)\,\mathrm{d}\nu\,\mathrm{d}z\right\rangle_{H^{0,m},H^{0,-m}}.\end{aligned}$$

Hence on a dense set of f, g,

$$\langle F_0(W_- - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}} = -i \int_{\mathbb{R}^+} \int_0^\infty \left\langle h_0(\lambda), \int_{\mathbb{R}} \mathrm{e}^{i\nu z} q_\lambda(\nu)\,\mathrm{d}\nu \right\rangle_{H^{0,m}, H^{0,-m}} \mathrm{d}z\,\mathrm{d}\lambda. \quad \square$$

Remark 4.3.13. The proof of Lemma 4.3.12 shows how the various requirements on ρ in Assumption 4.3.1 are obtained. In particular, in Lemma 2.4.10 we assumed $\rho > \frac{n+1}{2}$ and in Lemma 4.1.1 we required $t > \frac{n}{2}$. In Lemma 4.3.12 we required $\rho > n + t + 2$ which gives $\rho > \frac{3n+4}{2}$ for $n \geq 5$. The case $n = 4$ requires $\rho > 11$ to use Theorem 3.2.37.

4.3.3.4 The function of dilation and completion of proof

We recall from Section 2.2.3 D_+, the self-adjoint generator of dilations on $L^2(\mathbb{R}^+)$. Lemma 2.2.21 allows us to take functions of D_+ via

$$[\psi(D_+)f](x) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\psi](t)[U_+(t)f](x)\,\mathrm{d}t.$$

We introduce the function $\psi \in C(\mathbb{R}) \cap L^\infty(\mathbb{R})$ defined by

$$\psi(x) = \frac{1}{2}\left(1 - \tanh(2\pi x) - i\cosh(2\pi x)^{-1}\right). \tag{4.29}$$

The Hilbert spaces $L^2(\mathbb{R}^+, H^{s,t})$ and $\mathcal{H}_{spec}$ can be naturally identified with the Hilbert spaces $L^2(\mathbb{R}^+) \otimes H^{s,t}$ and $L^2(\mathbb{R}^+) \otimes \mathcal{P}$. We recall the operator G_- of Equation (4.21) and B of Lemma 4.3.9.

Theorem 4.3.14. *Let $n \geq 4$. Suppose that ρ, t satisfy Assumption 4.3.1, and that there are no resonances for $n = 4$. Then*

$$F_0(W_- - \mathrm{Id})F_0^* = -2\pi i G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,\rho-t}})B$$

in $\mathcal{B}(\mathcal{H}_{spec})$.

Proof. Take $f \in C_c(\mathbb{R}^+, \mathcal{P})$ and $g \in C_c^\infty(\mathbb{R}^+) \odot C(\mathbb{S}^{n-1})$, and set $m = \rho - t$. We show that $\langle F_0(W_- - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}}$ is equal to $\langle -2\pi i G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,m}})Bf, g\rangle_{\mathcal{H}_{spec}}$. Write χ_+ for the characteristic function of $\mathbb{R}^+$ and note that q_λ has compact support to obtain (in the sense of distributions with values in $H^{0,-m}$),

$$\begin{aligned}\int_0^\infty \int_{\mathbb{R}} \mathrm{e}^{i\nu z} q_\lambda(\nu)\,\mathrm{d}\nu\,\mathrm{d}z &= (2\pi)^{\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\chi_+](\nu) q_\lambda(\nu)\,\mathrm{d}\nu \\ &= (2\pi)^{\frac{1}{2}} \int_{-\lambda}^\infty [\mathcal{F}^*\chi_+](\nu) \left(\frac{\nu+\lambda}{\lambda}\right)^{\frac{1}{4}} p(\nu+\lambda)\,\mathrm{d}\nu \\ &= (2\pi)^{\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\chi_+](\lambda(\mathrm{e}^\mu-1))\lambda \mathrm{e}^{\frac{5\mu}{4}} p(\mathrm{e}^\mu\lambda)\,\mathrm{d}\mu \\ &= (2\pi)^{\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}^*\chi_+](\lambda(\mathrm{e}^\mu-1))\lambda \mathrm{e}^{\frac{3\mu}{4}} [(U_+(\mu)\otimes \mathrm{Id}_{H^{0,-m}})p](\lambda)\,\mathrm{d}\mu.\end{aligned}$$

Next, note that the inverse Fourier transform of the characteristic function χ_+ is the distribution $[\mathcal{F}^*\chi_+](y) = \pi^{\frac{1}{2}} 2^{-\frac{1}{2}}\delta(y) + i(2\pi)^{-\frac{1}{2}}\mathrm{Pv}\frac{1}{y}$ (here Pv denotes the principal value), from which we obtain

$$\int_0^\infty \int_{\mathbb{R}} \mathrm{e}^{i\nu z} q_\lambda(\nu)\,\mathrm{d}\nu\,\mathrm{d}z = \int_{\mathbb{R}} \left(\pi\delta(\mathrm{e}^\mu - 1) + i\mathrm{Pv}\frac{\mathrm{e}^{\frac{3\mu}{4}}}{\mathrm{e}^\mu - 1}\right) [(U_+(\mu)\otimes \mathrm{Id}_{H^{0,-s}})p](\lambda)\,\mathrm{d}\mu$$

Next, note that

$$\frac{\mathrm{e}^{\frac{3\mu}{4}}}{\mathrm{e}^\mu - 1} = \frac{1}{4}\left(\frac{1}{\sinh\left(\frac{\mu}{4}\right)} + \frac{1}{\cosh\left(\frac{\mu}{4}\right)}\right)$$

and the Fourier transform of the function ψ of Equation (4.29) is [84, Table 20.1]

$$[\mathcal{F}\psi](\mu) = \pi^{\frac{1}{2}} 2^{-\frac{1}{2}}\delta(\mathrm{e}^\mu - 1) + \frac{i}{4}(2\pi)^{-\frac{1}{2}}\mathrm{Pv}\left(\frac{1}{\sinh\left(\frac{\mu}{4}\right)} + \frac{1}{\cosh\left(\frac{\mu}{4}\right)}\right).$$

Combining these facts,

$$\begin{aligned}\langle F_0(W_- - \mathrm{Id} f, g\rangle_{\mathcal{H}_{spec}} = i \int_{\mathbb{R}^+} \Bigg\langle h_0(\lambda), \int_{\mathbb{R}} \Bigg(\pi\delta(\mathrm{e}^\mu - 1) + \frac{1}{4}\mathrm{Pv}\left(\frac{1}{\sinh\left(\frac{\mu}{4}\right)} + \frac{1}{\cosh\left(\frac{\mu}{4}\right)}\right) \\ \times [(U_+(\mu)\otimes \mathrm{Id}_{H^{0,-m}})p](\lambda)\Bigg)\,\mathrm{d}\mu \Bigg\rangle_{H^{0,m},H^{0,-m}} \mathrm{d}\lambda.\end{aligned}$$

Since $[Bf](\lambda) = h_0(\lambda)$, $p = G_-^* g$ and

$$(\psi(D_+)\otimes \mathrm{Id}_{H^{0,m}})^* p = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} [\mathcal{F}\psi](\mu)(U_+(\mu)\otimes \mathrm{Id}_{H^{0,m}})p\,\mathrm{d}\mu.$$

Combining these facts we obtain

$$\begin{aligned}\langle F_0(W_- - \mathrm{Id})F_0^* f, g\rangle_{\mathcal{H}_{spec}} &= 2\pi i \int_{\mathbb{R}^+} \big\langle [Bf](\lambda), [(\psi(D_+)^* \otimes \mathrm{Id}_{H^{0,-s}})G_-^* g](\lambda)\big\rangle_{H^{0,m},H^{0,-m}} \,\mathrm{d}\lambda \\ &= \langle -2\pi i G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,m}})Bf, g\rangle_{\mathcal{H}_{spec}}.\end{aligned}$$

Density of $C_c(\mathbb{R}^+, \mathcal{P})$ and $C_c^\infty(\mathbb{R}^+) \odot C(\mathbb{S}^{n-1})$ in $\mathcal{H}_{spec}$ concludes the proof. □

The following is a straightforward generalisation of [141, Lemma 2.7].

Lemma 4.3.15. *Take $s \geq 0$ and $t > \frac{n}{2}$, and suppose that there are no resonances for $n = 4$. Then the difference*

$$(\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}})G_- - G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{s,t}}) \tag{4.30}$$

is in $\mathcal{K}(L^2(\mathbb{R}^+, H^{s,t}), \mathcal{H}_{spec})$.

Proof. Define the unitary operator $J : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+)$ by

$$[Jf](\lambda) = \lambda^{-\frac{1}{2}} f(\ln(\lambda)).$$

Then J satisfies $[J^* U_+(t) J f](x) = f(x + t)$ and $[J^* \mathrm{e}^{it\ln(M)} J f](x) = \mathrm{e}^{itx} f(x)$ for each $x, t \in \mathbb{R}$, with M the operator of multiplication by the variable in $L^2(\mathbb{R}^+)$. It follows that $J^* D_+ J = D$ on $\mathrm{Dom}(D)$ and $J^* \ln(M) J = X$ on $\mathrm{Dom}(X)$, where D and X are the operators of momentum and position in $L^2(\mathbb{R})$.

Take $f_1, f_2 : \mathbb{R} \to \mathbb{C}$ with limits at $\pm\infty$. A result of Cordes [8, Theorem 4.1.10] implies $[f_1(D), f_2(X)] \in \mathcal{K}(L^2(\mathbb{R}))$. Conjugating with the unitary operator J, we find that $[f_1(D_+), f_3(M)] \in \mathcal{K}(L^2(\mathbb{R}^+))$, with $f_3 = f_2 \circ \ln$.

We know that $[Q\xi](\lambda) = q(\lambda)\xi(\lambda)$ for $\xi \in C_c(\mathbb{R}^+, H^{s,t})$ and $\lambda \in \mathbb{R}^+$, with $q \in C([0,\infty], \mathcal{K}(H^{s,t}, \mathcal{P}))$, when $C([0,\infty], \mathcal{K}(H^{s,t}, \mathcal{P}))$ is equipped with the uniform topology [133, Theorem 1.15]. So for each $\varepsilon > 0$ there exists $n \in \mathbb{N}$, $a_j \in C([0,\infty])$ and $b_j \in \mathcal{K}(H^{s,t}, \mathcal{P})$ such that

$$\left\| N - \sum_{j=1}^{k} a_j(M) \otimes b_j \right\|_{\mathcal{B}(L^2(\mathbb{R}^+, H^{s,t}), \mathcal{H}_{spec})} < \varepsilon.$$

So in order to prove our claim, it is sufficient to show that the operator

$$\begin{aligned}&(\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}) \left(\sum_{j=1}^{n} a_j(M) \otimes b_j \right) - \left(\sum_{j=1}^{n} a_j(M) \otimes b_j \right) (\psi(D_+) \otimes \mathrm{Id}_{H^{s,t}}) \\ &= \sum_{j=1}^{n} [\psi(D_+), a_j(M)] \otimes b_j\end{aligned}$$

is compact. We know that $b_j \in \mathcal{K}(H^{s,t}, \mathcal{P})$ and that $[\psi(D_+), a_j(M)] \in \mathcal{K}(L^2(\mathbb{R}^+))$. It follows that the operator (4.30) is compact, since finite sums and tensor products of compact operators are compact operators (see [77, Theorem 2]). □

Recall from Lemma 2.2.26 that the generator of dilations D_n satisfies $F_0 D_n F_0^* = -2D_+ \otimes \mathrm{Id}_{\mathcal{P}}$. Defining $\varphi(x) = \frac{1}{2}(1 + \tanh(\pi x) - i \cosh(\pi x)^{-1})$, we have

$$F_0 \varphi(D_n) F_0^* = \psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}. \tag{4.31}$$

We can now prove the main result.

Proof of Theorem 4.0.1. Using Equation (4.31) at the last equality, we deduce from Theorem 4.3.14 and Lemma 4.3.15 that

$$\begin{aligned} W_- - \mathrm{Id} &= -2\pi i F_0^* G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,\rho-t}}) B F_0 \\ &= -2\pi i F_0^* \big[G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,\rho-t}}) - (\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}) G_- + (\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}) G_-\big] B F_0 \\ &= -2\pi i F_0^* (\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}) G_- B F_0 + K \\ &= \varphi(D_n) F_0^* (-2\pi i) G_- B F_0 + K, \end{aligned}$$

with $K := -2\pi i F_0^* \big(G_-(\psi(D_+) \otimes \mathrm{Id}_{H^{0,\rho-t}}) - (\psi(D_+) \otimes \mathrm{Id}_{\mathcal{P}}) G_-\big) B F_0 \in \mathcal{K}(\mathcal{H})$. Note that the last equality follows from Equation (4.31). Using Theorem 2.4.32, we compute

$$-2\pi i [G_- B f](\lambda, \omega) = -2\pi i [\Gamma_0(\lambda) v M_0(\lambda)^{-1} v \Gamma_0(\lambda)^* f(\lambda, \cdot)](\omega) = [(S(\lambda) - \mathrm{Id}) f(\lambda, \cdot)](\omega).$$

Thus $F_0^*(-2\pi i) G_- B F_0 = S - \mathrm{Id}$, proving the claim. □

Corollary 4.3.16. *Suppose that V satisfies Assumption 4.3.1, that there are no p resonances in dimension $n = 2$ and no resonances in dimension $n = 4$. Then the operator K defined by Equation* (4.7) *is compact.*

In the next chapter we show that as an immediate consequence of Theorem 4.0.1 we can view Levinson's theorem in all dimensions as an index theorem as discussed in [98, Sections 4-6]. In Chapter 5 we discuss this topological interpretation and use the result of Theorem 4.0.1 to give a new topological interpretation of Levinson's theorem.

Chapter 5

Levinson's theorem as an index pairing

The form of the wave operator found in Theorem 4.0.1 allows us to view Levinson's theorem in a topological manner in multiple ways. In [97, 98, 140, 141, 142] it is shown in low dimensions that Levinson's theorem is an index theorem by considering the wave operator as an element of a particular C^*-algebra and computing the winding number of its image in a Toeplitz algebra. In Section 5.1 we describe in detail the Toeplitz algebra approach of Kellendonk and Richard [97, 98] and demonstrate using Theorem 4.0.1 how it applies to the wave operator of higher dimensional scattering. Of particular interest is the nature in which resonances contribute to the winding number as considered in dimension $n = 1$ [97] and dimension $n = 3$ [98].

We next demonstrate a new topological approach to Levinson's theorem by reinterpreting the problem as an index pairing. In Section 5.2 we construct a class of Fredholm operators W_U indexed by a particular family of unitaries $\{U\} \subset \mathcal{B}(\mathcal{H})$. Each such unitary U defines a K-theory class $[U]$ and can be paired with the K-homology class $[D_+]$ of the dilation operator, which we construct in Section 5.2.1. We show in Theorem 5.2.14 that such a pairing computes the quantity $\text{Index}(W_U)$. Theorem 4.0.1 shows that generically we have the equality $W_- = W_S$ and as a consequence we reinterpret Levinson's theorem as an index pairing in Theorem 5.3.2. This pairing is joint work with Adam Rennie and appears in the preprint [5] in the non-resonant case.

The existence of zero energy resonances causes obstructions to the existence of such a pairing and as such some care is required to modify the index pairing to handle this information. In Section 5.3.1 we provide the necessary modifications in dimension $n = 1$ to obtain an index pairing in all cases in Theorem 5.3.15. Using results of [97] we obtain the a new proof of the well-known Levinson's theorem [108] in dimension $n = 1$ in Theorem 5.3.16. Such a statement also allows us to completely determine the spectral shift function for the pair (H, H_0) in any generic or resonant case.

In Section 5.3.2 we provide the required modifications to obtain an index pairing in the resonant case in dimension $n = 3$ in Theorem 5.3.20. Unfortunately, the high energy behaviour of the scattering matrix in trace norm provides an additional obstruction to using the index pairing to obtain computational formulae for the index. In Section 5.3.2 we consider a unitary related to S with better trace norm decay at infinity in order to construct in Lemma 5.3.22 an element of the class $[W_-]$ which can be used to obtain a new proof of the well-known Levinson's theorem in dimension $n = 3$ [31], which we state and prove in Theorem 5.3.24. Such a statement of Levinson's theorem allows us to completely determine the spectral shift function for the pair (H, H_0) in both the generic and resonant case.

In Section 5.3.3 in dimension $n = 2$ we proceed as in dimension $n = 3$ by constructing in Lemma 5.3.28 an element of $[W_-]$ with better trace norm properties which can be used in Theorem 5.3.29 to obtain (in the case of no p-resonances) a new proof of the known Levinson theorem of [26, Theorem 6.3] (see also [50, Theorem 3.2]). We can further use Theorem 5.3.29 to completely determine the spectral shift function for the pair (H, H_0) in the case of no p-resonances.

In Section 5.3.4 we demonstrate the necessary modifications to construct in Lemma 5.3.33 an element of $[W_-]$ which we use in Theorem 5.3.34 a new proof of Levinson's theorem in higher dimensions (with the additional assumption that there are no resonances in dimension $n = 4$). Unfortunately Theorem 5.3.34 has the drawback that most of the correction terms provided by Lemma 5.3.33 are not easily computable. We demonstrate the easiest cases of dimension $n = 4, 5$ to illustrate this difficulty. We then use Theorem 5.3.34 to obtain a complete characterisation of the spectral shift function for the pair (H, H_0).

5.1 Levinson's theorem as an index theorem

As an immediate consequence of the form of the wave operator in Theorem 4.0.1 we can view Levinson's theorem as an index theorem by considering the wave operator as an element of a particular C^*-algebra and computing the winding number of its image under a quotient map. Such results have appeared in various forms in [97, 98, 138, 140, 141]. In particular we refer to the review article [138] for greater detail.

We construct a C^*-algebra which contains the wave operator as an element. Let

$$C(\overline{\mathbb{R}^+}, \mathcal{K}(\mathcal{P})) = \{f \in C(\mathbb{R}^+, \mathcal{K}(\mathcal{P})) : \lim_{y\to\infty} f(y) \text{ exists}\} \quad \text{and}$$
$$C(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P})) = \{g \in C(\mathbb{R}, \mathcal{K}(\mathcal{P})) : \lim_{x\to\pm\infty} g(x) \text{ exists}\},$$

each equipped with the sup norm. The ideals of functions vanishing at the endpoints are

$$C_0(\overline{\mathbb{R}^+}, \mathcal{K}(\mathcal{P})) = \{f \in C_0(\mathbb{R}^+, \mathcal{K}(\mathcal{P})) : \lim_{y\to\infty} f(y) = 0\} = C_0(\mathbb{R}^+, \mathcal{K}(\mathcal{P})) \quad \text{and}$$
$$C_0(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P})) = \{g \in C(\mathbb{R}, \mathcal{K}(\mathcal{P})) : \lim_{x\to\pm\infty} g(x) = 0\} = C_0(\mathbb{R}, \mathcal{K}(\mathcal{P})).$$

Note that the continuity here refers to norm continuity.

Definition 5.1.1. Define E to be the C^*-algebra generated by

$$E := \left\{g(D_n)f(H_0) : f \in C(\overline{\mathbb{R}^+}, \mathcal{K}(\mathcal{P})), g \in C(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P}))\right\}.$$

Define J to be the ideal generated by

$$J := \left\{g(D_n)f(H_0) : f \in C_0(\mathbb{R}, \mathcal{K}(\mathcal{P})), g \in C_0(\mathbb{R}^+, \mathcal{K}(\mathcal{P}))\right\}.$$

Note that the C^*-algebra E is nonunital, since the space $\mathcal{P}$ is not finite dimensional (except in dimension $n = 1$). C^*-algebras isomorphic to E and J have been studied in a different context in [68], where the isomorphism is given by the Mellin transform. The key relation is $\frac{1}{2}[D_n, \ln(H_0)] = i$, the canonical commutation relation. In a similar manner, we can consider the pair X of multiplication by the variable and the Dirac operator D acting on $L^2(\mathbb{R})$ and construct a C^*-algebra.

Definition 5.1.2. Define $E_{D,X}$ to be the C^*-algebra generated by all $f(D)g(X)$ such that $f, g \in C(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P}))$ (that is f, g are continuous with limits at $\pm\infty$) and $J_{D,X}$ to be the subalgebra generated by all $f(D)g(X)$ such that $f, g \in C_0(\mathbb{R}, \mathcal{K}(\mathcal{P}))$ (that is f, g are continuous and vanish at $\pm\infty$).

Lemma 5.1.3. *The subalgebra $J_{D,X}$ is a an ideal in $E_{D,X}$ and $J_{D,X} \cong \mathcal{K}(L^2(\mathbb{R}))$.*

Proof. That $J_{D,X}$ is an ideal in $E_{D,X}$ is a simple check. That $J_{D,X} \cong \mathcal{K}(L^2(\mathbb{R}))$ is the statement of [68, Corollary 2.18], however we provide also a more elementary proof based on the Stone-von Neumann theorem.

Since the pair (D, X) satisfy the canonical commutation relations, any $f, g \in C_0(\mathbb{R})$ satisfy $f(X)g(D) \in \mathcal{K}(L^2(\mathbb{R}))$ by [151, Theorem 4.1], so $J_{D,X} \subseteq \mathcal{K}(L^2(\mathbb{R}))$. For the reverse inclusion, fix $K \in \mathcal{K}(L^2(\mathbb{R}))$ and approximate K by a sequence (K_N) of finite rank operators, so that $||K - K_N|| \to 0$ as $N \to \infty$. Write

$$K_N = \sum_{j=1}^{N} \langle \xi_j, \cdot\rangle \eta_j$$

for $(\xi_j), (\eta_j) \subset L^2(\mathbb{R})$. Approximate each ξ_j and η_j by $\tilde{\xi}_j$ and $\tilde{\eta}_j$ with $\tilde{\xi}_j, \tilde{\eta}_j \in C_0(\mathbb{R}) \cap L^2(\mathbb{R})$

(and thus each $\tilde{\xi}_j, \tilde{\eta}_j$ vanishes at $\pm\infty$). Then

$$\tilde{K}_N := \sum_{j=1}^{N} \langle \tilde{\xi}_j, \cdot \rangle \tilde{\eta}_j$$

satisfies $\tilde{K}_N \in J_{D,X}$ and converges in norm to K. Since $J_{D,X}$ is a closed two-sided ideal, $K \in J_{D,X}$ also so $J_{D,X} = \mathcal{K}(L^2(\mathbb{R}))$. □

We provide a convenient description of the quotient $E_{D,X}/J_{D,X}$ for explicit computations. Let $q : E_{D,X} \to E_{D,X}/J_{D,X}$ be the quotient map. Consider the square $\blacksquare = [-\infty, \infty] \times [-\infty, \infty]$ whose boundary $\square$ is the union of the four edges $E_1 = \{-\infty\} \times [-\infty, \infty]$, $E_2 = [-\infty, \infty] \times \{\infty\}$, $E_3 = \{\infty\} \times [-\infty, \infty]$, and $E_4 = [-\infty, \infty] \times \{-\infty\}$. We identify the space $C(\square)$ with the subalgebra of $C([-\infty, \infty])^{\oplus 4}$ given by elements $\Gamma = (\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ which coincide at the corresponding endpoints. That is, $\Gamma_1(\infty) = \Gamma_2(-\infty)$, $\Gamma_2(\infty) = \Gamma_3(\infty)$, $\Gamma_3(-\infty) = \Gamma_4(\infty)$ and $\Gamma_4(-\infty) = \Gamma_1(-\infty)$.

Lemma 5.1.4. *The algebras $C(\square)$ and $E_{D,X}/J_{D,X}$ are isomorphic. In particular, for any $f, g \in C(\overline{\mathbb{R}})$ we have the relation*

$$q(f(D)g(X)) = (f(-\infty)g(\cdot), f(\cdot)g(\infty), f(\infty)g(\cdot), f(\cdot)g(-\infty)). \tag{5.1}$$

Proof. This is the statement of [68, Proposition 3.22]. □

From Lemma 5.1.4 we obtain a short exact sequence

$$0 \to \mathcal{K}(L^2(\mathbb{R})) \to E_{D,X} \xrightarrow{q} C(\square) \to 0. \tag{5.2}$$

Let $\mathcal{M} : L^2(\mathbb{R}^+) \to L^2(\mathbb{R}^+)$ be the Mellin transform of Definition 2.2.22 and let $B = -M_{\ln}$ be the operator of multiplication by $-\ln$ on $L^2(\mathbb{R}^+)$. Note that $B = -\ln(L)$ where L is the operator of multiplication by the variable in $L^2(\mathbb{R}^+)$, $\mathcal{M}D_+\mathcal{M}^* = X$, and $\mathcal{M}B\mathcal{M}^* = D$. For $f \in C(\overline{\mathbb{R}})$ we have the relation

$$\mathcal{M}^* f(D)\mathcal{M} = f(\mathcal{M}^* D\mathcal{M}) = f(B) = f(-\ln(L)) = g(L), \tag{5.3}$$

where $g = f \circ (-\ln) \in C(\overline{\mathbb{R}^+})$. This motivates the following definition.

Definition 5.1.5. Let E_{L,D_+} be the C^*-algebra generated by $f(L)g(D_+)$ with $f \in C(\overline{\mathbb{R}^+}, \mathcal{K}(\mathcal{P}))$ and $g \in C(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P}))$. Let J_{L,D_+} be the subalgebra generated by $f(L)g(D_+)$ with $f \in C_0(\overline{\mathbb{R}^+}, \mathcal{K}(\mathcal{P}))$ and $g \in C_0(\overline{\mathbb{R}}, \mathcal{K}(\mathcal{P}))$.

Lemma 5.1.6. *The C^*-algebras E_{L,D_+} and $E_{D,X}$ are isomorphic.*

Proof. This follows from the relations $\mathcal{M}D_+\mathcal{M}^* = X$ and $\mathcal{M}B\mathcal{M}^* = D$ combined with Equation (5.3). □

One can perform an identical identification procedure for $E_{L,D_+}/J_{L,D_+}$ with functions on a square. Consider the square $\blacksquare' = [0,\infty]\times[-\infty,\infty]$ whose boundary $\square'$ is the union of the four edges $B_1 = \{0\}\times[-\infty,\infty]$, $B_2 = [0,\infty]\times\{\infty\}$, $B_3 = \{\infty\}\times[-\infty,\infty]$ and $B_4 = [0,\infty]\times\{-\infty\}$. Identify the space $C(\square')$ with the subalgebra of $C([-\infty,\infty])\oplus C([0,\infty])\oplus C([-\infty,\infty])\oplus C([0,\infty])$ given by elements $\Gamma = (\Gamma_1,\Gamma_2,\Gamma_3,\Gamma_4)$ which coincide at the corresponding endpoints. That is, $\Gamma_1(\infty) = \Gamma_2(0)$, $\Gamma_2(\infty) = \Gamma_3(\infty)$, $\Gamma_3(-\infty) = \Gamma_4(\infty)$ and $\Gamma_4(0) = \Gamma_1(-\infty)$. After defining the quotient map $q' : E_{L,D_+} \to E_{L,D_+}/J_{L,D_+}$ one also obtains a short exact sequence

$$0 \to \mathcal{K}(L^2(\mathbb{R}^+)) \to E_{L,D_+} \xrightarrow{q'} C(\square') \to 0. \tag{5.4}$$

Lemma 5.1.7. *[138] We have the isomorphism* $E_{L,D_+}/J_{L,D_+} \cong C(\square')$.

The following index theoretic result is the basis of the interpretation of Levinson's theorem as an index theorem.

Theorem 5.1.8 ([138, Theorem 4.4])**.** *Suppose that $\mathcal{H}$ is a separable Hilbert space and that $E \subset \mathcal{B}(\mathcal{H})$ is a unital C^*-algebra with $\mathcal{K}(\mathcal{H}) \subset E$ and $E/\mathcal{K}(\mathcal{H}) \cong C(\mathbb{S}^1)$ (with quotient map q). Let $U \in E/\mathcal{K}(\mathcal{H})$ be a unitary. Then there exists an integer $m \in \mathbb{Z}$ such that for any Fredholm lift W of U with W a Fredholm partial isometry, we have the equality*

$$\mathrm{Wind}(U) = m\mathrm{Tr}([\mathrm{Id} - W^*W] - [\mathrm{Id} - WW^*]) = m\mathrm{Index}(W).$$

Proof. The existence of $m \in \mathbb{Z}$ is the statement of [145, Proposition 9.2.4]. In fact by [145, Example 8.3.2] we have $m = \pm 1$. □

Using the identification of Lemma 5.1.7 we can obtain more information about Fredholm elements of our C^*-algebra E_{L,D_+}. The following is the basic tool for computing the index of our wave operators, first stated in this context as [97, Proposition 7].

Theorem 5.1.9. *Suppose that $T \in E_{L,D_+}$ is a Fredholm operator and let the image of T under the quotient map be $q(T) = (\Gamma_1,\Gamma_2,\Gamma_3,\Gamma_4) \in E_{L,D_+}/J_{L,D_+}$. Suppose further that the maps Γ_j are piecewise differentiable and the integrals*

$$w_j = \frac{1}{2\pi i}\int_{B_j} \mathrm{Tr}(\Gamma_j(y)^*\Gamma_j(y)')\,\mathrm{d}y \tag{5.5}$$

exist. Then we have the equality

$$\mathrm{Index}(T) = \sum_{j=1}^{4} w_j. \tag{5.6}$$

That the index can be computed as a winding number this way is a consequence of the Gohberg-Kreĭn Theorem (see [69, Theorem 10.1]).

5.2 Constructing an index pairing

We now show how the formula for the wave operator implies that the number of bound states can be computed as an index pairing between K-theory and K-homology, see [45, 76]. The index pairing we present is based on the form of the wave operator constructed in Chapter 4, and thus the case of resonances in dimensions $n = 2, 4$ is ruled out. In dimension $n = 1$ generically and in dimension $n = 3$ in the case of resonances some subtleties are required to define an index pairing, since $S(0) \neq \mathrm{Id}$. In dimension $n \geq 2$, further subtleties are required to use the index pairing to deduce statements of Levinson's theorem due to the behaviour of $S(\lambda)$ as $\lambda \to \infty$ in trace norm.

5.2.1 The spectral triple

We first recall the definition of a spectral triple.

Definition 5.2.1. An *odd spectral triple* $(\mathcal{A}, \mathcal{H}, \mathcal{D})$ is given by a Hilbert space $\mathcal{H}$, a dense $*$-subalgebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ acting on $\mathcal{H}$, and a densely defined unbounded self-adjoint operator $\mathcal{D}$ such that:

1. $a \cdot \operatorname{dom} \mathcal{D} \subset \operatorname{dom} \mathcal{D}$ for all $a \in \mathcal{A}$, so that $da := [\mathcal{D}, a]$ is densely defined. Moreover, da extends to a bounded operator for all $a \in \mathcal{A}$;
2. $a(1 + \mathcal{D}^2)^{-1/2} \in \mathcal{K}(\mathcal{H})$ for all $a \in \mathcal{A}$.

Spectral triples define classes in the K-homology of the norm closure $\overline{\mathcal{A}}$, a C^*-algebra [16, 44]. We will produce a spectral triple for $C_c^\infty((0, \infty), \mathcal{K})$ where $\mathcal{K}$ is the compact operators on $L^2(\mathbb{S}^{n-1})$.

Lemma 5.2.2. *The spaces $L^2(\mathbb{R}, \mathrm{d}x)$ and $L^2(\mathbb{R}^+, \mathrm{d}y)$ are unitarily equivalent via the map $W : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+)$ given by*

$$[Wf](y) = y^{-\frac{1}{2}} f(\ln(y)) \tag{5.7}$$

with adjoint $W^* : L^2(\mathbb{R}^+, \mathrm{d}y) \to L^2(\mathbb{R}, \mathrm{d}x)$ given by $[W^*g](x) = \mathrm{e}^{\frac{x}{2}} g(\mathrm{e}^x)$.

Proof. This is a simple check. □

Lemma 5.2.3. *The two spectral triples*

$$\left(C_c^\infty(\mathbb{R}), L^2(\mathbb{R}, \mathrm{d}x), \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right) \quad \textit{and} \quad \left(C_c^\infty(\mathbb{R}^+), L^2(\mathbb{R}^+, \mathrm{d}y), \frac{y}{i}\frac{\mathrm{d}}{\mathrm{d}y} + \frac{1}{2i}\right)$$

are unitarily equivalent.

Proof. Conjugating $\frac{y}{i}\frac{\mathrm{d}}{\mathrm{d}} + \frac{1}{2i}$ by $W : L^2(\mathbb{R}) \to L^2(\mathbb{R}^+)$ gives $\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}$. □

Since $-i\frac{\mathrm{d}}{\mathrm{d}x}$ defines a non-trivial (indeed generating) K-homology class for $C_0(\mathbb{R})$, we see that the generator of dilations on the half-line defines a non-trivial K-homology class for $C_0(\mathbb{R}^+)$.

Using this identification we immediately get the following in our context.

Corollary 5.2.4. *The data* $(C_c^\infty(\mathbb{R}^+)\otimes\mathcal{K}(L^2(\mathbb{S}^{n-1})), L^2(\mathbb{R}^+)\otimes L^2(\mathbb{S}^{n-1}), D_+\otimes\mathrm{Id})$ *defines an odd spectral triple, and so a class* $[D_+]$ *in odd* K*-homology.*

5.2.2 Generalised wave operators

Motivated by the form of the wave operator demonstrated in Chapter 4 we define a class of Fredholm operators, parametrised by particular unitaries, which allow us to reinterpret Levinson's theorem as an index pairing, as well as accounting for the contribution of resonances in dimension 1 and 3. As usual, we let D_n be the generator of the dilation group on $\mathcal{H} = L^2(\mathbb{R}^n)$. Let $A \in \mathcal{B}(\mathcal{H})$ be a self-adjoint involution which commutes with D_n and define the operator

$$\varphi(D_n) = \mathrm{Id} + \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_n) - i\cosh(\pi D_n)^{-1}A\right). \tag{5.8}$$

If $T \in \mathcal{B}(\mathcal{H})$ commutes with H_0, there exists a family $\{T(\lambda)\}_{\lambda\in\mathbb{R}^+}$ of bounded operators on $L^2(\mathbb{S}^{n-1})$ such that $[F_0TF_0^*f](\lambda,\omega) = T(\lambda)f(\lambda,\omega)$ for all $f \in L^2(\mathbb{R}^+)\otimes L^2(\mathbb{S}^{n-1})$ and $(\lambda,\omega) \in \mathbb{R}^+\otimes\mathbb{S}^{n-1}$. We call $T(\cdot)$ the matrix of T.

Definition 5.2.5. We say that a unitary $U \in \mathcal{B}(\mathcal{H})$ is *admissable* if $[U, H_0] = 0$, the matrix of U is norm continuous in $\lambda \in \mathbb{R}^+$ and $U(\lambda) - \mathrm{Id} \in \mathcal{K}(\mathcal{P})$ for all $\lambda \in \mathbb{R}^+$. We say that U is *properly admissable* if in addition we have $U(0) = \lim_{\lambda\to\infty} U(\lambda) = \mathrm{Id}$ (where the limit is taken in $\mathcal{B}(\mathcal{P})$).

Lemma 5.2.6. *Let* $U \in \mathcal{B}(\mathcal{H})$ *be a properly admissable unitary. Then* U *defines a class* $[U] \in K_1\left((C_0(\mathbb{R}^+)\otimes\mathcal{K}(\mathcal{P}))^\sim\right)$.

Proof. By definition $U \in ((C_0(\mathbb{R}^+)\otimes\mathcal{K}(\mathcal{P}))^\sim$ and thus defines a K-theory class $[U] \in K_1\left((C_0(\mathbb{R}^+)\otimes\mathcal{K}(\mathcal{P}))^\sim\right)$. □

Lemma 5.2.7. *Let* $U \in \mathcal{B}(\mathcal{H})$ *be a properly admissable unitary and* $K \in \mathcal{K}(\mathcal{H})$*. Then the operator* $W_U \in \mathcal{B}(\mathcal{H})$ *defined by*

$$W_U = \mathrm{Id} + \varphi(D_n)(U - \mathrm{Id}) + K, \tag{5.9}$$

is a Fredholm operator. Furthermore, $F_0W_UF_0^* \in E_{L,D_+}$.

Proof. We show that W_U^* is an inverse for W_U up to compacts. We compute

$$\begin{aligned}W_U W_U^* &= (\mathrm{Id} + \varphi(D_n))(U - \mathrm{Id}) + K)\left(\mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + K^*\right) \\ &= \mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + \varphi(D_n)(U - \mathrm{Id}) + \varphi(D_n)(U - \mathrm{Id})(U^* - \mathrm{Id})\varphi(D_n)^* \\ &\quad + K\left(\mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + K^*\right) + \left(\varphi(D_n)(U - \mathrm{Id}) + K\right)K^*.\end{aligned}$$

The term $K_1 = K\left(\mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + K^*\right) + \left(\varphi(D_n)(U - \mathrm{Id}) + K\right)K^*$ is compact, since the compact operators form an ideal, so

$$W_U W_U^* = \mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + \varphi(D_n)(U - \mathrm{Id}) + \varphi(D_n)(U - \mathrm{Id})(U^* - \mathrm{Id})\varphi(D_n)^* + K_1.$$

Note that A is a self-adjoint involution which commutes with all functions of D_n. Then

$$\begin{aligned}\varphi(D_n)\varphi(D_n)^* &= \frac{1}{4}\Big(\mathrm{Id} + 2\tanh(\pi D_n) + i\cosh(\pi D_n)^{-1}A + i\tanh(\pi D_n)A^*\cosh(\pi D_n)^{-1} \\ &\quad + \tanh(\pi D_n)^2 - i\cosh(\pi D_n)^{-1}A + \cosh(\pi D_n)^{-1}A\cosh(\pi D_n)^{-1}A^* \\ &\quad - i\cosh(\pi D_n)^{-1}A\tanh(\pi D_n)\Big) \\ &= \frac{1}{4}\Big(\mathrm{Id} + 2\tanh(\pi D_n) + \tanh(\pi D_n)^2 + \cosh(\pi D_n)^{-2}\Big) \\ &= \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_n)\right),\end{aligned}$$

where in the last line we have used the equality $\cosh(y)^{-2} + \tanh(y)^2 = 1$. Since $\cosh(\cdot)^{-2} \in L^2(\mathbb{R})$ and $U(0) = \lim_{\lambda\to\infty} U(\lambda) = \mathrm{Id}$ (where the limit is taken in $\mathcal{B}(\mathcal{P})$), Lemma 4.2.6 shows that $\cosh(D_n)^{-1}(U - \mathrm{Id}) \in \mathcal{K}(L^2(\mathbb{R}^n))$. Thus, up to compacts, we have

$$\varphi(D_n)(U - \mathrm{Id}) = \varphi(D_n)^*(U - \mathrm{Id}) = \varphi(D_n)\varphi(D_n)^*(U - \mathrm{Id}) \tag{5.10}$$

and an analogous statement for U^*. We can then use commutators to compute that

$$\begin{aligned}W_U W_U^* &= \mathrm{Id} + (U^* - \mathrm{Id})\varphi(D_n)^* + \varphi(D_n)(U - \mathrm{Id}) + \varphi(D_n)(U - \mathrm{Id})(U^* - \mathrm{Id})\varphi(D_n)^* + K_1 \\ &= \mathrm{Id} + \varphi(D_n)^*(U^* - \mathrm{Id}) + [U^*, \varphi(D_n)^*] + \varphi(D_n)(U - \mathrm{Id}) \\ &\quad + \varphi(D_n)\varphi(D_n)^*(U - \mathrm{Id})(U^* - \mathrm{Id}) + \varphi(D_n)(U - \mathrm{Id})[U^*, \varphi(D_n)^*] \\ &\quad + \varphi(D_n)[U, \varphi(D_n)^*](U^* - \mathrm{Id}) + K_1 \\ &= \mathrm{Id} + \varphi(D_n)^*(U^* - \mathrm{Id} + \varphi(D_n)(U - \mathrm{Id}) + \varphi(D_n)\varphi(D_n)^*(U - \mathrm{Id})(U^* - \mathrm{Id}) + K_2.\end{aligned}$$

The term $K_2 = K_1 + [U^*, \varphi(D_n)^*] + \varphi(D_n)(U - \mathrm{Id})[U^*, \varphi(D_n)^*] + \varphi(D_n)[U, \varphi(D_n)^*](U^* - \mathrm{Id})$ is compact by the arguments of [8, Theorem 4.1.10]. Noting the multiplicative identity

$(U-\mathrm{Id})(U^*-\mathrm{Id}) = 2\mathrm{Id} - U - U^*$ we have

$$\begin{aligned} W_U W_U^* &= \mathrm{Id} + \varphi(D_n)^*(U^*-\mathrm{Id}) + \varphi(D_n)(U-\mathrm{Id}) + \varphi(D_n)\varphi(D_n)^*(U-\mathrm{Id})(U^*-\mathrm{Id}) + K_2 \\ &= \mathrm{Id} + \varphi(D_n)(U^*-\mathrm{Id} - U - \mathrm{Id} + (U-\mathrm{Id})(U^*-\mathrm{Id})) + K_2 + K_3 \\ &= \mathrm{Id} + K_2 + K_3, \end{aligned}$$

where the term $K_3 = 2iA\cosh(\pi D_n)^{-1}(U^*-\mathrm{Id}) + iA\cosh(\pi D_n)^{-1}(U-\mathrm{Id})(U^*-\mathrm{Id})$ is compact by Equation (5.10). Thus, W_U^* is a right inverse for W_U up to compacts. A similar calculation shows that W_U^* is a left inverse, so W_U is Fredholm. □

Since the composition of Fredholm operators is Fredholm, and the composition of two properly admissable unitaries is itself a properly admissable unitary, it is natural to ask whether there is a product rule for operators of the form W_U. The following result shows that this is the case.

Lemma 5.2.8. *Let $U_1, U_2 \in \mathcal{B}(\mathcal{H})$ be properly admissable unitaries. Defining, for $j = 1, 2$, operators W_{U_j} by Equation (5.9), we have $W_{U_1}W_{U_2} = W_{U_1U_2}$, modulo compacts.*

Proof. We compute

$$\begin{aligned} W_{U_1}W_{U_2} &= (\mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + K_1)(\mathrm{Id} + \varphi(D_n)(U_2-\mathrm{Id}) + K_2) \\ &= \mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + K_1 + \varphi(D_n)(U_2-\mathrm{Id}) + \varphi(D_n)(U_1-\mathrm{Id})\varphi(D_n)(U_2-\mathrm{Id}) \\ &\quad + K_1\varphi(D_n)(U_2-\mathrm{Id}) + (\mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + K_1)K_2. \end{aligned}$$

Define $K_3 = K_1 + K_1\varphi(D_n)(U_2-\mathrm{Id}) + (\mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + K_1)K_2$, which is compact. Then,

$$\begin{aligned} W_{U_1}W_{U_2} &= \mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + \varphi(D_n)(U_2-\mathrm{Id}) + \varphi(D_n)(U_1-\mathrm{Id})\varphi(D_n)(U_2-\mathrm{Id}) + K_3 \\ &= \mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + \varphi(D_n)(U_2-\mathrm{Id}) + \varphi(D_n)^2(U_1-\mathrm{Id})(U_2-\mathrm{Id}) + K_3 \\ &\quad + \varphi(D_n)[U_1, \varphi(D_n)](U_2-\mathrm{Id}) \\ &= \mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + \varphi(D_n)(U_2-\mathrm{Id}) + \varphi(D_n)(U_1-\mathrm{Id})(U_2-\mathrm{Id}) + K_3 \\ &\quad + \varphi(D_n)[U_1, \varphi(D_n)](U_2-\mathrm{Id}) + (\varphi(D_n)^2 - \varphi(D_n))(U_1-\mathrm{Id})(U_2-\mathrm{Id}). \end{aligned}$$

Note that by [8, Theorem 4.1.10] the commutator $[U_1, \varphi(D_n)]$ is compact. Noting that $\varphi(D_n)^2 - \varphi(D_n) = -\frac{1}{2}(i\cosh(\pi D_n)^{-1}\tanh(\pi D_n)A + 2\cosh(\pi D_n)^{-2})$ we find, by similar arguments to the proof of Lemma 5.2.7, that $(\varphi(D_n)^2 - \varphi(D_n))(U_1-\mathrm{Id})(U_2-\mathrm{Id})$ is compact also. Hence,

$$\begin{aligned} W_{U_1}W_{U_2} &= \mathrm{Id} + \varphi(D_n)(U_1-\mathrm{Id}) + \varphi(D_n)(U_2-\mathrm{Id}) + \varphi(D_n)(U_1-\mathrm{Id})(U_2-\mathrm{Id}) + K_4 \\ &= \mathrm{Id} + \varphi(D_n)(U_1U_2-\mathrm{Id}) + K_4, \end{aligned}$$

where K_4 is compact. Thus, $W_{U_1}W_{U_2} = W_{U_1U_2}$ modulo compacts as claimed. □

Lemma 5.2.8 can be extended to show that we have a partially defined product rule also.

Lemma 5.2.9. *Let $U_1, U_2 \in \mathcal{B}(\mathcal{H})$ be admissable unitaries with $U_1(0) = U_2(0)$ and $\lim_{\lambda\to\infty} U_1(\lambda) = \lim_{\lambda\to\infty} U_2(\lambda)$ (with the limits taken in $\mathcal{B}(\mathcal{P})$). Defining, for $j = 1, 2$, operators W_{U_j} by Equation (5.9), we have $W_{U_1} = W_{U_1U_2^*}W_{U_2}$, modulo compacts.*

Proof. Our assumptions show that the composition $U_1U_2^*$ is a properly admissable unitary. Let

$$W_{U_1U_2^*} = \mathrm{Id} + \varphi(D_n)(U_1U_2^* - \mathrm{Id}) + K_{12}, \quad \text{and} \quad W_{U_2} = \mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + K_2.$$

Define $K_3 = K_2 + \varphi(D_n)(U_1U_2^* - \mathrm{Id})K_2 + K_{12}(\mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + K_2)$, a compact operator. Then,

$$\begin{aligned}
W_{U_1U_2^*}W_{U_2} &= \mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id}) \\
&\quad + \varphi(D_n)(U_1U_2^* - \mathrm{Id})\varphi(D_n)(U_2 - \mathrm{Id}) + K_3 \\
&= \mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id}) + \varphi(D_n)^2(U_1U_2^* - \mathrm{Id})(U_2 - \mathrm{Id}) \\
&\quad + \varphi(D_n)[U_1U_2^*, \varphi(D_n)](U_2 - \mathrm{Id}) + K_3 \\
&= \mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id})(U_2 - \mathrm{Id}) \\
&\quad + (\varphi(D_n)^2 - \varphi(D_n))(U_1U_2^* - \mathrm{Id})(U_2 - \mathrm{Id}) + \varphi(D_n)[U_1U_2^*, \varphi(D_n)](U_2 - \mathrm{Id}) + K_3.
\end{aligned}$$

Since $U_1U_2^*$ is properly admissable, the proof of Lemma 5.2.8 shows that $(\varphi(D_n)^2 - \varphi(D_n))(U_1U_2^* - \mathrm{Id})(U_2 - \mathrm{Id})$ and $\varphi(D_n)[U_1U_2^*, \varphi(D_n)](U_2 - \mathrm{Id})$ define compact operators. Thus,

$$\begin{aligned}
W_{U_1U_2^*}W_{U_2} &= \mathrm{Id} + \varphi(D_n)(U_2 - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id}) + \varphi(D_n)(U_1U_2^* - \mathrm{Id})(U_2 - \mathrm{Id}) + K_4 \\
&= \mathrm{Id} + \varphi(D_n)(U_1 - \mathrm{Id}) + K_4 \\
&= W_{U_1},
\end{aligned}$$

as claimed. □

The following useful property shows that even if neither of the unitaries U_1 and U_2 are properly admissable, we may still be able to deduce the Fredholm property of W_{U_2} given that of W_{U_1} and that both are close enough in some sense.

Corollary 5.2.10. *Let $U_1, U_2 \in \mathcal{B}(\mathcal{H})$ be admissable unitaries with $U_1(0) = U_2(0)$ and $\lim_{\lambda\to\infty} U_1(\lambda) = \lim_{\lambda\to\infty} U_2(\lambda)$ (with the limits taken in $\mathcal{B}(\mathcal{P})$). Define, for $j = 1, 2$, operators W_{U_j} by Equation (5.9). Then if one of the W_{U_j} is Fredholm, so is the other.*

Proof. Suppose, without loss of generality, that W_{U_2} is Fredholm. Then since the unitary $U_1U_2^*$ is properly admissable, we have $W_{U_1U_2^*}$ is Fredholm by Lemma 5.2.7. Since the composition of Fredholm operators is also Fredholm, we deduce from Lemma 5.2.9 that W_{U_1} is Fredholm also. □

There is far more underlying algebraic structure to be analysed here. Let

$$G = \{U \in \mathcal{B}(\mathcal{H}) : U \text{ is properly admissable}\}.$$

Define the Calkin algebra of $\mathcal{H}$ by $Q(\mathcal{H}) = \mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H})$. Define the map $\eta : G \to Q(\mathcal{H})$ by $\eta(U) = [W_U]$. We have the following algebraic relationship.

Lemma 5.2.11. *The set G is a subgroup of $\mathcal{U}(\mathcal{H})$, the set $\eta(G)$ is a group under composition and $\eta : G \to \eta(G)$ is a group homomorphism.*

Proof. The group operation and identity of G are inherited from $\mathcal{U}(\mathcal{H})$, so we only need to check that G is closed under composition and inverses. Compute for $U_1, U_2 \in G$ that

$$\begin{aligned} U_1U_2 - \mathrm{Id} &= (U_1U_2 - U_1 - U_2 + \mathrm{Id}) + U_1 + U_2 - 2\mathrm{Id} \\ &= (U_1 - \mathrm{Id})(U_2 - \mathrm{Id}) + (U_1 - \mathrm{Id}) + (U_2 - \mathrm{Id}), \end{aligned}$$

which is compact since $U_1, U_2 \in G$ and so $U_1U_2 \in G$. The statement for inverses follows from the fact that $U^{-1} = U^*$. That the set $\eta(G)$ is a group follows from Lemma 5.2.8. To see that η is a group homomorphism, we again use Lemma 5.2.8 to see that

$$\eta(U_1U_2) = [W_{U_1U_2}] = [W_{U_1}W_{U_2}] = [W_{U_1}][W_{U_2}] = \eta(U_1)\eta(U_2).$$

That η preserves inverses follows in a similar manner. □

The index map $\mathrm{Index} : \mathrm{Fred}(Q(\mathcal{H})) \to \mathbb{Z}$ defines a map from Fredholm lifts of unitaries in $Q(\mathcal{H})$ to $\mathbb{Z}$. When considered on equivalence classes, we obtain a group homomorphism $\mathrm{Index} : \eta(G) \to \mathbb{Z}$ and thus can form the quotient group $G' = \eta(G)/\mathrm{Ker}(\mathrm{Index})$.

Lemma 5.2.12. *We have isomorphisms $G' \cong \pi_1(\mathcal{U}(\mathcal{P})) \cong K_0(\mathcal{K})$, where $\pi_1(\mathcal{U}(\mathcal{P}))$ denotes the connected components of the unitary group on $\mathcal{P}$.*

5.2.3 The index pairing

Corollary 5.2.4 and Lemma 5.2.6 tell us that we can pair the classes $[D_+]$ and $[U]$ to obtain an integer. See [76, Section 8.7] for details. Sadly, the fact that our algebra $C_0(\mathbb{R}^+) \otimes \mathcal{K}$ is nonunital (both $C_0(\mathbb{R}^+)$ and $\mathcal{K}$!), we need to be careful about applying index pairing formulae. See [43, Section 2.3] for a description of the problems.

In [43, Section 2.7] it was shown that for spectral triples $(\mathcal{A}, \mathcal{H}, \mathcal{D})$ over a nonunital algebra, the index pairing with the class of a unitary $U \in \mathcal{A}$ can be computed as $\mathrm{Index}(PUP - (\mathrm{Id} - P))$ where $P = \chi_{[0,\infty)}(\mathcal{D})$ is the non-negative spectral projection of $\mathcal{D}$.

In our setting, however, we will be using an approximation of the non-positive spectral projection of $D_+ \otimes \mathrm{Id}$ and we need to show that we still get a Fredholm operator.

Lemma 5.2.13. *If $B = GG^*$ is invertible modulo compacts then G is Fredholm.*

Proof. Write $B = A + K$ where A is invertible and K is compact. Then $GG^*A^{-1} = BA^{-1} = \mathrm{Id} + KA^{-1}$. So G is Fredholm with approximate right inverse G^*A^{-1}. □

Theorem 5.2.14. *Let $U \in \mathcal{B}(\mathcal{H})$ be a properly admissable unitary and define W_U by Equation* (5.9)*. Let $[D_+]$ be defined by Corollary 5.2.4. Then*

$$\langle [U], [D_+] \rangle = -\mathrm{Index}(W_U). \tag{5.11}$$

Proof. We know from [76, Section 8.7] that the pairing can be computed as

$$\langle [U], [D_+] \rangle = \mathrm{Index}(PUP - (\mathrm{Id} - P)) = \mathrm{Index}(PUP + (\mathrm{Id} - P)),$$

where P is the non-negative spectral projection for $D_+ \otimes \mathrm{Id}$. The second equality follows from the homotopy $t \mapsto \mathrm{e}^{i\pi(1-t)}(\mathrm{Id} - P)$. We note that the pairing can also be computed using the non-positive spectral projection P_- for $D_+ \otimes \mathrm{Id}$, at the expense of a minus sign, since $[2P_+ - 1] = -[2P_- - 1] \in K^1(C_0(\mathbb{R}^+, \mathcal{K}))$. The result is

$$\langle [U], [D_+] \rangle = -\mathrm{Index}(P_-UP_- - (\mathrm{Id} - P_-)) = -\mathrm{Index}(P_-UP_- + (\mathrm{Id} - P_-)).$$

We will use this second form, and for convenience drop the subscript '−'. To compute the pairing, we consider the wave operator in the spectral representation. Recall that the operator D_n satisfies $F_0 D_n F_0^* = -2(D_+ \otimes \mathrm{Id})$.

So we need to be able to approximate P with the operator $\varphi(-2D_+) \otimes \mathrm{Id}$. We initially work with D_n for convenience. Let $T = \varphi(D_n)$ and $t = \tanh(\pi D_n)$ for simplicity. A quick computation shows that

$$TT^* = T^*T = \frac{1}{2}(\mathrm{Id} + t).$$

Starting from W_U there is a compact operator K such that

$$W_U = \mathrm{Id} - \frac{1}{2}(\mathrm{Id} + t) + TUT^* + K.$$

We can also find a compact K_1 such that

$$\begin{aligned}\frac{1}{2}(\mathrm{Id}-t)TU^*T^* &= \frac{1}{2}(\mathrm{Id}-t)TT^*U^* + \frac{1}{2}(\mathrm{Id}-t)[T,U^*]T^* \\ &= \frac{1}{4}(\mathrm{Id}-t^2)U^* + \frac{1}{2}(\mathrm{Id}-t)[T,U^*]T^* \\ &= \frac{1}{4}(\mathrm{Id}-t^2) + \frac{1}{4}(\mathrm{Id}-t^2)(U^*-\mathrm{Id}) + \frac{1}{2}(\mathrm{Id}-t)[T,U^*]T^* \\ &:= \frac{1}{4}(\mathrm{Id}-t^2) + K_1.\end{aligned}$$

Similarly we find compacts K_2, K_3 such that

$$\frac{1}{2}TUT^*(\mathrm{Id}-t) = \frac{1}{4}(\mathrm{Id}-t^2) + K_2, \quad \text{and} \quad TUT^*TU^*T^* = \frac{1}{4}(\mathrm{Id}+t)^2 + K_3.$$

Then (with all equalities modulo compacts)

$$W_U W_U^* = (\mathrm{Id} - \frac{1}{2}(\mathrm{Id}+t) + TUT^*)(\mathrm{Id} - \frac{1}{2}(\mathrm{Id}+t) + TU^*T^*) = \mathrm{Id} - \frac{1}{2}(\mathrm{Id}-t^2)$$

which is invertible and hence $\mathrm{Id} - \frac{1}{2}(\mathrm{Id}+t) + TUT^*$ is invertible modulo compacts by Lemma 5.2.13. Now we compare $\mathrm{Id} - \frac{1}{2}(\mathrm{Id}+t) + TUT^*$ and $PSP + (\mathrm{Id}-P)$ to see that they have the same Fredholm index. Taking commutators we have (modulo compacts)

$$\mathrm{Id} - \frac{1}{2}(\mathrm{Id}+t) + TUT^* = \mathrm{Id} - TT^* + TUT^* = \mathrm{Id} + T(U-\mathrm{Id})T^*$$

and

$$PUP + (\mathrm{Id}-P) = \mathrm{Id} + P(U-\mathrm{Id})P.$$

Define, in the spectral representations, the operators $\tilde{T}$ and $\tilde{t}$ by

$$\tilde{T} = F_0 T F_0^* = \frac{1}{2}(\mathrm{Id} - \tanh(2\pi D_+) - i\cosh(2\pi D_+)^{-1}) \otimes \mathrm{Id}$$

and

$$\tilde{t} = F_0 t F_0^* = -\tanh(2\pi D_+) \otimes \mathrm{Id}.$$

Taking the difference, and using $P = \frac{1}{2}(\mathrm{Id} - \mathrm{sign}(D_+))$ we have

$$\begin{aligned}&(P\otimes\mathrm{Id})U(P\otimes\mathrm{Id}) + (\mathrm{Id} - (P\otimes\mathrm{Id})) - \big(\mathrm{Id} - \tilde{T}\tilde{T}^* + \tilde{T}U\tilde{T}^*\big) \\ &= P(U-\mathrm{Id})P - \tilde{T}(U-\mathrm{Id})\tilde{T}^* \\ &= (P - \tilde{T}\tilde{T}^*)(U-\mathrm{Id}) + \mathcal{K}(\mathcal{H}) \\ &= \frac{1}{2}(-\mathrm{sign} + \tanh)(D_+)(U-\mathrm{Id}) + \mathcal{K}(\mathcal{H}). \qquad (5.12)\end{aligned}$$

We note that the second equality, where we have commuted the exact spectral projection with U up to compacts, is justified by the arguments in [43, Section 2.7].

To complete the argument, observe that $\frac{1}{2}(-\mathrm{sign}+\tanh)$ is an L^2 function, and for any compactly supported function $\chi \in C_c(\mathbb{R}^+)$, $\lambda \mapsto \chi(\lambda)\|U(\lambda)-\mathrm{Id}\|_{\mathcal{B}(\mathcal{P})}$ is L^2 as well. Hence for any such χ we have

$$\begin{aligned}&\frac{1}{2}(-\mathrm{sign}+\tanh)(D_+)\chi(U(\cdot)-\mathrm{Id})\\&=\frac{1}{2}(-\mathrm{sign}+\tanh)(D_+)\chi\|(U(\cdot)-\mathrm{Id})\|_{\mathcal{B}(\mathcal{P})}\|(U(\cdot)-\mathrm{Id})\|^{-1}_{\mathcal{B}(\mathcal{P})}(U(\cdot)-\mathrm{Id})\end{aligned}$$

is a product of L^2 functions, one of D_+ and one of H_0, composed with a uniformly bounded compact operator-valued function $\|(U(\cdot)-\mathrm{Id})\|^{-1}_{\mathcal{B}(\mathcal{P})}(U(\cdot)-\mathrm{Id})$. Applying the standard $f(x)g(\nabla)$ result [151, Theorem 4.1] we obtain a compact operator times a uniformly bounded operator, which is then compact. As $\|(U(\cdot)-\mathrm{Id})\|_{\mathcal{B}(\mathcal{P})}$ is continuous and vanishes at $\lambda=0,\infty$, we can take an approximate unit $\chi_m \in C_c(\mathbb{R}^+)$ and see that

$$\frac{1}{2}(-\mathrm{sign}+\tanh)(D_+)\chi_m\|(U(\cdot)-\mathrm{Id})\|_{\mathcal{B}(\mathcal{P})}$$

converges in norm. Hence, the limit $\frac{1}{2}(-\mathrm{sign}+\tanh)(D_+)\|(U(\cdot)-\mathrm{Id})\|$ is compact.

Since the difference (5.12) is compact, the two Fredholm operators W_U and $P(U-\mathrm{Id})P$ have the same index. □

5.3 The index pairing for scattering operators

We now apply the results of Section 5.2 to the wave operator W_- and scattering operator S in order to reinterpret Levinson's theorem as an index pairing.

Lemma 5.3.1. *When* $S(0)=\mathrm{Id}$ *the scattering operator defines an element of the odd* K*-theory* $[S]\in K_1(C_0(\mathbb{R}^+)\otimes\mathcal{K})$. *For suitably decaying potentials, for example those satisfying Assumption 4.3.1,* $S(0)=\mathrm{Id}$ *in all dimensions except dimension 1 (generically) and dimension 3 (in the presence of resonances).*

Proof. The claim follows from Lemma 5.2.6 and the statement that when $S(0)=\mathrm{Id}$ we have that S defines a properly admissable unitary, since $\lim_{\lambda\to\infty}S(\lambda)=\mathrm{Id}$ in $\mathcal{B}(\mathcal{H})$ by Corollary 4.3.10 □

Theorem 5.3.2. *Let* $H=H_0+V$ *be such that the wave operators exist, are complete and are of the form of Equation* (4.1) *with* $S(0)=\mathrm{Id}$. *Let* S *be the corresponding scattering operator. We have the pairing*

$$\langle [S],[D_+]\rangle = -\mathrm{Index}(W_-)=N,$$

where N is the number of bound states of H (eigenvalues counted with multiplicity).

Proof. The scattering operator is a properly admissable unitary by Lemma 5.3.1, and so the first equality is just the statement of Theorem 5.2.14. The fact that $\mathrm{Index}(W_-) = -N$ is the statement of Proposition 2.3.9 □

Note that the case $S(0) \neq \mathrm{Id}$ cannot immediately be handled by the simple pairing described in Theorem 5.3.2, requiring some subleties which we demonstrate in the next two sections.

Corollary 5.3.3. *Let V_0 and V_1 be such that the wave operators exist, are complete and of the form of Equation* (4.1)*. Suppose further that $S_0(0) = S_1(0) = \mathrm{Id}$, where S_0 and S_1 denote the scattering operators for the potentials V_0 and V_1. If the number of eigenstates (counted with multiplicity) for V_0 differs from that of V_1 then their scattering matrices are not (stably) homotopic.*

Corollary 5.3.4. *Let V_0 and V_1 be such that the wave operators exist, are complete and of the form of Equation* (4.1)*. Suppose further that $S_0(0) = S_1(0) = \mathrm{Id}$, where S_0 and S_1 denote the scattering operators for the potentials V_0 and V_1. Consider the path $V_t = (1-t)V_0 + tV_1$ for $t \in [0,1]$ with corresponding scattering operators S_t. If the number of eigenstates (counted with multiplicity) for V_0 differs from that of V_1, then the path S_t is not norm continuous.*

In fact, Corollary 5.3.4 shows that there are a discrete number of points at which the path S_t fails to be norm continuous, corresponding to 'jumps' in the number of eigenvalues for the potential V_t. The norm holomorphy (which implies norm continuity) of the scattering operator as a function of t is discussed in [34, Theorem 4.2] where an equivalent condition to holomorphy of S_t is given. The points of failure of norm continuity in Corollary 5.3.4 are also points of failure of holomorphy in [34, Theorem 4.2]. In the case of a Rollnik class potential on $\mathbb{R}^3$ holomorphy of the scattering matrix as a function of t has been studied in [94, Theorem 6.1] and [34, Theorem 5.2].

Lemma 5.3.5. *Suppose that V_1, V_2 satisfy Assumption 2.2.14 and define the operators $H_j = H_0 + V_j$. Suppose further that the scattering operators S_1 and S_2 are properly admissable unitaries. Then the wave operator $W_-(H_2, H_1)$ is given by*

$$W_-(H_2, H_1) = \mathrm{Id} + \varphi(D_n)(S_2 S_1^* - \mathrm{Id}) + K$$

for a compact operator K.

Proof. The chain rule for wave operators (Proposition 2.1.4) gives that

$$W_-(H_2, H_0) = W_-(H_2, H_1) W_-(H_1, H_0).$$

Using that S_2 and S_1 are properly admissable unitaries and Lemma 5.2.8 we find that

$$\begin{aligned} W_-(H_2,H_1) &= W_-(H_2,H_0)W_-(H_1,H_0)^* \\ &= (\mathrm{Id}+\varphi(D_n)(S_2-\mathrm{Id}))(\mathrm{Id}+(S_1^*-\mathrm{Id})\varphi(D_n)^*) \\ &= \mathrm{Id}+\varphi(D_n)(S_2S_1^*-\mathrm{Id}), \end{aligned}$$

where all equalities are modulo compacts and we have used the inclusions $[S_1^*,\varphi(D_n)], (S^*-\mathrm{Id})(\varphi(D_n)-\varphi(D_n)^*)\in\mathcal{K}(\mathcal{H})$. □

Such an equality cannot be obtained when the scattering operators are only assumed to be admissable, since we no longer have the required compactness relations.

For $t\in[0,1]$ define the operator $H_t = H_0+tV$ and suppose that H_1 does not admit a zero energy resonance. The analytic Fredholm alternative gives that there is a discrete set $(t_j)_{j\leq J}\subset[0,1]$ such that each H_{t_j} admits a zero energy resonance. Choose a sequence $(\tilde{t}_j)_{j\leq J+1}\subset[0,1]$ with $\tilde{t}_0=0$, $\tilde{t}_{J+1}=1$ and $t_{j-1}<\tilde{t}_j<t_j$ for $1\leq j\leq J-1$. Then each $H_{\tilde{t}_j}$ does not admit a zero energy resonance, and Lemma 5.3.5 gives

$$W_-(H_{\tilde{t}_{j+1}},H_{\tilde{t}_j}) = \mathrm{Id}+\varphi(D_n)(S_{j+1}S_j^*-\mathrm{Id})+K_j$$

for some compact K_j, allowing us to prove the following.

Lemma 5.3.6. *Let V satisfy Assumption 2.2.14 and suppose that the scattering operator S is a properly admissable unitary. Then the wave operator W_- satisfies*

$$W_- = \prod_{j=0}^{J} W_-(H_{\tilde{t}_{j+1}},H_{\tilde{t}})$$

Proposition 5.3.7. *Let V satisfy Assumption 4.3.1 and suppose that $H_1=H_0+V$ admits a resonance. Then there exists a $t_0>0$ such that for all $t\in(1,1+t_0)$ the operator $H_t=H_0+tV$ does not admit a resonance and the number of bound states $N(t)$ of $H(t)$ is constant for all $t\in[1,1+t_0)$. Furthermore, for any $t\in(1,1+t_0)$ the scattering operator S_t defines a properly admissable unitary and*

$$W_-(H_t,H_0) = W_-(H_t,H_1)W_-(H_1,H_0)$$

and $\mathrm{Index}(W_-(H_t,H_0))=\mathrm{Index}(W_-(H_1,H_0))$. *In particular,* $\mathrm{Index}(W_-(H_t,H_1))=0$.

5.3.1 Low energy corrections in dimension $n=1$

Due to the generic failure of $S(0)=\mathrm{Id}$ in dimension $n=1$, the pairing of Theorem 5.3.2 is not applicable in dimension $n=1$. In each generic and resonant case, we construct a unitary σ such that $S\sigma^*$ is a properly admissable unitary and so defines a pairing by

Theorem 5.2.14. As a corollary, we obtain a new proof of the well-known Levinson's theorem [108].

The main tool in this section is the following result which allows us to compute the index of a generalised wave operator W_U by computing the winding number of the component functions described in Lemma 5.1.4.

Lemma 5.3.8. *Let $U \in \mathcal{B}(L^2(\mathbb{R}))$ be a properly admissable unitary such that the matrix of U is differentiable and $|\mathrm{Tr}(U(\cdot)^*U'(\cdot))| \in L^1(\mathbb{R}^+)$. Let $W_U \in \mathcal{B}(L^2(\mathbb{R}))$ be defined by*

$$W_U = \mathrm{Id} + \varphi(D_1)(U - \mathrm{Id}) + K, \tag{5.13}$$

with K compact. Then $W_U \in E_{L,D_+}$ and

$$\mathrm{Index}(W_U) = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(U(\lambda)^*U'(\lambda))\,\mathrm{d}\lambda. \tag{5.14}$$

Proof. This is a consequence of Proposition 5.1.9. Since $U(0) = \mathrm{Id}$, the only non-trivial winding number contribution around the square $\square'$ is from the edge corresponding to ∞ in $\sigma(D_1)$, which gives us the winding number of $\mathrm{Id} + \varphi(\infty)(U - \mathrm{Id}) = U$. □

Lemma 5.3.9. *Suppose that $n = 1$ and V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$ and let S be the corresponding scattering operator. Let $\sigma \in U(L^2(\mathbb{R}))$ be an admissable unitary with $\sigma(0) = S(0)$ and $\lim_{\lambda\to\infty}\sigma(\lambda) = \mathrm{Id}$ (with the limit in $\mathcal{B}(\mathcal{P})$). If we have $\mathrm{Tr}(\sigma(\cdot)\sigma'(\cdot)^*) \in L^1(\mathbb{R}^+)$ then*

$$\mathrm{Index}(W_{S\sigma^*}) = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^*S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)\sigma'(\lambda)^*)\,\mathrm{d}\lambda. \tag{5.15}$$

Proof. Since $\mathcal{B}(\mathcal{P}) = \mathcal{L}^1(\mathcal{P})$ we have $\sigma(\lambda)^*\sigma'(\lambda) \in \mathcal{L}^1(\mathcal{P})$ for all $\lambda \in \mathbb{R}^+$. The function $\lambda \mapsto \mathrm{Tr}(S(\cdot)^*S'(\cdot))$ is integrable by Theorem 2.5.34. The Leibniz rule for matrix valued functions shows that

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}(S(\lambda)\sigma(\lambda)^*) = S'(\lambda)\sigma(\lambda)^* + S(\lambda)\sigma'(\lambda)^*.$$

Multiplying by $(S(\lambda)\sigma(\lambda)^*)^* = \sigma(\lambda)S(\lambda)^*$ and taking the trace we obtain

$$\begin{aligned}\mathrm{Tr}\left(S(\lambda)\sigma(\lambda)^*)^*\frac{\mathrm{d}}{\mathrm{d}\lambda}S(\lambda)\sigma(\lambda)^*\right) &= \mathrm{Tr}\left(\sigma(\lambda)S(\lambda)^*(S'(\lambda)\sigma(\lambda)^* + S(\lambda)\sigma'(\lambda)^*)\right)\\ &= \mathrm{Tr}\left(\sigma(\lambda)S(\lambda)^*S'(\lambda)\sigma(\lambda)^*\right) + \mathrm{Tr}\left(\sigma(\lambda)S(\lambda)^*S(\lambda)\sigma'(\lambda)^*\right)\\ &= \mathrm{Tr}\left(S(\lambda)^*S'(\lambda)\right) + \mathrm{Tr}\left(\sigma(\lambda)\sigma'(\lambda)^*\right),\end{aligned}$$

where we have used unitarity and cyclicity of the trace. The result follows upon integrating the traces and applying Lemma 5.3.8. □

Remark 5.3.10. Equation (5.15) indicates that, in one dimension, Levinson's theorem is related to the Witten index. In particular, the contribution from the scattering operator is the Witten index of the pair (D_+, S^*D_+S). For more details regarding this observation, we direct the reader to [37, 38, 39, 40, 42] and the short note [41].

Definition 5.3.11. A map $\sigma : \mathbb{R}^+ \to M_2(\mathbb{C})$ is a *generic correction* if there exist differentiable functions $\theta : \mathbb{R}^+ \to \mathbb{R}$ and $f, g : \mathbb{R}^+ \to \mathbb{C}$ such that θ is increasing, $\theta(\infty) \in 2\pi\mathbb{Z}$, $\theta(0) \in (2\mathbb{Z}+1)\pi$, $\theta(\infty) - \theta(0) = \pi$, $g(0) = f(\infty) = 1$ and $f(0) = g(\infty) = 0$ such that $|f(\lambda)|^2 + |g(\lambda)|^2 = 1$ for all λ and

$$\sigma(\lambda) = \begin{pmatrix} f(\lambda) & g(\lambda) \\ -\mathrm{e}^{i\theta(\lambda)}\overline{g(\lambda)} & \mathrm{e}^{i\theta(\lambda)}\overline{f(\lambda)} \end{pmatrix}. \tag{5.16}$$

A map $\sigma : \mathbb{R}^+ \to M_2(\mathbb{C})$ is a *resonant correction* if there exist differentiable functions $\theta : \mathbb{R}^+ \to \mathbb{R}$ and $f, g : \mathbb{R}^+ \to \mathbb{C}$ such that θ is increasing, $\theta(\infty), \theta(0) \in 2\pi\mathbb{Z}$ and $\theta(\infty) - \theta(0) = 0$ with $f(0) = 2c_+c_-$, $g(0) = c_+^2 - c_-^2$, $f(\infty) = 1$ and $g(\infty) = 0$ for some $c_+, c_- \in \mathbb{R} \setminus \{0\}$ with $c_+^2 + c_-^2 = 1$ such that $|f(\lambda)|^2 + |g(\lambda)|^2 = 1$ for all λ and

$$\sigma(\lambda) = \begin{pmatrix} f(\lambda) & g(\lambda) \\ -\mathrm{e}^{i\theta(\lambda)}\overline{g(\lambda)} & \mathrm{e}^{i\theta(\lambda)}\overline{f(\lambda)} \end{pmatrix}. \tag{5.17}$$

For both generic and resonant corrections, $\sigma(\lambda)$ is unitary for all $\lambda \in \mathbb{R}^+$, and $\lim_{\lambda\to\infty} \sigma(\lambda) = \mathrm{Id}$, with the limit taken in $\mathcal{B}(\mathcal{P})$. To explicitly evaluate the index appearing in one dimension in terms of scattering data, we need the following result [97, Proposition 9].

Lemma 5.3.12. *Let σ be a correction (generic or resonant) and define $\Gamma_1 : \mathbb{R} \to M_2(\mathbb{C})$ by*

$$\Gamma_1(y) = \mathrm{Id} + \frac{1}{2}(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}A)(\sigma(0) - \mathrm{Id}),$$

where $[Af](x) = f(-x)$. Then

$$\frac{1}{2\pi i}\int_{\mathbb{R}} \mathrm{Tr}(\Gamma_1(y)^*\Gamma_1'(y))\,\mathrm{d}y = \begin{cases} -\frac{1}{2}, & \text{if } \sigma \text{ is a generic correction,} \\ 0, & \text{if } \sigma \text{ is a resonant correction.} \end{cases}$$

Proof. The proof consists of changing to a basis in which the operator $\tanh(\pi D_1) + iA\cosh(\pi D_1)$ is diagonal, from which the computation follows. We refer to [97, Proposition 9] for the details. □

We use Lemma 5.3.12 to compute directly the index of W_σ.

Lemma 5.3.13. *Let σ be a generic correction. Then the operator W_σ is Fredholm and* $\mathrm{Index}(W_\sigma) = 0$.

Proof. Example 2.5.35 shows that there exists a scattering matrix with $S(0) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$ and $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$, with the limit taken in $\mathcal{B}(\mathcal{P})$. By Proposition 2.3.9, $W_- = W_S$ is Fredholm. That W_σ is Fredholm then follows from Corollary 5.2.10. To compute the index we use Lemma 5.1.9. The image $q(W_\sigma) \in E_{L,D_+}/J_{L,D_+}$ is given by $(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ with

$$\Gamma_1(y) = \mathrm{Id} + \frac{1}{2}(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}A)(\sigma(0) - \mathrm{Id}),$$

$\Gamma_2(\lambda) = \sigma(\lambda)$ and $\Gamma_3(y) = \mathrm{Id} = \Gamma_4(\lambda)$. By Theorem 5.1.9 we find

$$\begin{aligned}\mathrm{Index}(W_\sigma) &= \frac{1}{2\pi i}\int_{\mathbb{R}} \mathrm{Tr}(\Gamma_1(y)^*\Gamma_1'(y))\,\mathrm{d}y + \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)^*\sigma'(\lambda))\,\mathrm{d}\lambda \\ &= -\frac{1}{2} + \frac{1}{2\pi}\int_0^\infty \theta'(\lambda)\,\mathrm{d}\lambda \\ &= 0,\end{aligned}$$

where we have used Lemma 5.3.12 to calculate the first integral. □

Lemma 5.3.14. *Let σ be a resonant correction. Then the operator W_σ is Fredholm and* $\mathrm{Index}(W_\sigma) = 0$.

Proof. Example 2.5.35 shows that for any $c_+, c_- \in \mathbb{R} \setminus \{0\}$ with $c_+^2 + c_-^2 = 1$ there exists a potential V with scattering matrix satisfying $S(0) = \begin{pmatrix} 2c_1c_2 & c_+^2 - c_-^2 \\ c_-^2 - c_+^2 & 2c_1c_2 \end{pmatrix}$ and $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$, with the limit taken in $\mathcal{B}(\mathcal{P})$. By Proposition 2.3.9, $W_- = W_S$ is Fredholm. That W_σ is Fredholm then follows from Corollary 5.2.10. To compute the index we use Lemma 5.1.9. The image $q(W_\sigma) \in E_{L,D_+}/J_{L,D_+}$ is given by $(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4)$ with

$$\Gamma_1(y) = \mathrm{Id} + \frac{1}{2}(1 + \tanh(\pi y) - i\cosh(\pi y)^{-1}A)(\sigma(0) - \mathrm{Id}),$$

$\Gamma_2(\lambda) = \sigma(\lambda)$ and $\Gamma_3(y) = \mathrm{Id} = \Gamma_4(\lambda)$. Thus,

$$\begin{aligned}\mathrm{Index}(W_\sigma) &= \frac{1}{2\pi i}\int_{\mathbb{R}} \mathrm{Tr}(\Gamma_1(y)^*\Gamma_1'(y)\,\mathrm{d}y + \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)^*\sigma'(\lambda))\,\mathrm{d}\lambda \\ &= -\frac{1}{2} + \frac{1}{2\pi i}\int_0^\infty \theta'(\lambda)\,\mathrm{d}\lambda \\ &= 0,\end{aligned}$$

where again we have used Lemma 5.3.12 to calculate the first integral. □

We can now use a generic or resonant correction to prove a modified index pairing in one dimension.

Theorem 5.3.15. *Let $n = 1$ and suppose V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$. If $H = H_0 + V$ has no resonances, then for any generic correction σ we have the pairing*

$$\langle [S\sigma^*], [D_+] \rangle = -\mathrm{Index}(W_-) = N, \tag{5.18}$$

where N is the number of bound states of H (eigenvalues counted with multiplicity). If $H = H_0 + V$ has resonances, then for any resonant correction σ the pairing of Equation (5.18) *holds.*

Proof. Since in both cases (generic and resonant) $S(0) = \sigma(0)$ and $\lim_{\lambda\to\infty} S(\lambda) = \lim_{\lambda\to\infty} \sigma(\lambda) = \mathrm{Id}$ (with the limits taken in $\mathcal{B}(\mathcal{P})$) we find that S and σ are admissable unitaries with $S\sigma^*$ a properly admissable unitary. Theorem 5.3.2 then gives us the equality

$$\langle [S\sigma^*], [D_+] \rangle = -\mathrm{Index}(W_{S\sigma^*}). \tag{5.19}$$

Since both $= W_S$ and W_{σ^*} are Fredholm we find that

$$\mathrm{Index}(W_{S\sigma^*}) = \mathrm{Index}(W_S) + \mathrm{Index}(W_\sigma) = -N + 0,$$

where we have used Proposition 2.3.9 and Lemma 5.3.13 (generic) or Lemma 5.3.14 (resonant) to evaluate the indices. The statement follows by noting that $W_- = W_S$ (modulo compacts) by Theorem 4.0.1. □

We also obtain an alternative proof of the integral form of Levinson's theorem in one dimension.

Theorem 5.3.16. *Let $n = 1$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$. Then the number of bound states of $H = H_0 + V$ is given by*

$$N = \begin{cases} -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda, & \textit{if there exists a resonance,} \\ -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2} & \textit{otherwise.} \end{cases} \tag{5.20}$$

Proof. Theorem 5.3.15 tells us that for any generic (or resonant if necessary) correction σ we have $N = -\mathrm{Index}(W_{S\sigma^*})$. Combining with Lemma 5.3.9 we find that

$$\begin{aligned} N = -\mathrm{Index}(W_{S\sigma^*}) &= -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)^* \sigma'(\lambda))\,\mathrm{d}\lambda \\ &= \begin{cases} -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda, & \text{if there exists a resonance,} \\ -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2} & \text{otherwise.} \end{cases} \end{aligned}$$

Here, the σ integral has been evaluated explicitly to $\frac{1}{2}$ in the generic case and 0 in the resonant case. □

Remark 5.3.17. Theorem 5.3.16 allows us to completely characterise the spectral shift function in dimension $n = 1$. The result is

$$\xi(\lambda) = -\sum_{k=1}^{K} M(\lambda_k)\chi_{[\lambda_k,\infty)}(\lambda) - \frac{1}{2}(1 - M_R(0))\chi_{[0,\infty)}(\lambda) \\ - \frac{1}{2\pi i}\chi_{[0,\infty)}(\lambda)\int_0^\lambda \mathrm{Tr}(S(\mu)^* S'(\mu))\,\mathrm{d}\mu,$$

where $M_R(0) = 1$ if there exists a zero-energy resonance and zero otherwise.

Corollary 5.3.18. *Suppose that $n = 1$ and V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$. Then we have*

$$\xi(0+) = -N - \frac{1}{2}(1 - M_R(0)).$$

5.3.2 Low and high energy corrections in dimension $n = 3$

In dimension $n = 3$ the pairing of Theorem 5.3.2 fails in the presence of resonances. In this section we emulate the ideas of the previous section to construct a resonant correction from which an index pairing can be proved. Due to the failure of $S(\lambda)$ to converge as $\lambda \to \infty$ in the trace norm, additional corrections are required to pass from the index pairing to an integral formula for the number of bound states. We construct an explicit high energy correction to S obtain a more useful representative of $[W_-]$ and as a corollary we obtain a new proof of the well known Levinson's theorem in dimension $n = 3$ [31].

Define the function

$$\varphi(D_3) = \frac{1}{2}\left(\mathrm{Id} + \tanh(\pi D_3) - i\cosh(\pi D_3)^{-1}\right). \tag{5.21}$$

We are interested in the resonant case, and so we are interested in finding a simple operator $\sigma \in U(L^2(\mathbb{R}^3))$ such that in the spectral representation we have $\sigma(0) = S(0)$ and $\lim_{\lambda\to\infty}\sigma(\lambda) = \mathrm{Id}$, with the limit taken in $\mathcal{B}(\mathcal{P})$.

Definition 5.3.19. Let $n = 3$. Then for any increasing differentiable $\theta : \mathbb{R}^+ \to \mathbb{R}$ with $\theta(\infty) = \pi$ and $\theta(0) = 0$ define

$$\sigma(\lambda) = \mathrm{Id} - (1 - \mathrm{e}^{i\theta(\lambda)})P_s, \tag{5.22}$$

where P_s denotes the projection onto the spherical harmonic subspace of order zero. We call σ a *resonant correction.* A particular choice of θ is given by $\theta = 2\tan^{-1}(\cdot)$.

Computation shows that for all $\lambda \in \mathbb{R}^+$ we have $\sigma(\lambda)$ is unitary and $\sigma(\lambda)^*\sigma'(\lambda) \in \mathcal{L}^1(\mathcal{P})$, and that

$$\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)^*\sigma'(\lambda))\,\mathrm{d}\lambda = \frac{1}{2}.$$

With such a σ we obtain the following pairing result.

Theorem 5.3.20. *Suppose that $n = 3$ and V satisfies Assumption 2.2.14 for some $\rho > 5$. Suppose further that the operator $H = H_0 + V$ admits a zero energy resonance. For any resonant correction σ we have*

$$\langle [S\sigma^*], [D_+] \rangle = -\mathrm{Index}(W_-) = N,$$

where N is the number of bound states of H (eigenvalues counted with multiplicity).

Proof. The operator $S\sigma^*$ is a properly admissable unitary by construction, and so the first equality is just the statement of Theorem 5.2.14. That $\mathrm{Index}(W_-) = -N$ follows from Proposition 2.3.9. That $\mathrm{Index}(W_\sigma) = 0$ is a consequence of Theorem 5.1.9. □

While Theorem 5.3.20 demonstrates that the index of W_- can be obtained as an index pairing, it does not supply a method for obtaining computational formulae. To do so requires more subleties of the scattering operator. It was noted in Remark 4.3.11 that while $S(\lambda) \to \mathrm{Id}$ as $\lambda \to \infty$ in $\mathcal{B}(\mathcal{P})$, this convergence does not happen in $\mathcal{L}^1(\mathcal{P})$. To remedy this we must find a representative of the class $[W_{S\sigma^*}]$ which has better trace class properties at infinity. This motivates the following definition.

Definition 5.3.21. Suppose that V satisfies Assumption 2.2.14 for some $\rho > 6$ and let S be the scattering operator for $H = H_0 + V$. Let $\beta : \mathbb{R}^+ \to \mathcal{B}(\mathcal{P})$ be a once continuously differentiable unitary valued function such that $\beta(\lambda) - \mathrm{Id} \in \mathcal{L}^1(\mathcal{P})$ for all $\lambda \in \mathbb{R}^+$ and $\beta(0) = \mathrm{Id}$ and $\lim_{\lambda\to\infty}\beta(\lambda) = \mathrm{Id}$ in $\mathcal{B}(\mathcal{P})$. Then $\mathrm{Det}(\beta(\lambda)) \in \mathbb{T}$ exists for all $\lambda \in \mathbb{R}^+$ and we say that β is a *high energy correction for S* if

$$\lim_{\lambda\to\infty} \mathrm{Det}(S(\lambda)\beta(\lambda)) = 1, \tag{5.23}$$

and $\mathrm{Index}(W_\beta) = 0$.

Note that the assumption $\lim_{\lambda\to\infty}(S(\lambda)\beta(\lambda) - \mathrm{Id}) = 0$ in $\mathcal{L}^1(\mathcal{H})$ implies Equation (5.23).

The following result is applicable to all dimensions $n \geq 2$. As usual we decompose the potential into $V = vUv$ with $v = |v|^{\frac{1}{2}}$ and $U = \mathrm{sign}(V)$.

Lemma 5.3.22. *Suppose that $n \geq 2$ and $q_1, q_2 \in C_c^\infty(\mathbb{R}^n)$ with $q_1q_2 = V$ and corresponding scattering operator S and fix $0 \neq \tilde{\chi} \in C_c^\infty(\mathbb{R}^+)$ with $\tilde{\chi}(\lambda) = 0$ for $\lambda \leq 1$. Define*

$\chi : \mathbb{R}^+ \to \mathbb{R}$ for $\lambda \in \mathbb{R}^+$ by

$$\chi(\lambda) = \frac{\int_0^\lambda \tilde{\chi}(u)\,\mathrm{d}u}{\int_0^\infty \tilde{\chi}(u)\,\mathrm{d}u}.$$

If $n = 2, 3$ let $p = 2$ and if $n \geq 4$ let $p \geq n$. For $\lambda > 0$ define the self-adjoint operator $\tilde{A}(\lambda) \in \mathcal{B}(\mathcal{P})$ by

$$\tilde{A}(\lambda) = -2\pi\Gamma_0(\lambda)q_2 \left(\sum_{\ell=1}^{p-1} \sum_{j=0}^{\ell-1} \frac{(-1)^\ell}{\ell} (q_1 R_0(\lambda + i0)q_2)^j \, (q_1 R_0(\lambda - i0)q_2)^{\ell-j-1} \right) q_1 \Gamma_0(\lambda)^*,$$

For $\lambda \in \mathbb{R}^+$ let $A(\lambda) = \chi(\lambda^{\frac{1}{2}})\tilde{A}(\lambda)$. Then the unitary operator $\beta(\lambda) = \mathrm{e}^{iA(\lambda)}$ satisfies $\mathrm{Index}(W_\beta) = 0$ and

$$\lim_{\lambda \to \infty} \mathrm{Det}(S(\lambda)\beta(\lambda)) = 1. \tag{5.24}$$

Proof. By construction we have that $A(\lambda)$ is self-adjoint for all $\lambda \in \mathbb{R}^+$. We have $A(0) = 0$ and the norm limit

$$\lim_{\lambda \to \infty} A(\lambda) = 0$$

by an application of the estimate (4.20) and [120, Theorem 1]. By Lemma 2.4.20 we have that $A(\lambda)$ is a trace-class operator and by cyclicity of the trace we have

$$\mathrm{Tr}(A(\lambda)) = i\chi(\lambda^{\frac{1}{2}}) \sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0)q_2)^\ell - (q_1 R_0(\lambda - i0)q_2)^\ell \right).$$

As a consequence of Hölder's inequality for Schatten ideals, $\beta(\lambda) - \mathrm{Id} \in \mathcal{L}^1(\mathcal{P})$ and so β defines a properly admissable unitary. Thus $\mathrm{Det}(\beta(\lambda)) = \mathrm{e}^{i\mathrm{Tr}(A(\lambda))}$ and so by Lemma 2.5.14 we find that

$$\begin{aligned}
&\mathrm{Det}(S(\lambda))\mathrm{Det}(\beta(\lambda)) \frac{\mathrm{Det}_p(\mathrm{Id} + q_1 R_0(\lambda + i0)q_2)}{\mathrm{Det}_p(\mathrm{Id} + q_1 R_0(\lambda - i0)q_2)} \\
&= \exp\left(\sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0)q_2)^\ell - (q_1 R_0(\lambda - i0)q_2)^\ell \right) + i\mathrm{Tr}(A(\lambda)) \right) \\
&= \exp\left((1 - \chi(\lambda^{\frac{1}{2}})) \sum_{\ell=1}^{p-1} \frac{(-1)^\ell}{\ell} \mathrm{Tr}\left((q_1 R_0(\lambda + i0)q_2)^\ell - (q_1 R_0(\lambda - i0)q_2)^\ell \right) \right).
\end{aligned}$$

An application of Theorem 2.5.29 and Lemma 2.5.16 gives that

$$\lim_{\lambda \to \infty} \mathrm{Det}(S(\lambda)\beta(\lambda)) = 1.$$

To see that $\mathrm{Index}(W_\beta) = 0$, we consider for $t \in [0,1]$ the homotopy

$$A_t(\lambda) = 2\pi\chi((1-t)\lambda^{\frac{1}{2}})\tilde{A}(\lambda).$$

The path $A_t(\lambda)$ defines a norm-continuous path in $\mathcal{B}(\mathcal{P})$ from $A_0(\lambda) = A(\lambda)$ to $A_1(\lambda) = 0$. Defining the path $A_t = A_t(L) \in \mathcal{B}(\mathcal{H})$ we obtain a norm continuous path in $\mathcal{B}(\mathcal{H})$ from A to 0. To see this, fix $t_1, t_2 \in [0,1)$ and define $d = (\min\{(1-t_1)^{-1}, (1-t_2)^{-1}\})^2 \geq 1$. Then for $g \in \mathcal{H}_{spec}$ we find

$$\begin{aligned}
&||(A_{t_2}(\cdot) - A_{t_1}(\cdot))g||^2_{\mathcal{H}_{spec}} \\
&= \int_0^\infty \int_{\mathbb{S}^{n-1}} |[(A_{t_2}(\lambda) - A_{t_1}(\lambda))g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega\,\mathrm{d}\lambda \\
&= \int_d^\infty \int_{\mathbb{S}^{n-1}} |[(A_{t_2}(\lambda) - A_{t_1}(\lambda))g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega\,\mathrm{d}\lambda \\
&\leq \int_d^\infty |\chi(\lambda^{\frac{1}{2}}(1-t_2)) - \chi(\lambda^{\frac{1}{2}}(1-t_1))|^2 \int_{\mathbb{S}^{n-1}} |[\tilde{A}(\lambda)g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega\,\mathrm{d}\lambda \\
&\leq C|t_2 - t_1|^2 \int_d^\infty \lambda \int_{\mathbb{S}^{n-1}} |[\tilde{A}(\lambda)g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega\,\mathrm{d}\lambda.
\end{aligned}$$

It remains to estimate $|[\tilde{A}(\lambda)g(\lambda,\cdot)](\omega)|$. We recall from [120, Theorem 1] that for sufficiently large λ we have

$$\left|\left|q_1 R_0(\lambda \pm i0)^j q_2\right|\right| = O(\lambda^{-\frac{j}{2}})$$

and so we may define

$$K = \sup\left\{2\pi \sum_{\ell=1}^{p-1}\sum_{j=0}^{\ell-1} \frac{1}{\ell}\left|\left|(q_1 R_0(\lambda + i0)q_2)^j (q_1 R_0(\lambda - i0)q_2)^{\ell-j-1}\right|\right| : \lambda \in [d,\infty)\right\}.$$

Using twice the estimate (4.20) we obtain

$$\begin{aligned}
&\int_{\mathbb{S}^{n-1}} |[\tilde{A}(\lambda)g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega = ||A(\lambda)g(\lambda,\cdot)||^2_{L^2(\mathbb{S}^{n-1})} \\
&\leq 2\pi\lambda^{-\frac{1}{2}} \sum_{\ell=1}^{p-1}\sum_{j=0}^{\ell-1} \frac{1}{\ell}\left|\left|(q_1 R_0(\lambda + i0)q_2)^j (q_1 R_0(\lambda - i0)q_2)^{\ell-j-1} q_1 \Gamma_0(\lambda)^* g(\lambda,\cdot)\right|\right|^2 \\
&\leq K\lambda^{-\frac{1}{2}} \left|\left|q_1\Gamma_0(\lambda)^* g(\lambda,\cdot)\right|\right|^2 \leq K\lambda^{-1} ||g(\lambda,\cdot)||^2_{L^2(\mathbb{S}^{n-1})}.
\end{aligned}$$

Combining these we find

$$\begin{aligned}||(A_{t_2}(\cdot) - A_{t_1}(\cdot))g||^2_{\mathcal{H}_{spec}} &\leq C|t_2 - t_1|^2 \int_d^\infty \lambda \int_{\mathbb{S}^{n-1}} |[\tilde{A}(\lambda)g(\lambda,\cdot)](\omega)|^2 \,\mathrm{d}\omega \,\mathrm{d}\lambda \\ &\leq CK|t_2 - t_1|^2 \int_d^\infty ||g(\lambda,\cdot)||^2_{L^2(\mathbb{S}^{n-1})} \,\mathrm{d}\lambda \\ &\leq CK|t_2 - t_1|^2 \, ||g||^2_{\mathcal{H}_{spec}}.\end{aligned}$$

The case when either or both of t_1, t_2 is one follows from a similar calculation.

As a result, the path $\beta_t = \mathrm{e}^{iA_t}$ defines a norm continuous path of unitary operators in $\mathcal{B}(\mathcal{H})$ from β to Id. Hence the path W_{β_t} defines a norm continuous path in $\mathcal{B}(\mathcal{H})$ from W_β to Id, along which the Fredholm index is constant and equal to zero. □

Remark 5.3.23. In dimension $n = 2, 3$ it is sufficient to take $\chi = \frac{2}{\pi}\tan^{-1}(\cdot)$ due to the milder growth of $A(\lambda)$ as $\lambda \to 0$.

Theorem 5.3.24. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > 6$ and let S be the scattering operator for $H = H_0 + V$. Let β be a high energy correction for S and let σ be a resonant correction if H admits a zero energy resonance. Otherwise, let $\sigma = \mathrm{Id}$. Then*

$$\begin{aligned}-N &= \mathrm{Index}(W_-) = \mathrm{Index}(W_{S\beta\sigma^*}) && (5.25)\\ &= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) + \frac{i}{4\pi}\lambda^{-\frac{1}{2}} \int_{\mathbb{R}^3} V(x)\,\mathrm{d}x\right)\mathrm{d}\lambda + \frac{1}{2}M_R(0), && (5.26)\end{aligned}$$

where we have defined

$$\frac{1}{2}M_R(0) = -\frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(\sigma(\lambda)^*\sigma'(\lambda))\,\mathrm{d}\lambda.$$

Proof. Since β defines a properly admissable unitary with $\mathrm{Index}(W_\beta) = 0$ we obtain the equality $-N = \mathrm{Index}(W_-) = \mathrm{Index}(W_{S\beta\sigma^*})$. By construction we have that the map $\lambda \mapsto \mathrm{Det}(S(\lambda)\beta(\lambda)\sigma(\lambda)^*)$ defines a loop, so has a well-defined winding number. The index of $W_{S\beta\sigma^*}$ can be computed via this winding number as

$$\begin{aligned}\mathrm{Index}(W_{S\beta\sigma^*}) &= \frac{1}{2\pi i}\int_0^\infty \frac{\frac{\mathrm{d}}{\mathrm{d}\lambda}(\mathrm{Det}(S(\lambda)\beta(\lambda)\sigma(\lambda)^*))}{\mathrm{Det}(S(\lambda)\beta(\lambda)\sigma(\lambda)^*)}\,\mathrm{d}\lambda \\ &= \frac{1}{2\pi i}\int_0^\infty (\mathrm{Tr}(S(\lambda)^*S'(\lambda)) + \mathrm{Tr}(\beta(\lambda)^*\beta'(\lambda)) - \mathrm{Tr}(\sigma(\lambda)^*\sigma'(\lambda)))\,\mathrm{d}\lambda \\ &= \frac{1}{2\pi i}\int_0^\infty (\mathrm{Tr}(S(\lambda)^*S'(\lambda)) + \mathrm{Tr}(\beta(\lambda)^*\beta'(\lambda)))\,\mathrm{d}\lambda + \frac{1}{2}M_R(0).\end{aligned}$$

Then Lemma 2.5.27 shows that $\mathrm{Tr}(S(\cdot)^*S'(\cdot)) - \frac{\mathrm{d}}{\mathrm{d}\lambda}\mathrm{Tr}(A(\cdot)) \in L^1(\mathbb{R}^+)$. Noting the equality

$\mathrm{Tr}(\beta(\lambda)^*\beta'(\lambda)) = \frac{\mathrm{d}}{\mathrm{d}\lambda}\mathrm{Tr}(A(\lambda))$, we obtain

$$\begin{aligned}\mathrm{Index}(W_{S\beta\sigma^*}) &= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) + \mathrm{Tr}(\beta(\lambda)^*\beta'(\lambda))\right)\mathrm{d}\lambda + \frac{1}{2}M_R(0)\\ &= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) + \frac{i}{4\pi}\lambda^{-\frac{1}{2}}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x\right)\mathrm{d}\lambda + \frac{1}{2}M_R(0). \quad \square\end{aligned}$$

Remark 5.3.25. With a statement of Levinson's theorem in hand, one can define the spectral shift function directly. Define the function $P_3 : \mathbb{R}^+ \to \mathbb{C}$ by

$$P_3(\lambda) = -\frac{i}{2\pi}\lambda^{\frac{1}{2}}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x.$$

Then the spectral shift function is given by the relation

$$\begin{aligned}\xi(\lambda) = &-\sum_{k=0}^{K} M(\lambda_k)\chi_{[\lambda_k,\infty)}(\lambda) - \frac{1}{2}M_R(0)\chi_{[0,\infty)}\\ &+ \chi_{[0,\infty)}\frac{1}{2\pi i}\left(\int_0^\lambda \left(\mathrm{Tr}(S(\mu)^*S'(\mu)) - P_3'(\mu)\right)\mathrm{d}\mu + p(\lambda)\right).\end{aligned}$$

This agrees with the normalisation convention of Theorem 2.5.13.

Corollary 5.3.26. *Suppose that $n = 3$ and V satisfies Assumption 2.2.14 for some $\rho > 5$. Then*

$$\xi(0+) = -N - \frac{1}{2}M_R(0).$$

5.3.3 High energy corrections in dimension $n = 2$

As we have seen in Theorem 4.1.5 we have, in dimension $n = 2$, the relation $S(0) = \mathrm{Id}$ always and so no low energy corrections are required to make the index pairing work. We do not however have $\lim_{\lambda\to\infty} S(\lambda) = \mathrm{Id}$ in trace norm, so a high energy correction is required to obtain a different representative of the class $[W_S]$ and use the index pairing to obtain a formula for the number of bound states. We demonstrate in this section how to obtain the 2-dimensional statement of Levinson's theorem in Theorem 2.5.32 in the case of no p-resonances, providing a new proof of [26, Theorem 6.3] and [50, Theorem 3.2].

Definition 5.3.27. Suppose that V satisfies Assumption 2.2.14 for some $\rho > 11$ and let S be the scattering operator for $H = H_0 + V$. Let $\beta : \mathbb{R}^+ \to \mathcal{B}(\mathcal{P})$ be a once continuously differentiable unitary valued function such that $\beta(\lambda) - \mathrm{Id} \in \mathcal{L}^1(\mathcal{P})$ for all $\lambda \in \mathbb{R}^+$ and $\beta(0) = \mathrm{Id}$ and $\lim_{\lambda\to\infty}\beta(\lambda) = \mathrm{Id}$ in $\mathcal{B}(\mathcal{P})$. Then $\mathrm{Det}(\beta(\lambda)) \in \mathbb{T}$ exists for all $\lambda \in \mathbb{R}^+$ and we say that β is a *high energy correction for S* if

$$\lim_{\lambda\to\infty}\mathrm{Det}(S(\lambda)\beta(\lambda)) = 1, \tag{5.27}$$

and $\mathrm{Index}(W_\beta) = 0$.

For a given potential V we construct a high energy correction for the corresponding scattering operator.

Lemma 5.3.28. *Suppose that $n = 2$ and V satisfies Assumption 2.2.14 for some $\rho > 11$ and let S be the corresponding scattering operator. For $\lambda > 0$ define the self-adjoint operator $A(\lambda) = -4i\tan^{-1}(\lambda) i\Gamma_0(\lambda)V\Gamma_0(\lambda)^*$. Then the unitary operator $\beta(\lambda) = \mathrm{e}^{iA(\lambda)}$ is a high energy correction for S.*

Proof. This follows directly from Lemma 5.3.22 and Remark 5.3.23. □

We note that the choice of the factor $\frac{2}{\pi}\tan^{-1}(\cdot)$ is simply for convenience, any increasing differentiable function vanishing at 0 and having limit 1 at infinity suffices.

Using the high energy correction of Lemma 5.3.28 we provide a new proof of Levinson's theorem in dimension $n = 2$ in the absence of p-resonances.

Theorem 5.3.29. *Suppose that $n = 2$ and V satisfies Assumption 2.2.14 for some $\rho > 11$ and let S be the corresponding scattering operator. Suppose further that there are no p-resonances and let β be a high energy correction for S. Then*

$$-N = \mathrm{Index}(W_-) = \mathrm{Index}(W_{S\beta}) = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x.$$

Proof. We only need to show the equality

$$\mathrm{Index}(W_{S\beta}) = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x$$

since the others have been established in Theorem 5.3.2. Compute

$$\begin{aligned}
\mathrm{Index}(W_{S\beta}) &= \frac{1}{2\pi i}\int_{\mathbb{R}^+} \frac{\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\mathrm{Det}(S(\lambda)\beta(\lambda))\right)}{\mathrm{Det}(S(\lambda)\beta(\lambda))}\,\mathrm{d}\lambda \\
&= \frac{1}{2\pi i}\int_{\mathbb{R}^+} \left(\mathrm{Tr}S(\lambda)^* S'(\lambda)) + \mathrm{Tr}(\beta(\lambda)^*\beta'(\lambda)\right)\,\mathrm{d}\lambda \\
&= \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2\pi i}\int_{\mathbb{R}^+} \frac{\mathrm{d}}{\mathrm{d}\lambda}\mathrm{Tr}(A(\lambda))\,\mathrm{d}\lambda \\
&= \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x,
\end{aligned}$$

where we have used Lemma 2.4.20 to compute the final integral. □

Thus, we have provided a new proof of Theorem 2.5.32 in the case of no p-resonances.

Remark 5.3.30. The result of Theorem 5.3.29 is enough to completely determine the spectral shift function for the pair (H, H_0) in the case of no p-resonances. We obtain

$$\xi(\lambda) = -\sum_{k=1}^{K} M(\lambda_k)\chi_{[\lambda_k,\infty)}(\lambda) + \frac{1}{2\pi i}\chi_{[0,\infty)}(\lambda)\int_0^{\lambda} \mathrm{Tr}(S(\mu)^* S'(\mu))\,\mathrm{d}\mu.$$

Corollary 5.3.31. *Suppose that $n = 2$ and V satisfies Assumption 2.2.14 for some $\rho > 11$. Suppose further that there are no p-resonances. Then*

$$\xi(0+) = -N.$$

5.3.4 High energy corrections in dimension $n \geq 4$

In dimension $n \geq 4$ the failure of the convergence of the scattering matrix at infinity in trace norm persists as an obstruction to obtaining an explicit formula. In this section we demonstrate how to construct a high energy correction to the scattering operator which will allow us to obtain a statement of Levinson's theorem in higher dimensions.

Definition 5.3.32. Suppose that V satisfies Assumption 4.3.1 and let S be the scattering operator for $H = H_0 + V$. Let $\beta : \mathbb{R}^+ \to \mathcal{B}(\mathcal{P})$ be a once continuously differentiable unitary-valued function such that $\beta(\lambda) - \mathrm{Id} \in \mathcal{L}^1(\mathcal{P})$ for all $\lambda \in \mathbb{R}^+$ and $\beta(0) = \mathrm{Id}$ and $\lim_{\lambda\to\infty} \beta(\lambda) = \mathrm{Id}$ in $\mathcal{B}(\mathcal{P})$. Then $\mathrm{Det}(\beta(\lambda)) \in \mathbb{T}$ exists for all $\lambda \in \mathbb{R}^+$ and we say that β is a *high energy correction for S* if

$$\lim_{\lambda\to\infty} \mathrm{Det}(S(\lambda)\beta(\lambda)) = 1, \tag{5.28}$$

and $\mathrm{Index}(W_\beta) = 0$.

For a given potential V we construct a high energy correction for the corresponding scattering operator. As usual we decompose the potential into $V = vUv$ with $v = |V|^{\frac{1}{2}}$ and $U = \mathrm{sign}(V)$.

Lemma 5.3.33. *Suppose that $V \in C_c^\infty(\mathbb{R}^n)$ and let S be the corresponding scattering operator. For $\lambda > 0$ define for $p \geq n$ the self-adjoint operator $\tilde{A}(\lambda) \in \mathcal{B}(\mathcal{P})$ by*

$$\tilde{A}(\lambda) = 2\pi\Gamma_0(\lambda)V\left(\sum_{\ell=1}^{p-1}\sum_{j=0}^{\ell-1}\frac{(-1)^\ell}{\ell}(vR_0(\lambda+i0)vU)^j(vR_0(\lambda-i0)vU)^{\ell-j-1}\right)\Gamma_0(\lambda)^*$$

Further define the self-adjoint operator $A(\lambda) \in \mathcal{B}(\mathcal{P})$ by

$$A(\lambda) = \chi(\lambda^{\frac{1}{2}})\tilde{A}(\lambda),$$

where χ is as in Lemma 5.3.22. Then the unitary $\beta(\lambda) = \mathrm{e}^{iA(\lambda)}$ is a high energy correction for S.

Proof. This follows directly from Lemma 5.3.22. □

We now use the high energy correction of Lemma 5.3.28 to provide an alternate proof of Levinson's theorem in dimension $n \geq 4$ in the absence of resonances. Define the function $Q_n : \mathbb{R}^+ \to \mathbb{C}$ by

$$Q_n(\lambda) = -\mathrm{Tr}(\tilde{A}(\lambda))$$

and recall the high-energy polynomials P_n, p_n from Definitions 2.5.28 and 2.5.26.

Theorem 5.3.34. *Suppose that $n \geq 4$, $V \in C_c^\infty(\mathbb{R}^n)$ and there are no resonances. Then the number of bound states of H is given by*

$$-N = \mathrm{Index}(W_-) = \mathrm{Index}(W_{S\beta}) = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - p_n(\lambda)\right)\,\mathrm{d}\lambda - \frac{1}{2\pi i}P_n(0).$$

Proof. The first two equalities have been established in Theorem 5.3.2. Since the operator $\mathrm{Det}(S(\lambda)\beta(\lambda)) \to 1$ as both $\lambda \to 0$ and $\lambda \to \infty$, the map $\lambda \mapsto \mathrm{Det}(S(\lambda)\beta(\lambda))$ defines a loop and we find

$$\begin{aligned}
&\mathrm{Index}(W_{S\beta})\\
&= \mathrm{Wind}(\mathrm{Det}(S(\cdot)\beta(\cdot)) = \frac{1}{2\pi i}\int_0^\infty \frac{\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathrm{Det}(S(\lambda)\beta(\lambda))}{\mathrm{Det}(S(\lambda)\beta(\lambda))}\,\mathrm{d}\lambda\\
&= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) + \frac{\mathrm{d}}{\mathrm{d}\lambda}\mathrm{Tr}(A(\lambda))\right)\mathrm{d}\lambda\\
&= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - p_n(\lambda)\right)\mathrm{d}\lambda + \frac{1}{2\pi i}\int_0^\infty \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\chi(\lambda)^{\frac{1}{2}}Q_n(\lambda) + P_n(\lambda)\right)\mathrm{d}\lambda\\
&= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - p_n(\lambda)\right)\mathrm{d}\lambda - \frac{1}{2\pi i}P_n(0),
\end{aligned}$$

where in the last line we have used the properties of χ and the fundamental theorem of calculus. □

Remark 5.3.35. We note that the statement of Levinson's theorem given in Theorem 5.3.34 completely determines the spectral shift function for the pair (H, H_0) as

$$\begin{aligned}
\xi(\lambda) = &-\sum_{k=1}^{K} M(\lambda_k)\chi_{[\lambda_k,\infty)}(\lambda)\\
&+ \frac{1}{2\pi i}\chi_{[0,\infty)}\left(\int_0^\lambda \left(\mathrm{Tr}(S(\mu)^*S'(\mu)) - p_n(\mu)\right)\mathrm{d}\mu + P_n(\lambda)\right).
\end{aligned}$$

Corollary 5.3.36. *Suppose that $n \geq 4$, V satisfies Assumption 4.3.1 and there are no resonances. Then $\xi(0+) = -N$.*

In higher dimensions we can determine the coefficients by performing more commutators, however these become difficult very quickly in a similar manner to the heat coefficients of Theorem 2.5.34. We describe in Proposition 5.3.37 the coefficients arising in dimensions $n \leq 7$. In Chapter 6 we provide an alternative method for determining some of these coefficients.

Proposition 5.3.37. *Let $n \in \{4,5,6,7\}$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > n+1$ and $V \in C^\infty(\mathbb{R}^n)$. Then the function Q_n of Lemma 5.3.33 satisfies $Q_n(\lambda) = P_n(\lambda) + q(\lambda)$, for some $q : \mathbb{R}^+ \to \mathbb{C}$. Explicitly we obtain*

$$Q_n(\lambda) = -\frac{(2\pi i)\lambda^{\frac{n-2}{2}}\mathrm{Vol}(\mathbb{S}^{n-1})}{2(2\pi)^n}\int_{\mathbb{R}^n} V(x)\,\mathrm{d}x + \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^{n-1})(n-2)\lambda^{\frac{n-4}{2}}}{8(2\pi)^n}\int_{\mathbb{R}^n} V(x)^2\,\mathrm{d}x$$
$$-\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^{n-1})(n-2)(n-4)\lambda^{\frac{n-6}{2}}}{48(2\pi)^n}\int_{\mathbb{R}^n}\left(V(x)^3 + \frac{1}{2}|[\nabla V](x)|^2\right)\mathrm{d}x + q(\lambda).$$

If n is even, then $q = 0$. In addition we have $q(0) = 0$ for n even.

Proposition 5.3.37 follows immediately from the computations in Theorem 2.5.29.

Remark 5.3.38. For explicitness and a later comparison, we record the statements of Levinson's theorem in dimensions $n = 4,5,6,7$. We use the notation of Theorem 2.5.34. In dimension $n = 4$ with no resonances we find

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - c_1(4,V)\right)\mathrm{d}\lambda - \beta_4(V),$$

where

$$c_1(4,V) - \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^3)}{2(2\pi)^4}\int_{\mathbb{R}^4} V(x)\,\mathrm{d}x \quad \text{and}$$
$$\beta_4(V) = \frac{1}{2\pi i}P_4(0) = \frac{\mathrm{Vol}(\mathbb{S}^3)}{4(2\pi)^2}\int_{\mathbb{R}^4} V(x)^2\,\mathrm{d}x.$$

In dimension $n = 5$ we find

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \lambda^{\frac{1}{2}}c_1(5,V) - \lambda^{-\frac{1}{2}}c_2(5,V)\right)\mathrm{d}\lambda,$$

where the coefficients are

$$c_1(5,V) = -\frac{3}{2}\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^4)}{2(2\pi)^5}\int_{\mathbb{R}^5} V(x)\,\mathrm{d}x \quad \text{and}$$
$$c_2(5,V) = \frac{1}{2}\frac{3(2\pi i)\mathrm{Vol}(\mathbb{S}^4)}{8(2\pi)^5}\int_{\mathbb{R}^5} V(x)^2\,\mathrm{d}x.$$

In dimension $n = 6$ we have

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - c_1(6,V)\lambda - c_2(6,V)\right)\,\mathrm{d}\lambda - \beta_6(V),$$

where

$$\begin{aligned} c_1 &= -\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6}\int_{\mathbb{R}^6} V(x)\,\mathrm{d}x, \\ c_2 &= \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^5)}{2(2\pi)^6}\int_{\mathbb{R}^6} V(x)^2\,\mathrm{d}x \quad \text{ and} \\ b_6 &= \frac{1}{2\pi i}P_6(0) = -\frac{\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\int_{\mathbb{R}^6}\left(V(x)^3 + \frac{1}{2}|[\nabla V](x)|^2\right)\,\mathrm{d}x. \end{aligned}$$

In dimension $n = 7$ we obtain

$$-N = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \lambda^{\frac{3}{2}}c_1(7,V) - \lambda^{\frac{1}{2}}c_2(7,V) - \lambda^{-\frac{1}{2}}c_3(7,V)\right)\,\mathrm{d}\lambda,$$

where

$$\begin{aligned} c_1(7,V) &= -\frac{5}{2}\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^6)}{2(2\pi)^7}\int_{\mathbb{R}^7} V(x)\,\mathrm{d}x, \\ c_2(7,V) &= \frac{3}{2}\frac{5(2\pi i)\mathrm{Vol}(\mathbb{S}^6)}{8(2\pi)^7}\int_{\mathbb{R}^7} V(x)^2\,\mathrm{d}x \quad \text{ and} \\ c_3(7,V) &= \frac{1}{2}\frac{15(2\pi i)}{48(2\pi)^7}\int_{\mathbb{R}^7}\left(V(x)^3 + \frac{1}{2}|[\nabla V](x)|^2\right)\,\mathrm{d}x. \end{aligned}$$

Chapter 6

Spectral flow for Schrödinger operators

In this chapter we consider the spectral flow along the path $H = H_0 + tV$ and show how Levinson's theorem can be obtained from the spectral flow along this path. To use the spectral flow formula of [47, Theorem 9] we require some simple adjustments to make our path of operators Fredholm. To analyse the terms appearing in [47, Theorem 9] requires an analogue of the Birman-Kreĭn trace formula of Theorem 2.5.19 and the pseudodifferential operator calculus of [43], modified appropriately to our second order operators.

In Section 6.1 we briefly recall the definition of spectral flow of [129, 130] for paths of unbounded self-adjoint Fredholm operators and in particular Equation 6.1 of [47, Theorem 9]. Since the operators H_0 and H are never Fredholm, we consider a family of modified operators $(H_0(\alpha), H(\alpha))$ which are Fredholm and describe their stationary scattering theory in Section 6.2. In Section 6.3 we briefly recall a number of results from the pseudodifferential operator calculus of [43, 46] modified to our operators $(H_0(\alpha), H(\alpha))$.

In Section 6.4 we apply [47, Theorem 9] to the path $H_t(\alpha) = H_0 + \alpha + tV$ to prove, using the Birman-Kreĭn trace formula and the pseudodifferential operator calculus of Section 6.3 to provide in Theorems 6.4.22 (odd dimensions) and 6.4.23 (even dimensions) an expression for the spectral flow along the path $H_t(\alpha)$. Finally, in Section 6.5 we use the high-energy behaviour of the time delay operator discussed in Section 2.5.1 and Chapter 5 to show that Levinson's theorem is a result of spectral flow. In particular, Section 6.4 onwards contains original results.

6.1 Spectral flow

The concept of spectral flow was used by Atiyah, Patodi and Singer in [10, 11] as a tool to develop APS index theory. Spectral flow is intuitively defined as the net number of eigenvalues which change sign along a path of self-adjoint operators, with the convention that an eigenvalue changing from negative to positive will contribute a 1 to the spectral flow. We use the definition due to Phillips [129, 130]. Phillips' definition of spectral flow is valid in the much broader setting of semifinite von Neumann algebras with faithful normal semifinite traces, although we do not need the full power of such a definition.

Consider $\mathcal{B}(\mathcal{H})$ with trace Tr, let $\pi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H})$ denote the projection onto the Calkin algebra. Let $\chi = \chi_{[0,\infty)}$ be the characteristic function of the interval $[0, \infty)$. Let (T_t) be any norm continuous path of bounded self-adjoint Fredholm operators in $\mathcal{B}(\mathcal{H})$. Then $\pi(\chi(T_t)) = \chi(\pi(T_t))$. Since the spectrum of the $\pi(T_t)$ are bounded away from zero, the path $\chi(\pi(T_t))$ is continuous. By compactness (and [20, Lemma 4.1]), we can choose a partition $0 = t_0 < t_1 < \cdots < t_k = 1$ such that

$$||\pi(\chi(T_t)) - \pi(\chi(T_s))|| < \frac{1}{2}$$

for all $t, s \in [t_{i-1}, t_i]$ and $1 \leq i \leq k$. Defining the projection $P_i = \chi(T_{t_i})$ we find that $P_{i-1}P_i : P_i\mathcal{H} \to P_{i-1}\mathcal{H}$ is Fredholm. We recall the following definition, due to Phillips [129, 130].

Definition 6.1.1. Let $\mathcal{H}$ be a Hilbert space. For $t \in [0, 1]$ let (T_t) be any norm continuous path of bounded self-adjoint Fredholm operators in $\mathcal{B}(\mathcal{H})$. For a partition $0 = t_0 < t_1 < \cdots < t_k = 1$ of the interval $[0, 1]$ define the operators $P_i = \chi(T_{t_i})$. Then we define the *spectral flow* of the path (T_t) by

$$\mathrm{sf}(T_t) := \sum_{i=1}^{k} \mathrm{Ind}(P_{i-1}P_i).$$

We note that the above definition of spectral flow is independent of the choice of partition [107, 129, 130] and agrees with the topological definition used in [10, 11], when both make sense. For unbounded operators, we make the following definition of spectral flow [47].

Definition 6.1.2. Let $\mathcal{H}$ be a Hilbert space with trace Tr. Let (D_t) be a graph norm continuous path of unbounded self-adjoint Fredholm operators on $\mathcal{H}$. Denote the function $F : \mathbb{R} \to [-1, 1]$ by $F(x) = x(1 + x^2)^{-\frac{1}{2}}$. The *spectral flow* along the path (D_t) is defined by

$$\mathrm{sf}(D_t) = \mathrm{sf}(F(D_t)).$$

Throughout the rest of this section $[0, 1] \ni t \mapsto D_t$ stands for a path of unbounded self-adjoint linear operators on $\mathcal{H} = L^2(\mathbb{R}^n)$. We denote by $(F_t) = (F(D_t))$ the *bounded transform* of the path (D_t). We must also impose a smoothness assumption on D_t to use analytic formulae for the spectral flow.

Definition 6.1.3. 1. A path $[0,1] \ni t \mapsto D_t$ is called Γ-*differentiable* at the point $t = t_0$ if and only if there exists a bounded linear operator T such that

$$\lim_{t \to t_0} \left|\left| t^{-1}(D_t - D_{t_0})(\mathrm{Id} + D_{t_0}^2)^{-\frac{1}{2}} - T \right|\right| = 0.$$

In this case we set $\dot{D}_{t_0} = T(\mathrm{Id} + D_{t_0}^2)^{-\frac{1}{2}}$. The operator $\dot{D}_t$ is a symmetric linear operator with domain $\mathrm{Dom}(D_t)$ [47, Lemma 25].

2. If the mapping $t \mapsto \dot{D}_t(\mathrm{Id} + D_t^2)^{-\frac{1}{2}}$ is defined and continuous with respect to the operator norm, then we call the path $t \mapsto D_t$ a *continuously* Γ-*differentiable* or a C^1_Γ *path.*

The most general analytic spectral flow formula for the case of unbounded operators on a Hilbert space is given by the following theorem [47, Theorem 9].

Theorem 6.1.4. *Let* $[0,1] \ni t \mapsto D_t$ *be a piecewise* C^1_Γ *path of linear operators and* $F_t \in \mathcal{F}_* = \{F \in \mathcal{B}(\mathcal{H}) : F = F^* \text{ is Fredholm and } ||F|| \leq 1\}$. *Let* $g : \mathbb{R} \to \mathbb{R}$ *be a positive* C^2 *function such that*

1. $\int_{\mathbb{R}} g(x)\,\mathrm{d}x = 1$;
2. $\int_0^1 \left|\left| \dot{D}_t g(D_t) \right|\right|_1 \mathrm{d}t < \infty$; *and*
3. $G(D_1) - \frac{1}{2}B_1 - G(D_0) + \frac{1}{2}B_0 \in \mathcal{L}^1(\mathcal{H})$ *(the trace class), where* $B_j = 2\chi_{[0,\infty)}(D_j) - 1$, *and* G *is the antiderivative of* g *such that* $G(\pm\infty) = \pm\frac{1}{2}$.

Then

$$\mathrm{sf}(D_t) = \int_0^1 \mathrm{Tr}(\dot{D}_t g(D_t))\,\mathrm{d}t - \mathrm{Tr}\left(G(D_1) - \frac{1}{2}B_1 - G(D_0) + \frac{1}{2}B_0\right). \tag{6.1}$$

Remark 6.1.5. There is a sign difference on the second term on the right-hand side of Equation (6.1) when compared to the statement of [47, Theorem 9]. This is due to a sign error in the proof of [47, Theorem 9]. In particular, on p. 1823 there is a diagram illustrating the path of integration for the succeeding argument. The diagram is correct, however in the following formula the signs on the terms γ_1, γ_2 are incorrect due to the wrong choice of orientation of the path in their definition.

Fix $s > \frac{n+2}{2}$ and make the explicit choice $g_s(x) = \frac{1}{C_s}(1 + x^2)^{-s}$ with C_s chosen such that $||g_s||_1 = 1$. In this case we can determine the antiderivative G_s of g_s which satisfies the hypotheses of Theorem 6.1.4 as

$$G_s(x) = -\frac{1}{2} + \int_{-\infty}^{x} g_s(u)\,\mathrm{d}u.$$

Since we are using the functional calculus on G_s, we require a simpler expression which does not have the variable as an integration limit. Since G_s is an odd function, for $x > 0$ we find

$$\begin{aligned} G_s(x) &= \frac{1}{C_s}\int_0^x (1+u^2)^{-s}\,\mathrm{d}u = \frac{1}{C_s}\left(\int_0^\infty (1+u^2)^{-s}\,\mathrm{d}u - \int_x^\infty (1+u^2)^{-s}\,\mathrm{d}u\right) \\ &= \frac{1}{2} - \frac{1}{C_s}\int_x^\infty (1+u^2)^{-s}\,\mathrm{d}u = \frac{1}{2} - \frac{1}{2C_s}\int_1^\infty x(1+wx^2)^{-s}w^{-\frac{1}{2}}\,\mathrm{d}w \\ &=: \frac{1}{2} - \frac{1}{2}\eta_s(x). \end{aligned}$$

If $x < 0$ we use the fact G_s is odd, so $G_s(-x) = -\frac{1}{2} + \eta_s(-x)$. The requirement $s > \frac{n+2}{2}$ is to ensure η_s satisfies Equation (2.84) so that we are able to use Theorem 2.5.13 and in particular (an analogue of) the Birman-Kreĭn trace formula which we state in Lemma 6.2.8. We remark that the function η_s is defined for $\mathrm{Re}(s) > \frac{1}{2}$, holomorphic in s with a simple pole at $s = \frac{1}{2}$, a fact to be exploited repeatedly at a later point.

6.2 Making the operators Fredholm

As usual we let $H = H_0 + V$ where we make for the rest of this chapter the following assumption on V.

Assumption 6.2.1. We assume that V satisfies Assumption 4.3.1 so that we may use the results of Chapter 5 regarding the behaviour of the spectral shift function. We impose the additional assumption that V is smooth.

The assumption on the differentiability of the potential becomes necessary when we employ the pseudodifferential operator calculus, where we must take derivatives of the potential.

To use the spectral flow formulae of the previous section, we consider pairs of Fredholm operators, which H_0 and H are not since 0 is contained in the essential spectrum of both. We construct a pair of Fredholm operators as follows. Enumerate the distinct eigenvalues of H in increasing order as $\lambda_1 < \lambda_2 < \cdots < \lambda_K \leq 0$. Let $\mu \in \{\lambda_{K-1}, \lambda_K\}$ be the closest non-zero eigenvalue of H to zero. Then for any $\alpha \in (0, -\mu)$ the operators $H_0(\alpha) = H_0 + \alpha$ and $H(\alpha) = H_0 + V + \alpha$ are invertible and hence are Fredholm operators.

The operators $H_0(\alpha)$ and $H(\alpha)$ depend norm-resolvent continuously on $\alpha \in (0, -\mu)$. The operator $H_0(\alpha)$ has purely absolutely continuous spectrum $\sigma(H_0(\alpha)) = \sigma_{ac}(H_0(\alpha)) = [\alpha, \infty)$. The operator $H(\alpha)$ has finitely many eigenvalues in $(-\infty, \alpha]$ and has absolutely continuous spectrum $\sigma_{ac}(H(\alpha)) = \sigma_{ac}(H_0(\alpha)) = [\alpha, \infty)$. We enumerate the distinct eigenvalues of $H(\alpha)$ in ascending order as $\lambda_1(\alpha) < \lambda_2(\alpha) < \cdots < \lambda_K(\alpha)$ and note that for each j we have $\lambda_j(\alpha) = \lambda_j + \alpha$, where the λ_j denote the distinct eigenvalues of H. We also note that the number of eigenvalues of H is equal to the number of eigenvalues of $H(\alpha)$, independent of α.

For each $\alpha \in (0, -\mu)$, $z \in \mathbb{C} \setminus \mathbb{R}$ and any $p \geq n$ we have by (an analogue of) Lemma 2.5.11 that the difference $(H(\alpha) - z)^{-p} - (H_0(\alpha) - z)^{-p} \in \mathcal{L}^1(\mathcal{H})$ and the wave operators

$$W_\pm(\alpha) = \underset{t\to\pm\infty}{\text{s-lim}}\, \mathrm{e}^{itH(\alpha)}\mathrm{e}^{-itH_0(\alpha)}P_{ac}(H_0(\alpha)) = \underset{t\to\pm\infty}{\text{s-lim}}\, \mathrm{e}^{itH}\mathrm{e}^{-itH_0} = W_\pm$$

exist and are asymptotically complete by the invariance principle [137, Theorem XI.11] (or an adaptation of the results of Chapter 2). We also note that the wave operators are independent of α. The α dependence is seen in the spectral representation for $H_0(\alpha)$, which we now describe.

Definition 6.2.2. For $\lambda \in (\alpha, \infty)$, $s \in \mathbb{R}$ and $t > \frac{1}{2}$ we define the operator $\Gamma_\alpha(\lambda) : H^{s,t} \to \mathcal{P}$ by

$$[\Gamma_\alpha(\lambda)f](\omega) = 2^{-\frac{1}{2}}(\lambda - \alpha)^{\frac{n-2}{4}}[\mathcal{F}f]((\lambda - \alpha)^{\frac{1}{2}}\omega) = [\Gamma_0(\lambda - \alpha)f](\omega).$$

The operator $F_\alpha : \mathcal{H} \to L^2([\alpha, \infty)) \otimes \mathcal{P}$, which diagonalises the Hamiltonian $H_0(\alpha)$, is given by

$$[F_\alpha f](\lambda, \omega) = [\Gamma_\alpha(\lambda)f](\omega) = [F_0 f](\lambda - \alpha, \omega).$$

Since the operators F_α and Γ_α are simply translations of F_0 and Γ_0 one can easily check the following.

Lemma 6.2.3. *The operator F_α is unitary. Moreover for $\lambda \in (\alpha, \infty)$, $\omega \in \mathbb{S}^{n-1}$ and $f \in L^2([\alpha, \infty)) \otimes \mathcal{P}$ we have*

$$[F_\alpha H_0(\alpha) F_\alpha^* f](\lambda, \omega) = \lambda f(\lambda, \omega).$$

The scattering operator $S_\alpha = W_+(\alpha)^* W_-(\alpha)$ is unitary and commutes with $H_0(\alpha)$ and so there exists a family $\{S_\alpha(\lambda)\}_{\lambda\in[\alpha,\infty)}$ of unitary operators on $\mathcal{P}$ such that the relation $[F_\alpha S_\alpha f](\lambda, \omega) = S_\alpha(\lambda)[F_\alpha f](\lambda, \omega)$ holds. We call $S_\alpha(\lambda)$ the (translated) scattering matrix at energy λ.

The next result is proved in an identical fashion to Theorem 2.4.32.

Theorem 6.2.4. *Suppose that V satisfies Assumption* (6.2.1). *The scattering matrix is given for all $\lambda \in [\alpha, \infty)$ by the equation*

$$S_\alpha(\lambda) = \mathrm{Id} - 2\pi i \Gamma_\alpha(\lambda)(V - VR(\lambda - \alpha + i0)V)\Gamma_\alpha(\lambda)^* = S(\lambda - \alpha).$$

For each $\lambda \in [\alpha, \infty)$, the operator $S_\alpha(\lambda)$ is unitary in $\mathcal{P} = L^2(\mathbb{S}^{n-1})$ and depends norm continuously on $\lambda \in [\alpha, \infty)$.

Since the scattering matrix $S_\alpha(\lambda)$ is simply a translation of the scattering matrix $S(\lambda)$, the properties of the time-delay and spectral shift function for the pair $(H_0(\alpha), H(\alpha))$ also follow immediately.

The time delay satisfies $T_\alpha(\lambda) = -iS_\alpha^*(\lambda)S_\alpha'(\lambda) = T(\lambda-\alpha)$, its existence is guaranteed by the following result, whose proof is identical to that of Theorem 2.5.3.

Lemma 6.2.5. *Suppose that V satisfies Assumption 6.2.1 and let $P_0(\alpha)$ denote the spectral family for $H_0(\alpha)$. Then the scattering matrix is differentiable. Define T_α by*

$$\mathrm{Dom}(T_\alpha) = \{f \in \mathcal{H}_{ac} : P_0(\alpha)([a,b])f = f \text{ for some } [a,b] \subset (0,\infty)\},$$
$$[F_\alpha T_\alpha f](\lambda,\omega) = -iS_\alpha(\lambda)^* S_\alpha'(\lambda)[F_\alpha f](\lambda,\omega).$$

Then T_α is essentially self-adjoint on $\mathrm{Dom}(T_\alpha)$*,* $\mathrm{Dom}(T_\alpha) \subset \mathrm{Dom}(H_0(\alpha))$*, and T_α commutes with $H_0(\alpha)$. Furthermore, the operator $T_\alpha(\lambda)$ is trace class for all $\lambda \in [\alpha,\infty)$.*

Theorem 6.2.6. *Suppose that V satisfies Assumption 2.2.14 for some $\rho > n$. Then there exists a real-valued function ξ_α such that the trace formula*

$$\mathrm{Tr}\left(f(H(\alpha)) - f(H_0(\alpha))\right) = \int_{\mathbb{R}} \xi_\alpha(\lambda) f'(\lambda)\, \mathrm{d}\lambda \tag{6.2}$$

holds at least for all $f \in C_c^\infty(\mathbb{R})$. The function ξ_α satisfies $\xi_\alpha(\lambda) = \xi(\lambda-\alpha)$, where ξ is the spectral shift function for the pair (H, H_0).

The function $\xi_\alpha = \xi(H_0(\alpha), H(\alpha))$ is known as the spectral shift function for the pair $(H_0(\alpha), H(\alpha))$. As before the trace formula of Equation (6.2) fixes ξ_α up to an additive constant. This constant is fixed by the condition that $\xi_\alpha(\lambda) = 0$ for $\lambda < |\inf(\sigma_p(H(\alpha)))|$.

Lemma 6.2.7. *Suppose that V satisfies Assumption 6.2.1. Then for $\lambda \in [\alpha,\infty)$ the spectral shift function and the scattering matrix are related by the formula*

$$\mathrm{Det}(S_\alpha(\lambda)) = \mathrm{e}^{-2\pi i \xi_\alpha(\lambda)}.$$

For $\lambda \in [\alpha,\infty)$ the spectral shift function and time-delay operator are related by the formula

$$-2\pi i \xi_\alpha'(\lambda) = \mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)).$$

Our main use of the spectral shift function is the Birman-Kreĭn formula for the pair $(H(\alpha), H_0(\alpha))$, which follows immediately from Theorem 2.5.19 by an identical proof.

Lemma 6.2.8. *Suppose that V satisfies Assumption 6.2.1 and $f \in C_c^\infty(\mathbb{R})$. Then*

$$\mathrm{Tr}(f(H(\alpha)) - f(H_0(\alpha))) = \frac{1}{2\pi i}\int_\alpha^\infty f(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\mathrm{d}\lambda + \sum_{k=1}^K M(\lambda_k(\alpha))f(\lambda_k(\alpha))$$
$$+ f(\alpha)(\xi_\alpha(\alpha-) - \xi(\alpha+) - M(\alpha)).$$

6.3 Pseudodifferential operator calculus

In this section we use the pseudodifferential theory of [43, 46] to obtain a number of trace class and resolvent estimates which will be used to eliminate remainder terms in our use of Theorem 6.1.4 in Section 6.1. We are not able to directly use the results of [46] and [43], since they are formulated for first order pseudodifferential operators and our Hamiltonians are second order. We thus provide analogous results to keep track of the resulting numerology, although we omit the proofs since they are essentially identical.

The following definition captures the notion of a pseudodifferential operator associated to the operator $H_0(\alpha)$.

Definition 6.3.1. Define the space $\mathcal{H}_\infty = \cap_{k\geq 0}\mathrm{Dom}(H_0^k)$. For $T \in \mathcal{B}(\mathcal{H})$ with $T : \mathcal{H}_\infty \to \mathcal{H}_\infty$ we let $\delta(T) = [H_0(\alpha)^{\frac{1}{2}}, T]$. We define for $p \in \mathbb{R}$ the set of *regular order p pseudodifferential operators* associated with $H_0(\alpha)$ by

$$OP^p := (1 + H_0(\alpha)^2)^{\frac{p}{4}} \left(\bigcap_{n\in\mathbb{N}} \mathrm{Dom}(\delta^n) \right).$$

The topology of OP^p is associated with the family of norms

$$\sum_{k=0}^{\ell} \left|\left|\delta^k((1 + H_0(\alpha)^2)^{-\frac{p}{4}}T)\right|\right|$$

for $\ell \in \mathbb{N} \cup \{0\}$.

For the remainder of this chapter we let $r = \frac{1}{2}\min\{\alpha^2, (\mu+\alpha)^2\}$, so that the inequality $0 < r < \inf\{\sigma(H_t(\alpha)^2)\}$ holds.

We first give basic estimates for the operator norm of resolvents of certain operators.

Lemma 6.3.2. *Let $\alpha \in (0, -\mu)$ and $\lambda = a + iv$ with $a \in (0, r)$ Then for all $t \in [0, 1]$ we have*

$$\left|\left|(\lambda - (\mathrm{Id} + H_t(\alpha)^2))^{-1}\right|\right| \leq (v^2 + (r - a)^2)^{-\frac{1}{2}} \leq (r - a)^{-1}.$$

We will use the notation $Q = \mathrm{Id} + (H_0 + \alpha)^2$ and for $A \in OP^\ell$ we use the notation $A^{(k)} = [H_0(\alpha)^2, \cdots [H_0(\alpha)^2, A] \cdots]$, where the expression has k commutators. It is useful to note that the operator $A^{(k)}$ has order $\ell + 3k$ (each commutator raises the order by 3, one less than the order of $H_0(\alpha)^2$). For $\mathrm{Re}(s) > n$ we can use Cauchy's integral formula to write

$$Q^{-s} = \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s}(\lambda - Q)^{-1}\,\mathrm{d}\lambda$$

where γ_α is a vertical line with real part fixed in $(0, r)$. It can be checked using the spectral theorem that this integral converges in operator norm to Q^{-s}. We can thus reduce computing commutators of $T \in OP^p$ with Q^{-s} to iterated calculations of commutators of T with $(\lambda - Q)^{-1}$. This leads to the following, an analogue of [46, Lemma 6.9].

Lemma 6.3.3. *Let p, j, k be non-negative integers and $A \in OP^\ell$. Then*

$$(\lambda - Q)^{-p}A = \sum_{j=0}^{k} \binom{p+j-1}{j} A^{(j)}(\lambda - Q)^{-p+j} + P(\lambda)$$

where the remainder term $P(\lambda)$ has order $-(4p + k - \ell + 1)$ and is given explicitly by

$$P(\lambda) = \sum_{j=1}^{p} \binom{j+k+1}{k} (\lambda - Q)^{j-p-1} A^{(k+1)}(\lambda - Q)^{-j-k}.$$

Corollary 6.3.4. *Let p, M be positive integers and $A \in OP^k$. Let $R = (\lambda - Q)^{-1}$. Then*

$$R^p A R^{-p} = \sum_{j=0}^{M} \binom{p+j-1}{j} A^{(j)} R^j + P,$$

where P is of order $k - M - 1$ and given explicitly by

$$P = \sum_{j=1}^{p} \binom{j+M-1}{M} R^{p+1-j} A^{(M+1)} R^{M+j-p}.$$

The following is an analogue of [46, Lemma 6.10], allowing us to uniformly bound pseudodifferential operators when weighted by enough resolvents.

Lemma 6.3.5. *Let k, p be non-negative integers and suppose $\lambda \in \mathbb{C}$ with $a = \mathrm{Re}(\lambda) \in (0, r)$. Then for $A \in OP^k$ and with $R_\alpha(\lambda) = (\lambda - (\mathrm{Id} + (H_0 + \alpha)^2))^{-1}$ we have*

$$\left|\left| R_\alpha(\lambda)^{\frac{p}{4}+\frac{k}{4}} A R_\alpha(\lambda)^{-\frac{p}{4}} \right|\right| \leq C_{p,k}, \quad \text{and} \quad \left|\left| R_\alpha(\lambda)^{-\frac{p}{4}} A R_\alpha(\lambda)^{\frac{p}{4}+\frac{k}{4}} \right|\right| \leq C_{p,k}$$

where $C_{p,k}$ is a constant independent of λ.

Remark 6.3.6. We think of the operator X in the following lemmas as $t\{H_0, V\} + 2t\alpha V + t^2V^2$, and thus $H_0(\alpha)^2 + X = (H_t(\alpha))^2 \geq 0$. With $a = \mathrm{Re}(\lambda) \in (0, r)$ (and r fixed as before) we see that the spectrum of $(\mathrm{Id} + H_0(\alpha)^2 + X)$ is bounded away from the line $\mathrm{Re}(\lambda) = a$ by at least $1-a$ independent of λ and t. This fact is crucial in our next results.

Lemma 6.3.7. *Let $A_i \in OP^{p_i}$ for $i = 1, \ldots, \ell$ and let $0 < a = \mathrm{Re}(\lambda) < r$ as above. We consider the operator*

$$R_\alpha(\lambda)A_1R_\alpha(\lambda)A_2R_\alpha(\lambda)\cdots R_\alpha(\lambda)A_\ell\tilde{R}_\alpha(\lambda),$$

where $R_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1}$ and $\tilde{R}_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2 + X))^{-1}$, where X is self-adjoint and $H_0(\alpha)^2 + X \geq 0$. Then for all $M \geq 0$

$$R_\alpha(\lambda)A_1R_\alpha(\lambda)A_2\cdots A_\ell\tilde{R}_\alpha(\lambda) = \sum_{|k|=0}^{M} C_\ell(k)A_1^{(k_1)}\cdots A_\ell^{(k_\ell)}R_\alpha(\lambda)^{\ell+|k|}\tilde{R}_\alpha(\lambda) + P_{M,\ell}$$

where $P_{M,\ell}$ is of order at most $|p| - M - 4\ell - 5$, and k and p are multi-indices. The constant $C_\ell(k)$ is given by

$$C_\ell(k) = \frac{(|k|+\ell)!}{k_1!k_2!\cdots k_\ell!(k_1+1)(k_1+k_2+2)\cdots(|k|+\ell)}.$$

We now show that when weighted by sufficiently many resolvents, the remainder term $P_{M,\ell}$ can be uniformly bounded.

Lemma 6.3.8. *With the assumptions and notation of the previous lemma including the assumption that $A_i \in OP^{p_i}$ for each i, there is a positive constant C such that*

$$\left|\left|(\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{\ell+\frac{M}{4}+1-\frac{|p|}{4}}P_{M,\ell}\right|\right| \leq C$$

independent of λ and t (although depending on M and ℓ and the A_i). If the final $\tilde{R}_\alpha(\lambda)$ is replaced by $R_\alpha(\lambda)$ then the factor 1 in the exponent can be replaced by $\frac{5}{4}$.

We require two more estimates to guarantee that the operators which arise from the resolvent expansion and the Cauchy integral formula are trace class.

Lemma 6.3.9. *Let ℓ be a non-negative integer, and for $j = 0, \ldots, \ell$ let $A_j \in OP^{p_j}$. Fix $a \in (0, r)$ and define the vertical line $\gamma_\alpha = \{a + iv : v \in \mathbb{R}\}$. For $\lambda \in \gamma_\alpha$ let $R_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1}$ and $\tilde{R}_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2 + X))^{-1}$. Then for all $\varepsilon > 0$ and for $s \in \mathbb{C}$ with $\mathrm{Re}(s) > \frac{1}{2}$ the operator*

$$B_\alpha(t) = \frac{1}{2\pi i}\int_{\gamma_\alpha} \lambda^{-s}A_0R_\alpha(\lambda)A_1R_\alpha(\lambda)\cdots R_\alpha(\lambda)A_\ell\tilde{R}_\alpha(\lambda)\,\mathrm{d}\lambda$$

is trace class for $\mathrm{Re}(s) + \ell > \frac{p_0+|p|+n+\varepsilon}{4}$, and the function $t \mapsto ||B_\alpha(t)||_1$ is integrable on $[0, 1]$.

In the case where the final resolvent is actually an $R_\alpha(\lambda)$, we can use Cauchy's integral formula to explicitly evaluate the expression obtained after performing the expansion and get sharper trace class estimates.

Lemma 6.3.10. *Let ℓ be a non-negative integer, and for $j = 0, \dots, \ell$ let $A_j \in OP^{p_j}$, $p_j \geq 0$. Fix $a \in (0, r)$ and define the vertical line $\gamma_\alpha = \{a + iv : v \in \mathbb{R}\}$. For $\lambda \in \gamma_\alpha$ let $R_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1}$ and $\tilde{R}_\alpha(\lambda) = (\lambda - (\mathrm{Id} + H_0(\alpha)^2 + X))^{-1}$. Then the operator*

$$B_\alpha(t) = \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} A_0 R_\alpha(\lambda) A_1 R_\alpha(\lambda) A_2 \cdots R_\alpha(\lambda) A_\ell R_\alpha(\lambda) \, \mathrm{d}\lambda$$

is trace class for $\mathrm{Re}(s) + \ell > \frac{n+p_0+|p|}{4}$, and $t \mapsto ||B_\alpha(t)||_1$ is integrable on $[0, 1]$.

Our application of this result will have $p_0 = 0$ and each $p_i = 2$ (since $A_i = X$ for all i), giving $|p| = 2\ell$ and so, if we enforce $\mathrm{Re}(s) > \frac{1}{2}$, then a sufficient condition for ℓ is to take $\ell > \frac{n}{2} - 1$. If n is even we take $L = \frac{n}{2}$ and if n is odd we take $L = \frac{n-1}{2}$.

6.4 Spectral flow for Schrödinger operators

The resolvent expansions of the previous section and the Birman-Kreĭn trace formula of Lemma 6.2.8 will be the crucial elements in computing our spectral flow. Define for $\mathrm{Re}(s) > \frac{1}{2}$ the constants

$$C_s = \int_{\mathbb{R}} (1 + x^2)^{-s} \, \mathrm{d}x.$$

The C_s have a pole at $s = \frac{1}{2}$ with residue equal to one, a fact to be exploited later. Recall that for $\mathrm{Re}(s) > \frac{1}{2}$ we have defined the η function by

$$\eta_s(x) = \frac{1}{C_s} \int_1^\infty x(1 + wx^2)^{-s} w^{-\frac{1}{2}} \, \mathrm{d}w = \frac{2}{C_s} \int_x^\infty (1 + v^2)^{-s} \, \mathrm{d}v,$$

with the second formula only valid for $x > 0$. Note that η_s is odd and vanishes at 0 and $\pm\infty$. The result of Theorem 6.1.4 with $s > \frac{n+2}{2}$ now reads

$$\mathrm{sf}(D_t) = \frac{1}{C_s} \int_0^1 \mathrm{Tr}(\dot{D}_t (\mathrm{Id} + D_t^2)^{-s}) \, \mathrm{d}t + \frac{1}{2} \mathrm{Tr}(\eta_s(D_1) - \eta_s(D_0) + (P_{\mathrm{Ker}(D_1)} - P_{\mathrm{Ker}(D_0)})). \tag{6.3}$$

Multiplying both sides of Equation (6.3) by C_s we obtain

$$C_s\mathrm{sf}(D_t) = \int_0^1 \mathrm{Tr}(\dot{D}_t(\mathrm{Id}+D_t^2)^{-s})\,\mathrm{d}t + \frac{1}{2}C_s\mathrm{Tr}(\eta_s(D_1)-\eta_s(D_0)+(P_{\mathrm{Ker}(D_1)}-P_{\mathrm{Ker}(D_0)})). \tag{6.4}$$

The term C_s can be analytically continued for $\mathrm{Re}(s) > \frac{1}{2}$ to a meromorphic function with simple pole of residue 1 at $s = \frac{1}{2}$. Thus the left-hand side of Equation (6.4) is a meromorphic function and so the right hand side has a meromorphic continuation. We take the residue at $s = \frac{1}{2}$ of both sides to obtain

$$\begin{aligned}&\mathrm{sf}(D_t)\\ &= \operatorname*{Res}_{s=\frac{1}{2}}\bigg(\int_0^1 \mathrm{Tr}(\dot{D}_t(\mathrm{Id}+D_t^2)^{-s})\,\mathrm{d}t + \frac{1}{2}C_s\mathrm{Tr}(\eta_s(D_1)-\eta_s(D_0)+(P_{\mathrm{Ker}(D_1)}-P_{\mathrm{Ker}(D_0)})\bigg).\end{aligned} \tag{6.5}$$

We apply Equation (6.5) to the path $H_t(\alpha) = H_0 + \alpha + tV$, so that $\dot{H}_t(\alpha) = V$. The Birman-Kreĭn formula of Lemma 6.2.8 will be fundamental to our evaluation of this spectral flow formula. We denote the total number of bound states (eigenvalues counted with multiplicity) by

$$N(\alpha) = \sum_{k=1}^{K} M(\lambda_k(\alpha)).$$

Recall that by construction, $N(\alpha) = N$ (the number of bound states for H) independent of α. We refer to the term

$$\operatorname*{Res}_{s=\frac{1}{2}}\bigg(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\bigg)$$

as the 'integral of one form' contribution to the spectral flow, with this labelling justified by [47]. We refer to the term

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2}C_s\mathrm{Tr}(\eta_s(H(\alpha))-\eta_s(H_0(\alpha))+(P_{\mathrm{Ker}(H(\alpha))}-P_{\mathrm{Ker}(H_0(\alpha))})\right)$$

as the Birman-Kreĭn contribution to the spectral flow and the term

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2}C_s\mathrm{Tr}(\eta_s(D_1)-\eta_s(D_0))\right)$$

as the η contribution to the spectral flow.

6.4.1 The Birman-Kreĭn term

In this subsection we use the Birman-Kreĭn trace formula to determine the kernel and η contributions to the spectral flow in Equation (6.5).

Lemma 6.4.1. *By construction, the operators $P_{\mathrm{Ker}(H(\alpha))}$ and $P_{\mathrm{Ker}(H_0(\alpha))}$ are both zero.*

Since the kernel terms both vanish we are now able to evaluate the η contributions.

Lemma 6.4.2. *The η contribution to the Hamiltonian spectral flow is given by*

$$\begin{aligned}&\operatorname*{Res}_{s=\frac{1}{2}}\left(C_s \mathrm{Tr}(\eta_s(H_1(\alpha)) - \eta_s(H_0(\alpha)))\right)\\&= -(N(\alpha) - 2M_\alpha(\alpha)) + \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s \eta_s(\lambda)\mathrm{Tr}(S_\alpha^*(\lambda)S_\alpha'(\lambda))\,\mathrm{d}\lambda\right)\\&\quad + \left(\xi_\alpha(\alpha-) - \xi_\alpha(\alpha+) - M_\alpha(\alpha)\right),\end{aligned}$$

with $M_\alpha(\alpha)$ the multiplicity of the eigenvalue at energy α.

Proof. Suppose that $\lambda_K(\alpha) = \alpha$, that is H has zero as an eigenvalue. Apply the Birman-Kreĭn formula to obtain

$$\begin{aligned}\mathrm{Tr}(\eta_s(H(\alpha)) - \eta_s(H_0(\alpha))) &= \frac{1}{2\pi i}\int_\alpha^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha^*(\lambda)S_\alpha'(\lambda))\,\mathrm{d}\lambda + \sum_{k=1}^{K-1} M(\lambda_k(\alpha))\eta_s(\lambda_k(\alpha))\\&\quad + \eta_s(\alpha)\left(\xi_\alpha(\alpha-) - \xi_\alpha(\alpha+) - M(\alpha)\right).\end{aligned}$$

To simplify this expression, for $k < K$ we make the computation

$$\eta_s(\lambda_k(\alpha)) = -\eta_s(|\lambda_k(\alpha)|) = -\frac{2}{C_s}\int_{|\lambda_k(\alpha)|}^\infty (1+v^2)^{-s}\,\mathrm{d}v = -1 + \frac{2}{C_s}\int_0^{|\lambda_k(\alpha)|}(1+v^2)^{-s}\,\mathrm{d}v.$$

We further compute that

$$\eta_s(\alpha) = 1 - \frac{2}{C_s}\int_0^\alpha (1+v^2)^{-s}\,\mathrm{d}v.$$

Multiplying the trace by C_s and taking the residue we obtain

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(C_s \mathrm{Tr}(\eta_s(H_1) - \eta_s(H_0))\right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \Bigg(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha^*(\lambda) S_\alpha'(\lambda)) \, \mathrm{d}\lambda + \sum_{k=1}^{K-1} M(\lambda_k(\alpha)) C_s \eta_s(\lambda_k(\alpha)) + \\
&\quad + C_s \eta_s(\alpha) \left(\xi_\alpha(\alpha-) - \xi_\alpha(\alpha+)\right) \Bigg) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha^*(\lambda) S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) - \sum_{k=1}^{K-1} M(\lambda_k(\alpha)) \\
&\quad + M(\alpha) + \left(\xi_\alpha(\alpha-) - \xi_\alpha(\alpha+) - M(\alpha)\right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha^*(\lambda) S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) - (N(\alpha) - 2M(\alpha)) \\
&\quad + \left(\xi_\alpha(\alpha-) - \xi_\alpha(\alpha+) - M(\alpha)\right).
\end{aligned}$$

The case when $\lambda_K(\alpha) \neq \alpha$ follows by considering $M(\alpha) = 0$ in the above arguments. □

It is not surprising that the spectral flow is linked to the behaviour of the spectral shift function, such a relationship has been demonstrated in a number of contexts see, for example [12, 13, 14, 37, 38, 39, 40, 42].

We now show how the Birman-Kreĭn formula of Lemma 6.4.2 can be used in conjunction with the high energy behaviour of the function $\mathrm{Tr}(S(\cdot)^* S'(\cdot))$ to relate to Levinson's theorem.

The key observation for n odd is the following.

Lemma 6.4.3. *Fix $f \in C(\mathbb{R}^+)$ and suppose there exists a polynomial p such that $g(\lambda) = \lambda^{-\frac{1}{2}} p(\lambda)$ satisfies $|f - g| \in L^1(\mathbb{R}^+)$. Then*

$$\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) f(\lambda) \, \mathrm{d}\lambda \right) = \int_{\mathbb{R}^+} (f(\lambda) - g(\lambda)) \, \mathrm{d}\lambda.$$

Proof. We compute that

$$\begin{aligned}
\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) f(\lambda) \, \mathrm{d}\lambda \right) &= \operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) (f(\lambda) - g(\lambda) + g(\lambda)) \, \mathrm{d}\lambda \right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) (f(\lambda) - g(\lambda)) \, \mathrm{d}\lambda \right) \\
&\quad + \operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) g(\lambda) \, \mathrm{d}\lambda \right).
\end{aligned}$$

Note that $(s - \frac{1}{2}) C_s \eta_s(\lambda)$ is uniformly bounded and thus the fact that $|f - g| \in L^1(\mathbb{R}^+)$

allows us to use the dominated convergence theorem to obtain

$$\begin{aligned}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} C_s\eta_s(\lambda)(f(\lambda)-g(\lambda))\,\mathrm{d}\lambda\right) &= \int_{\mathbb{R}^+}\operatorname*{Res}_{s=\frac{1}{2}}(C_s\eta_s(\lambda))(f(\lambda)-g(\lambda))\,\mathrm{d}\lambda \\ &= \int_{\mathbb{R}^+}(f(\lambda)-g(\lambda))\,\mathrm{d}\lambda.\end{aligned}$$

It remains to show that

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} C_s\eta_s(\lambda)g(\lambda)\,\mathrm{d}\lambda\right) = 0.$$

For $r \neq -1$ we use integration by parts to calculate

$$\begin{aligned}\int_{\mathbb{R}^+}\lambda^r C_s\eta_s(\lambda)\,\mathrm{d}\lambda &= \int_{\mathbb{R}^+}\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{\lambda^{r+1}}{r+1}\right)C_s\eta_s(\lambda)\,\mathrm{d}\lambda \\ &= \left[\frac{\lambda^{r+1}}{r+1}C_s\eta_s(\lambda)\right]_0^\infty - \frac{1}{r+1}\int_{\mathbb{R}^+}\lambda^{r+1}C_s\eta_s'(\lambda)\,\mathrm{d}\lambda \\ &= \frac{2}{r+1}\int_{\mathbb{R}^+}\lambda^{r+1}(1+\lambda^2)^{-s}\,\mathrm{d}\lambda.\end{aligned}$$

The final integral can be reduced to a form of the Beta function with the substitution $\lambda = u^{\frac{1}{2}}$, which yields

$$\int_{\mathbb{R}^+}\lambda^{r+1}(1+\lambda^2)^{-s}\,\mathrm{d}\lambda = \frac{1}{2}\int_{\mathbb{R}^+}u^{\frac{r}{2}}(1+u)^{-s}\,\mathrm{d}u = \frac{\Gamma\left(\frac{r}{2}+1\right)\Gamma\left(s-\frac{r}{2}-1\right)}{\Gamma(s)}.$$

Thus,

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+}\lambda^r C_s\eta_s(\lambda)\,\mathrm{d}\lambda\right) = \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{\Gamma\left(\frac{r}{2}+1\right)\Gamma\left(s-\frac{r}{2}-1\right)}{(r+1)\Gamma(s)}\right) = 0,$$

provided $r \neq -2+k$ for any $k \in \mathbb{N}$. We are interested in the case $r = -\frac{1}{2}+k$ for $k \in \mathbb{N}$, since g is a linear combination of such powers. Hence,

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} C_s\eta_s(\lambda)g(\lambda)\,\mathrm{d}\lambda\right) = 0,$$

which completes the proof. □

We now compute the residue of the η contribution in odd dimensions.

Proposition 6.4.4. *Suppose that V satisfies Assumption 6.2.1 and n is odd. Then we* *have*

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right)$$
$$=\frac{1}{2\pi i}\int_0^\infty\left(\mathrm{Tr}(S(\lambda)^*S'(\lambda))-\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)\lambda^{\frac{n-2}{2}-j}\right)\mathrm{d}\lambda,$$

where the c_j *are as defined in Theorem 2.5.34. Note that this statement is independent of the choice of* $\alpha\in(0,-\mu)$*.*

Proof. By Theorem 2.5.34 the map

$$[\alpha,\infty)\ni\lambda\mapsto\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))-\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j}$$

is integrable. Thus we compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s\eta_s(\lambda)\left(\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))-\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j}\right)\mathrm{d}\lambda\right)\\
&\quad+\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s\eta_s(\lambda)-\left(\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j}\right)\mathrm{d}\lambda\right)\\
&=\frac{1}{2\pi i}\int_\alpha^\infty\left(\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))-\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j}\right)\mathrm{d}\lambda\\
&\quad+\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_0^\infty C_s\eta_s(u+\alpha)-\left(\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}c_j(n,V)u^{\frac{n-2}{2}-j}\right)\mathrm{d}u\right),
\end{aligned}$$

where we have used the observation $(s-\frac{1}{2})C_s\eta_s(\lambda)$ is uniformly bounded to apply the dominated convergence theorem. For $k\in\mathbb{N}$ the estimate

$$\begin{aligned}
\left|\int_0^\infty\int_{u+\alpha}^u u^{k-\frac{1}{2}}(1+v^2)^{-s}\,\mathrm{d}v\,\mathrm{d}u\right|&\le\int_0^\infty\int_u^{u+\alpha}u^{k-\frac{1}{2}}(1+v^2)^{-\mathrm{Re}(s)}\,\mathrm{d}v\,\mathrm{d}u\\
&\le\alpha\int_0^\infty u^{k-\frac{1}{2}}(1+u^2)^{-\mathrm{Re}(s)}\,\mathrm{d}u\\
&=\alpha\frac{\Gamma\left(\frac{k}{2}-\frac{1}{4}\right)\Gamma\left(\mathrm{Re}(s)-\frac{k}{2}+\frac{1}{4}\right)}{2\Gamma(\mathrm{Re}(s))}
\end{aligned}$$

shows that the map

$$s \mapsto \left(\frac{1}{2\pi i} \int_0^\infty C_s(\eta_s(u+\alpha) - \eta_s(u)) \left(\sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V) u^{\frac{n-2}{2}-j} \right) \mathrm{d}u \right)$$

is holomorphic at $s = \frac{1}{2}$. So we find

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) \\ &= \frac{1}{2\pi i} \int_\alpha^\infty \left(\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \\ &\quad + \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_0^\infty C_s \eta_s(u) \left(\sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V) u^{\frac{n-2}{2}-j} \right) \mathrm{d}u \right). \end{aligned}$$

Let $f(\lambda) = (\mathrm{Tr}(S(\lambda)^* S'(\lambda))$ and $g(\lambda) = p_n(\lambda)$ with p_n as in Definition 2.5.26. An application of Lemma 6.4.3 to the functions f, g then gives that the second residue in the above vanishes and thus

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) \\ &= \frac{1}{2\pi i} \int_\alpha^\infty \left(\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda. \end{aligned}$$

The statement of the proposition follows from the substitution $\lambda = u + \alpha$. □

For n even the residue of the η term is non-zero and can be computed using Theorem 2.5.34 as follows.

Proposition 6.4.5. *Suppose that n is even and V satisfies Assumption 6.2.1. Then*

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) \\ &= \frac{1}{2\pi i} \int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V) \lambda^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \\ &\quad + \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{0 \le \ell \le \frac{n-2}{2} - j \text{ odd}} \binom{\frac{n-2}{2} - j}{\ell} c_j(n,V)(-1)^{j-\ell} \alpha^{j-\ell} \frac{\Gamma\left(\frac{\ell}{2}+1\right)(-1)^{\frac{\ell+1}{2}}}{(\ell+1)\left(\frac{\ell+1}{2}\right)! \Gamma\left(\frac{1}{2}\right)} \\ &\quad - \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\ell=0}^{\frac{n-2}{2}-j} c_j(n,V) \binom{\frac{n-2}{2} - j}{\ell} (-1)^{\frac{n-2}{2}-j-\ell} \alpha^{\frac{n-2}{2}-j-\ell} \frac{\alpha^{\ell+1}}{2(\ell+1)}, \end{aligned}$$

where the $c_j(n, V)$ *are defined in Definition 2.5.26.*

Proof. By Theorem 2.5.34 the map

$$[\alpha, \infty) \ni \lambda \mapsto \mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n, V)(\lambda - \alpha)^{\frac{n-2}{2}-j}$$

is integrable. Thus we compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda))\, \mathrm{d}\lambda \right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \left(\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n, V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \right) \\
&\quad + \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \left(\sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n, V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \right) \\
&= \frac{1}{2\pi i} \int_\alpha^\infty \left(\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n, V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \\
&\quad + \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \left(\sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n, V)(\lambda - \alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \right),
\end{aligned}$$

where we have used the observation $(s - \frac{1}{2}) C_s \eta_s(\lambda)$ is uniformly bounded to apply the dominated convergence theorem. For $k \in \mathbb{N}$ we use the binomial theorem to obtain

$$\int_\alpha^\infty C_s \eta_s(\lambda)(\lambda - \alpha)^k\, \mathrm{d}\lambda = \sum_{\ell=0}^{k} (-1)^{k-\ell} \binom{k}{\ell} \alpha^{k-\ell} \int_\alpha^\infty C_s \eta_s(\lambda) \lambda^\ell\, \mathrm{d}\lambda. \tag{6.6}$$

We integrate by parts to obtain

$$\begin{aligned}
&\int_\alpha^\infty C_s \eta_s(\lambda) \lambda^\ell\, \mathrm{d}\lambda \\
&= \frac{1}{\ell+1} \int_\alpha^\infty \lambda^{\ell+1}(1+\lambda^2)^{-s}\, \mathrm{d}\lambda - \frac{1}{\ell+1} \alpha^{\ell+1} \int_\alpha^\infty (1+v^2)^{-s}\, \mathrm{d}v \\
&= \frac{1}{\ell+1} \int_0^\infty \lambda^{\ell+1}(1+\lambda^2)^{-s}\, \mathrm{d}\lambda - \frac{1}{\ell+1} \alpha^{\ell+1} \int_0^\infty (1+v^2)^{-s}\, \mathrm{d}v \\
&\quad - \frac{1}{\ell+1} \int_0^\alpha \lambda^{\ell+1}(1+\lambda^2)^{-s}\, \mathrm{d}\lambda + \frac{1}{\ell+1} \alpha^{\ell+1} \int_0^\alpha (1+v^2)^{-s}\, \mathrm{d}v \\
&= \frac{1}{2(\ell+1)} \frac{\Gamma\left(\frac{\ell}{2}+1\right) \Gamma\left(s - \frac{\ell}{2} - 1\right)}{\Gamma(s)} - \frac{C_s}{2(\ell+1)} \alpha^{\ell+1} \\
&\quad - \frac{1}{\ell+1} \int_0^\alpha \lambda^{\ell+1}(1+\lambda^2)^{-s}\, \mathrm{d}\lambda + \frac{1}{\ell+1} \alpha^{\ell+1} \int_0^\alpha (1+v^2)^{-s}\, \mathrm{d}v
\end{aligned}$$

Noting that the integrals from 0 to α are over a finite region and thus define a holomorphic function of s, we can take the residue at $s = \frac{1}{2}$ to obtain

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_\alpha^\infty C_s \eta_s(\alpha) \lambda^\ell \, \mathrm{d}\lambda \right) \\
&= -\frac{\alpha^{\ell+1}}{2(\ell+1)} + \begin{cases} 0, & \text{if } \ell \text{ is even,} \\ \frac{\Gamma\left(\frac{\ell}{2}+1\right)(-1)^{\frac{\ell+1}{2}}}{(\ell+1)\left(\frac{\ell+1}{2}\right)!\Gamma\left(\frac{1}{2}\right)}, & \text{if } \ell \text{ is odd.} \end{cases}
\end{aligned}$$

Returning to Equation (6.6) we have

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_\alpha^\infty C_s \eta_s(\lambda)(\lambda - \alpha)^k \, \mathrm{d}\lambda \right) \\
&= \sum_{0 \le \ell \le k \text{ odd}} \binom{k}{\ell} (-1)^{k-\ell} \alpha^{k-\ell} \frac{\Gamma\left(\frac{\ell}{2}+1\right)(-1)^{\frac{\ell+1}{2}}}{(\ell+1)\left(\frac{\ell+1}{2}\right)!\Gamma\left(\frac{1}{2}\right)} \\
&\quad - \sum_{\ell=0}^{k} \binom{k}{\ell} (-1)^{k-\ell} \alpha^{k-\ell} \frac{\alpha^{\ell+1}}{2(\ell+1)}
\end{aligned}$$

So we find

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \left(\sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \right) \\
&= \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{0 \le \ell \le \frac{n-2}{2}-j \text{ odd}} \binom{\frac{n-2}{2}-j}{\ell} c_j(n,V)(-1)^{j-\ell} \alpha^{j-\ell} \frac{\Gamma\left(\frac{\ell}{2}+1\right)(-1)^{\frac{\ell+1}{2}}}{(\ell+1)\left(\frac{\ell+1}{2}\right)!\Gamma\left(\frac{1}{2}\right)} \\
&\quad - \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\ell=0}^{\frac{n-2}{2}-j} c_j(n,V) \binom{\frac{n-2}{2}-j}{\ell} (-1)^{\frac{n-2}{2}-j-\ell} \alpha^{\frac{n-2}{2}-j-\ell} \frac{\alpha^{\ell+1}}{2(\ell+1)}.
\end{aligned}$$

Hence we have

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{1}{2\pi i} \int_\alpha^\infty C_s \eta_s(\lambda) \operatorname{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) \, \mathrm{d}\lambda \right) \\
&= \frac{1}{2\pi i} \int_\alpha^\infty \left(\operatorname{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)(\lambda-\alpha)^{\frac{n-2}{2}-j} \right) \mathrm{d}\lambda \\
&\quad + \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{0 \le \ell \le \frac{n-2}{2}-j \text{ odd}} \binom{\frac{n-2}{2}-j}{\ell} c_j(n,V)(-1)^{j-\ell} \alpha^{j-\ell} \frac{\Gamma\left(\frac{\ell}{2}+1\right)(-1)^{\frac{\ell+1}{2}}}{(\ell+1)\left(\frac{\ell+1}{2}\right)!\Gamma\left(\frac{1}{2}\right)} \\
&\quad - \frac{1}{2\pi i} \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} \sum_{\ell=0}^{\frac{n-2}{2}-j} c_j(n,V) \binom{\frac{n-2}{2}-j}{\ell} (-1)^{\frac{n-2}{2}-j-\ell} \alpha^{\frac{n-2}{2}-j-\ell} \frac{\alpha^{\ell+1}}{2(\ell+1)}.
\end{aligned}$$

The statement of the proposition follows from the substitution $\lambda = u + \alpha$. □

In practice it is easier to take the limit as $\alpha \to 0^+$ before taking the residue. To do so requires the following technical result.

Lemma 6.4.6. *Fix $f \in C(\mathbb{R}^+)$ and suppose there exists a polynomial $p(\lambda) = \sum_{j=0}^k a_j \lambda^j$ such that $|f - p| \in L^1(\mathbb{R}^+)$. Then*

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} C_s \eta_s(\lambda) f(\lambda)\,\mathrm{d}\lambda\right) = \int_{\mathbb{R}^+} (f(\lambda) - p(\lambda))\,\mathrm{d}\lambda + \sum_{m=1}^{\lfloor \frac{k}{2} \rfloor} \frac{\Gamma\left(m + \frac{1}{2}\right)(-1)^m}{2m(m!)\Gamma\left(\frac{1}{2}\right)} a_{2m-1}.$$

Proof. The same computations as Lemma 6.4.3 apply until the evaluation of the residue. Recall that for $r \neq -1$ we have

$$\int_{\mathbb{R}^+} \lambda^r C_s \eta_s(\lambda)\,\mathrm{d}\lambda = \frac{\Gamma\left(\frac{r}{2} + 1\right)\Gamma\left(s - \frac{r}{2} - 1\right)}{(r+1)\Gamma(s)}.$$

We use the fact that the Gamma function has a pole of order 1 at each non-positive integer $-k$ with residue $\frac{(-1)^k}{\Gamma(k+1)}$ to find for a positive integer j that

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} \lambda^j C_s \eta_s(\lambda)\,\mathrm{d}\lambda\right) = \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{\Gamma\left(\frac{j}{2} + 1\right)\Gamma\left(s - \frac{j}{2} - 1\right)}{(j+1)\Gamma(s)}\right).$$

If j is even, the residue vanishes. If $j = 2m - 1$ for some $m \in \mathbb{N}$ then we find

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^+} \lambda^j C_s \eta_s(\lambda)\,\mathrm{d}\lambda\right) = \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{\Gamma\left(m + \frac{1}{2}\right)\Gamma\left(s - m - \frac{1}{2}\right)}{2m\Gamma(s)}\right) = \frac{\Gamma\left(m + \frac{1}{2}\right)(-1)^m}{2m(m!)\Gamma\left(\frac{1}{2}\right)},$$

which completes the proof. □

Corollary 6.4.7. *Suppose that n is even and V satisfies Assumption 6.2.1. Then*

$$\begin{aligned}
&\lim_{\alpha \to 0^+} \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) \\
&= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)\lambda^{\frac{n-2}{2} - j}\right)\mathrm{d}\lambda \\
&\quad + \frac{1}{2\pi i}\sum_{1 \le j \le \lfloor \frac{n-1}{2} \rfloor \text{ odd}} \binom{\frac{n-2}{2} - j}{j} c_j(n,V) \frac{\Gamma\left(\frac{j}{2} + 1\right)(-1)^{\frac{j+1}{2}}}{(j+1)\left(\frac{j+1}{2}\right)!\,\Gamma\left(\frac{1}{2}\right)} \\
&= \operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_0^\infty C_s \eta_s(\lambda) \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda\right),
\end{aligned}$$

where the $c_j(n,V)$ are defined in Theorem 2.5.34.

Proof. By Theorem 2.5.34 we have that there exists $c_j(n,V) \in \mathbb{C}$ with

$$\left(\mathbb{R}^+ \ni \lambda \mapsto \mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)\lambda^{\frac{n-2}{2}-j}\right) \in L^1(\mathbb{R}^+).$$

An application of Lemma 6.4.6 then gives

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_0^\infty C_s \eta_s(\lambda)\mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda\right)\\
&= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - \sum_{j=1}^{\lfloor \frac{n-1}{2} \rfloor} c_j(n,V)\lambda^{\frac{n-2}{2}-j}\right) \mathrm{d}\lambda\\
&\quad + \frac{1}{2\pi i}\sum_{1 \le j \le \lfloor \frac{n-1}{2} \rfloor \text{ odd}} \binom{\frac{n-2}{2}-j}{j} c_j(n,V) \frac{\Gamma\left(\frac{j}{2}+1\right)(-1)^{\frac{j+1}{2}}}{(j+1)\left(\frac{j+1}{2}\right)!\Gamma\left(\frac{1}{2}\right)}.
\end{aligned}$$

Taking the limit as $\alpha \to 0^+$ in Proposition 6.4.5 completes the proof. □

Since there are far less terms to consider, in practice it is more convenient to use Corollary 6.4.7 than Proposition 6.4.5. We demonstrate the use of Proposition 6.4.5 in dimension $n = 4$, the lowest dimension in which non-trivial α dependence is found.

Corollary 6.4.8. *Suppose that $n = 4$ and V satisfies Assumption 6.2.1. Let $c_1(4,V)$ be as in Theorem 2.5.34. Then*

$$\begin{aligned}
\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_\alpha^\infty C_s \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) &= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - c_1(4,V)\right)\mathrm{d}\lambda\\
&\quad - \frac{c_1(4,V)}{2(2\pi i)}\alpha.
\end{aligned}$$

These computations will be used to relate spectral flow to Levinson's theorem in Section 6.5.

6.4.2 The "integral of one form" term

Finally we determine the contribution of the "integral of one form" term to the spectral flow formula with the aid of some technical results. As before we fix $r = \frac{1}{2}\min\{\alpha^2, (\mu+\alpha)^2\}$.

Lemma 6.4.9. *For $\alpha \in (0, -\mu)$, $\mathrm{Re}(s) > \frac{1}{2}$ and $a \in (0, r)$ define the vertical line $\gamma_\alpha = \{a + iv : v \in \mathbb{R}\}$. Define the perturbation $X = X(t,\alpha) = t\{H_0, V\} + 2t\alpha V + t^2V^2$. Then* *for each $L \in \mathbb{N}$, we have*

$$\begin{aligned}(\mathrm{Id} + H_t(\alpha)^2)^{-s} &= \sum_{\ell=0}^{L} \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} (X(\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1})^{\ell} (\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1} \,\mathrm{d}\lambda \\ &+ \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} (X(\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1})^{L+1} (\lambda - (\mathrm{Id} + H_t(\alpha)^2))^{-1} \,\mathrm{d}\lambda.\end{aligned} \tag{6.7}$$

Proof. An application of Cauchy's integral formula gives

$$(\mathrm{Id} + H_t(\alpha)^2)^{-s} = \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} (\lambda - (\mathrm{Id} + H_t(\alpha)^2))^{-1} \,\mathrm{d}\lambda.$$

For self-adjoint X, Y the resolvent identity

$$(\lambda - (X+Y))^{-1} = \sum_{\ell=0}^{L} (X(\lambda - Y)^{-1})^{\ell} (\lambda - Y)^{-1} + (X(\lambda - Y)^{-1})^{L} (\lambda - (X+Y))^{-1}$$

completes the proof. □

Lemma 6.4.10. *If n is even, let $L = \frac{n}{2}$ and if n is odd, let $L = \frac{n-1}{2}$. Let $X = X(t,\alpha)$ by given by $X = t\{H_0, V\} + 2t\alpha V + t^2 V^2$ and $\mathrm{Re}(s) > \frac{1}{2}$. For a multi-index k and $0 \le \ell \le L$, define the constant $Y_\ell(k,s)$ by*

$$Y_\ell(k,s) = (-1)^{\ell + |k|} C_\ell(k) \frac{\Gamma(\ell + |k| + s)}{\Gamma(s)(\ell + |k|)!}.$$

For $4\mathrm{Re}(s) + L > n$ we have

$$\mathrm{Tr}(V(\mathrm{Id} + (H_t(\alpha))^2)^{-s}) = \sum_{\ell=0}^{L} \sum_{|k|=0}^{M_\ell} Y_\ell(k,s) \mathrm{Tr}\left(V X^{(k_1)} \cdots X^{(k_\ell)} (\mathrm{Id} + H_0(\alpha)^2)^{-s-\ell-|k|}\right) + P, \tag{6.8}$$

where $M_\ell = \frac{n}{2} + 2 + \ell$ and P is holomorphic at $s = \frac{1}{2}$.

Proof. Apply Lemma 6.4.9 to obtain

$$\begin{aligned}(\mathrm{Id} + H_t(\alpha)^2)^{-s} &= \sum_{\ell=0}^{L} \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} (X(\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1})^{\ell} (\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1} \,\mathrm{d}\lambda \\ &+ \frac{1}{2\pi i} \int_{\gamma_\alpha} \lambda^{-s} (X(\lambda - (\mathrm{Id} + H_0(\alpha)^2))^{-1})^{L+1} (\lambda - (\mathrm{Id} + H_t(\alpha)^2))^{-1} \,\mathrm{d}\lambda.\end{aligned}$$

An application of Lemma 6.3.10 shows that the term

$$\frac{1}{2\pi i}\int_{\gamma_\alpha}\lambda^{-s}(X(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1})^{L+1}(\lambda-(\mathrm{Id}+H_t(\alpha)^2))^{-1}\,\mathrm{d}\lambda$$

is trace class for $L+1>\frac{n}{2}$. An argument similar to the proof of [46, Lemma 7.4] shows that this term is holomorphic in s also. An application of Lemma 6.3.9 shows that the term

$$\frac{1}{2\pi i}\int_{\gamma_\alpha}\lambda^{-s}(X(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1})^{\ell}(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1}\,\mathrm{d}\lambda$$

is trace class for $\mathrm{Re}(s)>\frac{n}{4}-\ell+\frac{|p|+p_0}{4}$. We have $0\leq|p|+p_0\leq 2\ell$ and so we require $\mathrm{Re}(s)>\frac{n}{4}-\frac{\ell}{2}$. Thus for $\ell\geq\frac{n}{2}-1$ we find that each term in the sum will have a non-zero residue and all terms with $L>\frac{n}{2}$ will have vanishing residue. We now apply Lemma 6.3.7 to obtain for any $M\geq 0$ the expansion

$$\begin{aligned}&\frac{1}{2\pi i}\int_{\gamma_\alpha}\lambda^{-s}(X(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1})^{\ell}(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1}\,\mathrm{d}\lambda\\&=\sum_{|k|=0}^{M}\frac{1}{2\pi i}\int_{\gamma_\alpha}\lambda^{-s}C_\ell(k)X^{(k_1)}\cdots X^{(k_\ell)}(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-\ell-|k|-1}\,\mathrm{d}\lambda\\&\quad+\frac{1}{2\pi i}\int_{\gamma_\alpha}P_{M,\ell}(\lambda)(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1}\,\mathrm{d}\lambda.\end{aligned}$$

An application of Cauchy's integral formula shows that the first term can be evaluated explicitly to obtain

$$\begin{aligned}&\frac{1}{2\pi i}\int_{\gamma_\alpha}\lambda^{-s}(X(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1})^{\ell}(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1}\,\mathrm{d}\lambda\\&=\sum_{|k|=0}^{M}Y_\ell(k,s)X^{(k_1)}\cdots X^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2))^{-\ell-|k|-s}\\&\quad+\frac{1}{2\pi i}\int_{\gamma_\alpha}P_{M,\ell}(\lambda)(\lambda-(\mathrm{Id}+H_0(\alpha)^2))^{-1}\,\mathrm{d}\lambda.\end{aligned}$$

The above expressions are trace class and for $M\geq\frac{n}{2}+1+\ell$ the remainder is holomorphic at $s=\frac{1}{2}$. □

6.4.3 The spectral flow formulae

In this subsection we combine the results of Sections 6.4.1 and 6.4.2 to determine an expression for the spectral flow along the path $H_t(\alpha)$. Such a formula is dependent on the parity of the dimension and the expressions we obtain are rather complicated, with many terms obtained by combinatorial arguments which are difficult to evaluate explicitly. To do so requires the following integral computations.

Lemma 6.4.11. *For $a, b > 0$ with $b > \frac{a}{4}$ we have*

$$\int_0^\infty r^{a-1}(1+r^4)^{-b}\,\mathrm{d}r = \frac{\Gamma\left(\frac{a}{4}\right)\Gamma\left(b-\frac{a}{4}\right)}{4\Gamma(b)}. \tag{6.9}$$

For $b > \frac{n+2}{4}$ and $1 \le m \le n$ we have

$$\int_{\mathbb{R}^n} \xi_m^2(1+|\xi|^4)^{-b}\,\mathrm{d}\xi = \frac{\mathrm{Vol}(\mathbb{S}^{n-1})}{n}\frac{\Gamma\left(\frac{n+2}{4}\right)\Gamma\left(b-\frac{n+2}{4}\right)}{4\Gamma(b)}, \tag{6.10}$$

independent of the direction ξ_m.

Proof. Making the substitution $u = r^4$ we find

$$\int_0^\infty r^{a-1}(1+r^4)^{-b}\,\mathrm{d}r = \frac{1}{4}\int_0^\infty u^{\frac{a}{4}-1}(1+u)^{-b}\,\mathrm{d}u = \frac{\Gamma\left(\frac{a}{4}\right)\Gamma\left(b-\frac{a}{4}\right)}{4\Gamma(b)},$$

where the integral was evaluated as a known form of the Beta function. For the second integral, we note that by symmetry we have

$$\int_{\mathbb{R}^n} \xi_m^2(1+|\xi|^4)^{-\beta}\,\mathrm{d}\xi = \frac{1}{n}\int_{\mathbb{R}^n} |\xi|^2(1+|\xi|^4)^{-b}\,\mathrm{d}\xi.$$

Changing to polar coordinates and using Equation (6.9) gives Equation (6.10). □

Lemma 6.4.12. *For $m = 2k$ a positive even integer and $q \in \mathbb{N}_0$ we have*

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^\infty r^{m-1}(1+(r^2+\alpha)^2)^{-s}\,\mathrm{d}r\right)\\
&= \operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{k-1}\binom{k-1}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\frac{\Gamma\left(\frac{\ell+1}{2}\right)\Gamma\left(s+q-\frac{\ell+1}{2}\right)}{4\Gamma(s+q)}\right).
\end{aligned}$$

Proof. Let $m = 2k$ and compute that

$$\begin{aligned}
\int_0^\infty r^{2k-1}(1+(r^2+\alpha)^2)^{-s-q}\,\mathrm{d}r &= \frac{1}{2}\int_0^\infty u^{k-1}(1+(u+\alpha)^2)^{-s-q}\,\mathrm{d}u\\
&= \frac{1}{2}\int_\alpha^\infty (v-\alpha)^{k-1}(1+v^2)^{-s-q}\,\mathrm{d}v.
\end{aligned}$$

Applying the binomial expansion we have

$$\begin{aligned}
\int_0^\infty r^{2k-1}(1+(r^2+\alpha)^2)^{-s}\,\mathrm{d}r &= \frac{1}{2}\int_\alpha^\infty (v-\alpha)^{k-1}(1+v^2)^{-s-q}\,\mathrm{d}v\\
&= \frac{1}{2}\sum_{\ell=0}^{k-1}\binom{k}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\int_\alpha^\infty v^\ell(1+v^2)^{-s-q}\,\mathrm{d}v.
\end{aligned}$$

Note that

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^\alpha v^j(1+v^2)^{-s-q}\,\mathrm{d}v\right)=0.$$

Thus we obtain

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^\infty r^{2k-1}(1+(r^2+\alpha)^2)^{-s}\,\mathrm{d}r\right)\\
&=\frac{1}{2}\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{k-1}\binom{k-1}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\int_\alpha^\infty v^\ell(1+v^2)^{-s-q}\,\mathrm{d}v\right)\\
&=\frac{1}{2}\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{k-1}\binom{k-1}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\int_0^\infty v^\ell(1+v^2)^{-s-q}\,\mathrm{d}v\right)\\
&=\frac{1}{4}\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{k-1}\binom{k-1}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\int_0^\infty w^{\frac{\ell+1}{2}-1}(1+w)^{-s-q}\,\mathrm{d}v\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{k-1}\binom{k-1}{\ell}(-1)^{k-\ell-1}\alpha^{k-\ell-1}\frac{\Gamma\left(\frac{\ell+1}{2}\right)\Gamma\left(s+q-\frac{\ell+1}{2}\right)}{4\Gamma(s+q)}\right),
\end{aligned}$$

which is the statement of the lemma. ☐

To avoid confusion, we introduce the notation (ΔV) for the action of the Laplacian H_0 on the potential V.

Lemma 6.4.13. *For n even we define*

$$X_0=2t\alpha V+t^2V^2+t(\Delta V),\quad X_1=-2t\sum_{j=1}^n\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j}\quad\text{and}\quad X_2=2tVH_0.$$

For $0\le\ell\le\frac{n}{2}$ define the set

$$J_\ell(n)=\left\{(k,p)\in\mathbb{N}_0^\ell\times\{0,1,2\}^\ell:|p|+n\ge 2+4\ell+|k|\right\}.$$

Then we have

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1\operatorname{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(n)}Y_\ell(k,s)\int_0^1\operatorname{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\mathrm{d}t\right).
\end{aligned}\tag{6.11}$$

Proof. By Lemma 6.4.10 we can write the expression (modulo holomorphic terms)

$$\mathrm{Tr}(V(\mathrm{Id}+(H(\alpha))^2)^{-s}) = \sum_{\ell=0}^{L}\sum_{|k|=0}^{M} Y_\ell(k,s)\mathrm{Tr}\left(VX^{(k_1)}\cdots X^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right).$$

We have written

$$X = \left(2t\alpha V + t^2V^2 + t(\Delta V)\right) - 2t\sum_{j=1}^{n}\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j} + 2tVH_0 = X_0 + X_1 + X_2$$

as the sum of an order zero, an order one and an order two component. The terms in the summand which are not trace class satisfy $|p| + 3|k| - 4\mathrm{Re}(s) - 4\ell - 4|k| \geq -n$ and with our decomposition of X we have $p_i \in \{0,1,2\}$. Thus for fixed n, ℓ the terms which are not trace class are precisely those with $(k,p) \in J_\ell(n)$. Summing over these terms and taking the residue at $s = \frac{1}{2}$ gives the result. □

Lemma 6.4.14. *For n odd we have*

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right) = 0.$$

Proof. For n odd, the same argument as n even in Lemma 6.4.13 shows that Equation (6.11) holds with X_1, X_2, X_3 defined as in Lemma 6.4.13. We show that all residues vanish for one of two reasons. Write $X_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)} = \sum_{j=0}^{|p|+3|k|} G_j$, where G_j is an operator of order j. By performing commutators, we can assume without loss of generality that G_j is of the form

$$G_j = g\sum_{|\beta|=j} g_\beta \partial^\beta$$

for some multi-index β of length n and $g_\beta \in C_c^\infty(\mathbb{R}^n)$. Then we find

$$\begin{aligned}&\mathrm{Tr}\left(VG_j(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\\ &= (2\pi)^{-n}\sum_{|\beta|=j}\left(\int_{\mathbb{R}^n} V(x)g_\beta(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n}\xi^\beta(1+(|\xi|^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}\xi\right).\end{aligned}$$

If any of the elements of the multi-index β are odd, the trace vanishes for the same reason. Thus we may assume that j is even and each component β_i of α is even. Write $\beta_i = 2b_i$ for a multi-index b of length n. Then we can write

$$G_j = \sum_{2|b|=j} g_{2b}\partial_1^{2b_1}\cdots\partial_n^{2b_n}.$$

We find that

$$\begin{aligned}
&\operatorname{Tr}\left(VG_j(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\\
&= i^{|\beta|}(2\pi)^{-n}\sum_{2|b|=j}\left(\int_{\mathbb{R}^n}V(x)g_{2b}(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n}\xi_1^{2b_1}\cdots\xi_n^{2b_n}(1+(|\xi|^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}\xi\right)\\
&= i^{|\beta|}(2\pi)^{-n}\sum_{2|b|=j}\left(\int_{\mathbb{R}^n}V(x)g_{2b}(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{S}^{n-1}}\omega_1^{2b_1}\cdots\omega_n^{2b_n}\,\mathrm{d}\omega\right)\times\\
&\quad\left(\int_0^\infty r^j(1+(r^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}r\right)\\
&= i^{|\beta|}\frac{2\Gamma\left(\frac{1}{2}+b_1\right)\cdots\Gamma\left(\frac{1}{2}+b_n\right)}{\Gamma\left(\frac{n}{2}+|b|\right)(2\pi)^n}\sum_{2|b|=j}\left(\int_{\mathbb{R}^n}V(x)g_{2b}(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{S}^{n-1}}\omega_1^{2b_1}\cdots\omega_n^{2b_n}\,\mathrm{d}\omega\right)\times\\
&\quad\left(\int_0^\infty r^{n+j-1}(1+(r^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}r\right),
\end{aligned}$$

where we have used Lemma 2.5.20 to evaluate the integral over $\mathbb{S}^{n-1}$. We make the estimate

$$\begin{aligned}
\left|\int_0^\infty |r^{n+j-1}(1+(r^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}r\right| &\le \int_0^\infty r^{n+j-1}(1+r^4)^{-\mathrm{Re}(s)-\ell-|k|}\,\mathrm{d}r\\
&= \frac{\Gamma\left(\frac{n+j}{4}\right)\Gamma\left(\mathrm{Re}(s)+\ell+|k|-\frac{n+j}{4}\right)}{4\Gamma\left(\mathrm{Re}(s)+\ell+|k|\right)}.
\end{aligned}$$

Since n is odd and j is even, we find that $\frac{1}{2}+\ell+|k|-\frac{n+j}{4}$ is never an integer and so

$$s\mapsto\int_0^\infty r^{n+j-1}(1+(r^2+\alpha)^2)^{-s-\ell-|k|}\,\mathrm{d}r$$

is holomorphic at $s=\frac{1}{2}$. Thus $\operatorname{Tr}\left(VG_j(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)$ is holomorphic at $s=\frac{1}{2}$ and we have shown that for n odd all residues at $s=\frac{1}{2}$ vanish, independent of $\alpha>0$. □

In higher even dimensions the terms appearing in Lemma 6.4.13 become cumbersome to compute rather quickly, however in dimension $n=2,4,6$ they can be computed directly, with the aid of Lemmas 6.4.11 and 6.4.12.

Lemma 6.4.15. *Let $n=2$ and suppose V satisfies Assumption 6.2.1. Then*

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1\operatorname{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right)=\frac{1}{8\pi}\int_{\mathbb{R}^2}V(x)\,\mathrm{d}x,$$

independent of $\alpha>0$.

Proof. Since $n=2$ we find that $J_0(2)=\{(0,0)\}$ and $J_1(2)=\emptyset$. Noting that for $\ell=0$ we have $Y_0(0, \frac{1}{2}) = 1$ we thus have

$$\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id} + H_t(\alpha)^2)^{-s})\, \mathrm{d}t \right) = \operatorname*{Res}_{s=\frac{1}{2}} \left(\mathrm{Tr}(V(\mathrm{Id} + H_0(\alpha)^2)^{-s}) \right).$$

So we compute that

$$\begin{aligned} \mathrm{Tr}(V(\mathrm{Id} + H_0(\alpha)^2)^{-s}) &= (2\pi)^{-2} \left(\int_{\mathbb{R}^2} V(x)\, \mathrm{d}x \right) \left(\int_{\mathbb{R}^2} (1 + (|y|^2 + \alpha)^2)^{-s}\, \mathrm{d}y \right) \\ &= (2\pi)^{-2} \mathrm{Vol}(\mathbb{S}^1) \left(\int_{\mathbb{R}^2} V(x)\, \mathrm{d}x \right) \left(\int_0^\infty r(1 + (r^2 + \alpha)^2)^{-s}\, \mathrm{d}r \right), \end{aligned}$$

where we have used polar coordinates and Lemma 6.4.11 to evaluate the y integral. Taking the residue at $s = \frac{1}{2}$ using Lemma 6.4.12 we find

$$\begin{aligned} \operatorname*{Res}_{s=\frac{1}{2}} \left(\mathrm{Tr}(V(\mathrm{Id} + H_0(\alpha)^2)^{-s}) \right) &= (2\pi)^{-2} \operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^2} V(x)\, \mathrm{d}x \right) \left(\mathrm{Vol}(\mathbb{S}^1) \frac{\Gamma\left(\frac{1}{2}\right) \Gamma\left(s - \frac{1}{2}\right)}{4\Gamma(s)} \right) \\ &= \frac{\mathrm{Vol}(\mathbb{S}^1)}{4(2\pi)^2} \left(\int_{\mathbb{R}^2} V(x)\, \mathrm{d}x \right), \end{aligned}$$

independent of α. □

Remark 6.4.16. In the notation of Theorems 2.5.34 and 5.3.29, the statement of Lemma 6.4.15 is

$$\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id} + H_t(\alpha)^2)^{-s})\, \mathrm{d}t \right) = \frac{1}{2} b_2,$$

independent of $\alpha > 0$.

Lemma 6.4.17. *Let $n = 4$ and suppose V satisfies Assumption 6.2.1. Then*

$$\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id} + H_t(\alpha)^2)^{-s})\, \mathrm{d}t \right) = -\alpha \frac{\mathrm{Vol}(\mathbb{S}^3)}{8(2\pi)^4} \int_{\mathbb{R}^4} V(x)\, \mathrm{d}x - \frac{\mathrm{Vol}(\mathbb{S}^3)}{8(2\pi)^6} \int_{\mathbb{R}^4} V(x)^2\, \mathrm{d}x.$$

Proof. Since $n = 4$ we have $J_1(4) = \{(0, 2)\}$, $J_0(4) = \{(0, 0)\}$ and $J_\ell(4) = \emptyset$ for $\ell \geq 2$. Thus only two terms corresponding to $\ell = 1, k = 0, p = 2$ and $\ell = 0, k = 0 = p$ will contribute. We first consider $\ell = 0, k = 0, p = 0$. We find

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}} \left(Y_0(0, s) \int_0^1 \mathrm{Tr}(V(\mathrm{Id} + H_0(\alpha)^2)^{-s})\, \mathrm{d}t \right) \\ &= (2\pi)^{-4} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_0(0, s) \left(\int_{\mathbb{R}^4} V(x)\, \mathrm{d}x \right) \left(\int_{\mathbb{R}^4} (1 + (|\xi|^2 + \alpha)^2)^{-s}\, \mathrm{d}\xi \right) \right) \\ &= \frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_0(0, s) \left(\int_{\mathbb{R}^4} V(x)\, \mathrm{d}x \right) \left(\int_0^\infty r^{4-1}(1 + (r^2 + \alpha)^2)^{-s}\, \mathrm{d}r \right) \right). \end{aligned}$$

Applying Lemma 6.4.12 we have

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_0(\alpha)^2)^{-s})\,\mathrm{d}t\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\left(\int_{\mathbb{R}^4}V(x)\,\mathrm{d}x\right)\left(\int_0^\infty r^{4-1}(1+(r^2+\alpha)^2)^{-s}\,\mathrm{d}r\right)\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\left(\int_{\mathbb{R}^4}V(x)\,\mathrm{d}x\right)\left(-\alpha\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(s-\frac{1}{2}\right)}{4\Gamma(s)}+\frac{\Gamma\left(1\right)\Gamma\left(s-1\right)}{4\Gamma(s)}\right)\right)\\
&=-\alpha\frac{\mathrm{Vol}(\mathbb{S}^3)}{8(2\pi)^4}\int_{\mathbb{R}^4}V(x)\,\mathrm{d}x.
\end{aligned}$$

We next consider the case $\ell=1,k=0,p=2$. We observe that $Y_1(0,\frac{1}{2})=-\frac{1}{2}$ and find

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 2t\mathrm{Tr}(V^2H_0(\mathrm{Id}+H_0(\alpha)^2)^{-s-1})\,\mathrm{d}t\right)\\
&=(2\pi)^{-4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^4}V(x)^2\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^4}|\xi|^2(1+(|\xi|^2+\alpha)^2)^{-s-1}\,\mathrm{d}\xi\right)\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^4}V(x)^2\,\mathrm{d}x\right)\left(\int_0^\infty r^{6-1}(1+(r^2+\alpha)^2)^{-s-1}\,\mathrm{d}r\right)\right).
\end{aligned}$$

Applying Lemma 6.4.12 we have

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 2t\mathrm{Tr}(V^2H_0(\mathrm{Id}+H_0(\alpha)^2)^{-s-1})\,\mathrm{d}t\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^4}V(x)^2\,\mathrm{d}x\right)\left(\int_0^\infty r^{6-1}(1+(r^2+\alpha)^2)^{-s-1}\,\mathrm{d}r\right)\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^3)}{(2\pi)^4}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^4}V(x)^2\,\mathrm{d}x\right)\left(\alpha^2\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(s+\frac{1}{2}\right)}{4\Gamma(s+1)}-2\alpha\frac{\Gamma\left(1\right)\Gamma\left(s\right)}{4\Gamma(s+1)}\right.\right.\\
&\qquad\left.\left.+\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(s-\frac{1}{2}\right)}{4\Gamma(s+1)}\right)\right)\\
&=-\frac{\mathrm{Vol}(\mathbb{S}^3)}{8(2\pi)^4}\int_{\mathbb{R}^4}V(x)^2\,\mathrm{d}x.
\end{aligned}$$

Adding the two contributions gives the statement. □

Remark 6.4.18. In the notation of Theorem 2.5.34 and Definition 2.5.26, the statement of Lemma 6.4.17 is

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right)=\frac{1}{2}\beta_4(V)+\frac{\alpha}{4(2\pi i)}c_1(4,V).$$

In fact the $n=2,4$ calculations suggest the following observation.

Proposition 6.4.19. *Suppose that n is even and V satisfies Assumption 6.2.1. Then*

$$\lim_{\alpha\to 0^+}\operatorname{Res}_{s=\frac{1}{2}}\left(\int_0^1 \operatorname{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right)$$
$$=\operatorname{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(n)} Y_\ell(k,s)\int_0^1 \operatorname{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

That is, the limit as $\alpha\to 0^+$ commutes with the residue at $s=\frac{1}{2}$.

Proof. By the same arguments as the proof of Lemma 6.4.14 is suffices to prove for any $q\in\mathbb{N}$, $g\in C_c^\infty(\mathbb{R}^n)$ and multi-index $\beta=(2b_1,\ldots,2b_n)$ that

$$\lim_{\alpha\to 0}\operatorname{Res}_{s=\frac{1}{2}}\left(\operatorname{Tr}\left(Vg\frac{\partial^\beta}{\partial x^\beta}(\mathrm{Id}+H_0(\alpha)^2)^{-s-q}\right)\right)=\operatorname{Res}_{s=\frac{1}{2}}\left(\operatorname{Tr}\left(Vg\frac{\partial^\beta}{\partial x^\beta}(\mathrm{Id}+H_0^2)^{-s-q}\right)\right). \tag{6.12}$$

So we compute that

$$\operatorname{Res}_{s=\frac{1}{2}}\left(\operatorname{Tr}\left(Vg\frac{\partial^\beta}{\partial x^\beta}(\mathrm{Id}+H_0(\alpha)^2)^{-s-q}\right)\right)$$
$$=i^{|\beta|}(2\pi)^{-n}\operatorname{Res}_{s=\frac{1}{2}}\left(\left(\int_{\mathbb{R}^n}V(x)g(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^n}\xi_1^{\beta_1}\cdots\xi_n^{\beta_n}(1+(|\xi|^2+\alpha)^2)^{-s-q}\,\mathrm{d}\xi\right)\right)$$
$$=i^{|\beta|}\frac{2\Gamma\left(\frac{1+\beta_1}{2}\right)\cdots\Gamma\left(\frac{1+\beta_n}{2}\right)}{\Gamma\left(\frac{n+|\beta|}{2}\right)(2\pi)^n}\operatorname{Res}_{s=\frac{1}{2}}\left(\left(\int_{\mathbb{R}^n}V(x)g(x)\,\mathrm{d}x\right)\times\right.$$
$$\left.\left(\int_0^\infty r^{n+|\beta|-1}(1+(r^2+\alpha)^2)^{-s-q}\,\mathrm{d}r\right)\right),$$

where we have changed to polar coordinates and used Lemma 2.5.20 to evaluate the integral over $\mathbb{S}^{n-1}$. Applying Lemma 6.4.12 we have

$$\operatorname{Res}_{s=\frac{1}{2}}\left(\int_{\mathbb{R}^n}r^{n+|\beta|-1}(1+(r^2+\alpha)^2)^{-s-q}\,\mathrm{d}r\right)$$
$$=\operatorname{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n+|\beta|}{2}-1}(-1)^{\frac{n+|\beta|}{2}-\ell-1}\alpha^{\frac{n+|\beta|}{2}-\ell-1}\frac{\Gamma\left(\frac{\ell+1}{2}\right)\Gamma\left(s+q-\frac{\ell+1}{2}\right)}{4\Gamma(s+q)}\right)$$
$$=\sum_{\ell=0}^{\frac{n+|\beta|}{2}-1}(-1)^{\frac{n+|\beta|}{2}-\ell-1}\alpha^{\frac{n+|\beta|}{2}-\ell-1}\operatorname{Res}_{s=\frac{1}{2}}\left(\frac{\Gamma\left(\frac{\ell+1}{2}\right)\Gamma\left(s+q-\frac{\ell+1}{2}\right)}{4\Gamma(s+q)}\right).$$

Taking the limit as $\alpha \to 0^+$ we have

$$\lim_{\alpha\to 0^+} \operatorname*{Res}_{s=\frac{1}{2}} \left(\int_{\mathbb{R}^n} r^{n+|\beta|-1}(1+(r^2+\alpha)^2)^{-s-q}\,\mathrm{d}r \right) = \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{\Gamma\left(\frac{n+|\beta|}{4}\right)\Gamma\left(s+q-\frac{n+|\beta|}{4}\right)}{4\Gamma(s+q)} \right),$$

from which we see that

$$\begin{aligned}
&\lim_{\alpha\to 0^+} \operatorname*{Res}_{s=\frac{1}{2}} \left(\operatorname{Tr}\left(Vg\frac{\partial^\beta}{\partial x^\beta}(\mathrm{Id}+H_0(\alpha)^2)^{-s-q} \right) \right) \\
&= i^{|\beta|}\frac{2\Gamma\left(\frac{1+\beta_1}{2}\right)\cdots\Gamma\left(\frac{1+\beta_n}{2}\right)}{\Gamma\left(\frac{n+|\beta|}{2}\right)(2\pi)^n} \left(\int_{\mathbb{R}^n} V(x)g(x)\,\mathrm{d}x \right) \operatorname*{Res}_{s=\frac{1}{2}} \left(\frac{\Gamma\left(\frac{n+|\beta|}{2}\right)\Gamma\left(s+q-\frac{n+|\beta|}{2}\right)}{4\Gamma(s+q)} \right).
\end{aligned}$$

For the right hand side of Equation (6.12) we can compute directly using Lemma 6.4.11 that

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\operatorname{Tr}\left(Vg\frac{\partial^\beta}{\partial x^\beta}(\mathrm{Id}+H_0^2)^{-s-q} \right) \right) \\
&= i^{|\beta|}(2\pi)^{-n}\operatorname*{Res}_{s=\frac{1}{2}} \left(\left(\int_{\mathbb{R}^n} V(x)g(x)\,\mathrm{d}x \right) \left(\int_{\mathbb{R}^n} \xi_1^{\beta_1}\cdots\xi_n^{\beta_n}(1+|\xi|^4)^{-s-q}\,\mathrm{d}\xi \right) \right) \\
&= i^{|\beta|}\frac{2\Gamma\left(\frac{1+\beta_1}{2}\right)\cdots\Gamma\left(\frac{1+\beta_n}{2}\right)}{\Gamma\left(\frac{n+|\beta|}{2}\right)(2\pi)^n}\operatorname*{Res}_{s=\frac{1}{2}} \left(\left(\int_{\mathbb{R}^n} V(x)g(x)\,\mathrm{d}x \right) \left(\int_0^\infty r^{n+|\beta|-1}(1+r^4)^{-s-q}\,\mathrm{d}r \right) \right) \\
&= i^{|\beta|}\frac{2\Gamma\left(\frac{1+\beta_1}{2}\right)\cdots\Gamma\left(\frac{1+\beta_n}{2}\right)}{\Gamma\left(\frac{n+|\beta|}{2}\right)(2\pi)^n}\operatorname*{Res}_{s=\frac{1}{2}} \left(\left(\int_{\mathbb{R}^n} V(x)g(x)\,\mathrm{d}x \right) \left(\frac{\Gamma\left(\frac{n+|\beta|}{4}\right)\Gamma\left(s+q-\frac{n+|\beta|}{4}\right)}{4\Gamma(s+q)} \right) \right),
\end{aligned}$$

which proves the claim. □

In practice, it is much easier to compute the residue in Equation (6.11) after taking the limit as $\alpha \to 0^+$. The number of terms required increases significantly as the dimension increases, with 8 terms required for $n = 6$ (after taking the limit as $\alpha \to 0$ and using Proposition 6.4.19). Only some of these terms are non-zero, the result is the following.

Lemma 6.4.20. *Let $n = 6$ and suppose V satisfies Assumption 6.2.1. Then*

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(\int_0^1 \operatorname{Tr}(V(\mathrm{Id}+H_t(0)^2)^{-s})\,\mathrm{d}t \right) \\
&= \frac{\mathrm{Vol}(\mathbb{S}^5)}{12(2\pi)^6}\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x + \frac{\mathrm{Vol}(\mathbb{S}^5)}{24(2\pi)^6}\int_{\mathbb{R}^6} |[\nabla V](x)|^2\,\mathrm{d}x - \frac{\mathrm{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6} V(x)\,\mathrm{d}x.
\end{aligned}$$

The proof of Lemma 6.4.20 is similar to, but much more involved than, Lemma 6.4.17 and as such is provided in Appendix A.1.

Remark 6.4.21. In the notation of Theorem 2.5.34 and Definition 2.5.26, the statement of Lemma 6.4.20 is

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(0)^2)^{-s})\,\mathrm{d}t\right) = \frac{1}{2}\beta_6(V) + \frac{c_1(6,V)}{4}.$$

We now return to more general statements. As a result of Lemma 6.4.13 we obtain the following formula for the spectral flow along the path $H_t(\alpha)$.

Theorem 6.4.22. *Let n be odd and V satisfy Assumption 6.2.1. The spectral flow from $H_0(\alpha)$ to $H(\alpha)$ is given by*

$$\begin{aligned}\mathrm{sf}(H(\alpha),H_0(\alpha)) &= \frac{1}{4\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - \frac{1}{2}(N-2N_0)\\ &\quad - \frac{1}{2}(\xi(0+)-\xi(0-)-N_0). \end{aligned} \tag{6.13}$$

The number of bound states N of H can be computed via the formula

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+)-\xi(0-)-N_0). \tag{6.14}$$

Proof. A combination of Lemmas 6.4.2, 6.4.1 and 6.4.13 applied to Equation (6.3) gives

$$\begin{aligned}\mathrm{sf}(H_t(\alpha)) &= \frac{1}{4\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - \frac{1}{2}(N-2N_0)\\ &\quad - \frac{1}{2}(\xi(0+)-\xi(0-)-N_0),\end{aligned}$$

where we have made the identifications $\xi_\alpha(\lambda+\alpha)=\xi(\lambda)$, $N(\alpha)=N$ and $M_\alpha(\alpha)=N_0$, the multiplicity of the zero eigenvalue for H. For the final statement note that the spectral flow is given by N_0-N, independent of α, and solve for N to obtain the result. □

Theorem 6.4.23. *Let n be even and V satisfy Assumption 6.2.1. The spectral flow from $H_0(\alpha)$ to $H(\alpha)$ is given by*

$$\begin{aligned}&\mathrm{sf}(H(\alpha),H_0(\alpha)) \\ &= \frac{1}{4\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - \frac{1}{2}(N-2N_0) - \frac{1}{2}(\xi(0+)-\xi(0-)-N_0)\\ &\quad + \operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\mathrm{d}t\right).\end{aligned} \tag{6.15}$$

The number of bound states N of H can be computed via the formula

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+) - \xi(0-) - N_0) \tag{6.16}$$
$$+ 2\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

Proof. A combination of Lemmas 6.4.2, 6.4.1 and 6.4.13 applied to Equation (6.3) gives

$$\mathrm{sf}(H_t(\alpha)) = \frac{1}{4\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - \frac{1}{2}(N-2N_0) - \frac{1}{2}(\xi(0+) - \xi(0-))$$
$$+ \operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

We know that $\mathrm{sf}(H_t(\alpha)) = N_0 - N$, independent of α. Equating the left hand side to $N_0 - N$ and solving for N gives the second statement. □

We remark that there are far more terms than necessary, although carefully indexing the terms with non-zero residue is a tedious task which we do not complete here.

6.5 Levinson's theorem

In this section we show how Theorems 6.4.22 and 6.4.23 imply that Levinson's theorem is a result of the spectral flow along the path $H_t(\alpha)$.

Lemma 6.5.1 (Levinson's Theorem in dimension $n = 1$)**.** *Let $n = 1$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > \frac{5}{2}$. Then*

$$-N = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + \frac{1}{2}(1 - M_R(0)),$$

where $M_R(0) = 1$ if there exists a resonance and $M_R(0) = 0$ otherwise.

Proof. By Theorem 6.4.22 we have

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+) - \xi(0-) - N_0).$$

By Proposition 6.4.5 we have

$$\frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda.$$

Corollary 5.3.18 then gives $\xi(0+) - \xi(0-) - N_0 = -\frac{1}{2}(1 - M_R(0))$, which completes the proof. □

Lemma 6.5.2 (Levinson's Theorem in dimension $n = 2$)**.** *Let $n = 2$ and suppose that V satisfies Assumption 2.2.14 for some $\rho > 11$. Then the number of bound states for $H = H_0 + V$ is given by*

$$-N = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda + M_p(0) + \frac{1}{4\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x,$$

where $M_p(0) = -(\xi(0+) - \xi(0-) - N_0)$, ξ is the spectral shift function for the pair (H, H_0) and N_0 is the number of zero eigenvalues for H.

Proof. By Theorem 6.4.23 we have

$$\begin{aligned}-N = &\frac{1}{2\pi i}\mathop{\mathrm{Res}}_{s=\frac{1}{2}}\left(\int_\alpha^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+) - \xi(0-) - N_0)\\ &+ 2\mathop{\mathrm{Res}}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{1}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).\end{aligned}$$

Lemma 6.4.15 shows that

$$\mathop{\mathrm{Res}}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right) = \frac{1}{8\pi}\int_{\mathbb{R}^2} V(x)\,\mathrm{d}x.$$

By Proposition 6.4.5 we have

$$\frac{1}{2\pi i}\mathop{\mathrm{Res}}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) = \frac{1}{2\pi i}\int_0^\infty \mathrm{Tr}(S(\lambda)^* S'(\lambda))\,\mathrm{d}\lambda.$$

Corollary 5.3.31 gives $\xi(0+) - \xi(0-) - N_0 = 0$, which completes the proof. □

We note that in the case of no p-resonances, we have $M_p(0) = (\xi(0+) - \xi(0-) - N_0) = 0$ by Corollary 5.3.31. Lemma 6.5.2 demonstrates that the value $\xi(0+)$ of the spectral shift function at zero is an integer determined by the number of p resonances.

Lemma 6.5.3 (Levinson's Theorem in higher odd dimensions)**.** *Let $n \geq 3$ be odd and suppose that V satisfies Assumption 6.2.1 and define for $1 \leq j \leq \lfloor\frac{n-1}{2}\rfloor$ constants $c_j(n, V)$ as in Theorem 2.5.34. Let $p_n(\lambda) = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} c_j(n, V)\lambda^{\frac{n-2}{2}-j}$ be the high-energy polynomial of Definition 2.5.26. Then*

$$-N = \frac{1}{2\pi i}\int_{\mathbb{R}^+} (\mathrm{Tr}(S(\lambda)^* S'(\lambda)) - p_n(\lambda))\,\mathrm{d}\lambda + \frac{1}{2}M_R(0),$$

where $M_R(0) = 1$ if there is a resonance in dimension $n = 3$ and $M_R(0) = 0$ otherwise.

Proof. By Theorem 6.4.22 we have

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+)-\xi(0-)-N_0).$$

By Proposition 6.4.5 we have

$$\frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) = \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - p_n(\lambda)\right)\mathrm{d}\lambda.$$

Noting that $-(\xi(0+)-\xi(0-)-N_0) = \frac{1}{2}M_R(0)$ by Corollaries 5.3.26 (for $n=3$) and 5.3.36 (for $n \geq 5$) completes the proof. □

The polynomial p_n is determined by Theorem 2.5.34. In dimension $n=3$ we have

$$p_3(\lambda) = -\frac{i\lambda^{-\frac{1}{2}}}{4\pi}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x.$$

In dimension $n=5$ we have

$$p_5(\lambda) = -\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^4)\lambda^{\frac{1}{2}}}{(2\pi)^5}\int_{\mathbb{R}^5} V(x)\,\mathrm{d}x + \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^4)\lambda^{-\frac{1}{2}}}{2(2\pi)^5}\int_{\mathbb{R}^5} V(x)^2\,\mathrm{d}x.$$

In dimension $n=7$ we have

$$\begin{aligned}p_7(\lambda) = &-\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^6)\lambda^{\frac{3}{2}}}{(2\pi)^7}\int_{\mathbb{R}^7} V(x)\,\mathrm{d}x + \frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^6)\lambda^{\frac{1}{2}}}{2(2\pi)^7}\int_{\mathbb{R}^7} V(x)^2\,\mathrm{d}x\\ &- \frac{15(2\pi i)\mathrm{Vol}(\mathbb{S}^6)\lambda^{-\frac{1}{2}}}{48(2\pi)^7}\int_{\mathbb{R}^7}\left(V(x)^3 + \frac{1}{2}|[\nabla V](x)|^2\right)\mathrm{d}x.\end{aligned}$$

We do not compute p_n for higher n, since the computations become tedious quickly.

Lemma 6.5.4 (Levinson's Theorem in dimension $n=4$)**.** *Let $n=4$ and suppose that V satisfies Assumption 6.2.1 and define*

$$c_1(4,V) = -\frac{(2\pi i)\mathrm{Vol}(\mathbb{S}^3)}{2(2\pi)^4}\int_{\mathbb{R}^4} V(x)\,\mathrm{d}x.$$

as in Theorem 2.5.34. Then

$$-N = \frac{1}{2\pi i}\int_{\mathbb{R}^+}\left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - c_1(4,V)\right)\mathrm{d}\lambda + M_R(0) + \frac{\mathrm{Vol}(\mathbb{S}^3)}{4(2\pi)^4}\int_{\mathbb{R}^4} V(x)^2\,\mathrm{d}x,$$

where $M_R(0) = -(\xi(0+)-\xi(0-)-N_0)$.

Proof. By Theorem 6.4.23 we have

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+) - \xi(0-) - N_0)$$
$$+ 2\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{2}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

Corollary 6.4.8 shows that

$$\operatorname*{Res}_{s=\frac{1}{2}}\frac{1}{2\pi i}\left(\int_\alpha^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) = \frac{1}{2\pi i}\int_0^\infty (\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - c_1(4,V))\,\mathrm{d}\lambda$$
$$- \frac{c_1(4,V)}{2(2\pi i)}\alpha.$$

Lemma 6.4.17 gives

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(\alpha)^2)^{-s})\,\mathrm{d}t\right) = -\frac{\mathrm{Vol}(\mathbb{S}^3)}{8(2\pi)^4}\int_{\mathbb{R}^4} V(x)^2\,\mathrm{d}x + \frac{c_1(4,V)}{4(2\pi i)}\alpha,$$

which completes the proof. □

We note that by Corollary 5.3.36, if there are no resonances then $M_R(0) = 0$. Thus the value $\xi(0+)$ of the spectral shift function at zero is an integer determined by the number of resonances.

Lemma 6.5.5 (Levinson's theorem in dimension $n = 6$)**.** *Suppose that $n = 6$ and V satisfies Assumption 6.2.1. Then the number of bound states of $H = H_0 + V$ is given by*

$$-N = \frac{1}{2\pi i}\int_0^\infty (\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - c_1(6,V)\lambda - c_2(6,V))\,\mathrm{d}\lambda - \beta_6(V),$$

where the constants $c_1(n,V), c_2(n,V), \beta_6(V)$ are defined by Theorem 2.5.34.

Proof. By Theorem 6.4.23 we have

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_\alpha^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^* S_\alpha'(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+) - \xi(0-) - N_0)$$
$$+ 2\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{3}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0(\alpha)^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

Since the left hand side is independent of α, we use Corollary 6.4.7 and Proposition 6.4.19

to take the limit as $\alpha \to 0^+$ and find

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^\infty \eta_s(\lambda)\mathrm{Tr}(S_\alpha(\lambda)^*S'_\alpha(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+)-\xi(0-)-N_0)$$
$$+ 2\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{3}\sum_{(k,p)\in J_\ell(n)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right).$$

Proposition 6.4.5 then shows

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\frac{1}{2\pi i}\int_0^\infty C_s\eta_s(\lambda)\mathrm{Tr}(S(\lambda)^*S'(\lambda))\,\mathrm{d}\lambda\right)$$
$$= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - c_1(6,V)\lambda - c_2(6,V)\right)\,\mathrm{d}\lambda + \frac{c_1(6,V)}{4(2\pi i)}.$$

We have the explicit expression $\frac{c_1(6,V)}{4(2\pi i)} = -\frac{\mathrm{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6}V(x)\,\mathrm{d}x$. Recall the constant $\beta_6(V)$ from Theorem 2.5.34. From Lemma 6.4.20 we find

$$\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{3}\sum_{(k,p)\in J_\ell(6)}Y_\ell(k)\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right)$$
$$= -\frac{\mathrm{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^4}V(x)\,\mathrm{d}x - \frac{\mathrm{Vol}(\mathbb{S}^5)}{12(2\pi)^6}\int_{\mathbb{R}^6}\left(V(x)^3+\frac{1}{2}|[\nabla V](x)|^2\right)\,\mathrm{d}x$$
$$= \frac{c_1(6,V)}{8(2\pi i)} + \frac{1}{2}\beta_6(V).$$

Note that by Corollary 5.3.36 we have $(\xi(0+)-\xi(0-)-N_0) = 0$. An application of Theorem 6.4.23 then gives

$$-N = \frac{1}{2\pi i}\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^\infty \eta_s(\lambda)\mathrm{Tr}(S(\lambda)^*S'(\lambda))\,\mathrm{d}\lambda\right) - (\xi(0+)-\xi(0-))$$
$$+ 2\operatorname*{Res}_{s=\frac{1}{2}}\left(\sum_{\ell=0}^{\frac{n}{2}}\sum_{(k,p)\in J_\ell(6)}\int_0^1 \mathrm{Tr}\left(VX_{p_1}^{(k_1)}\cdots X_{p_\ell}^{(k_\ell)}(\mathrm{Id}+H_0^2)^{-s-\ell-|k|}\right)\,\mathrm{d}t\right)$$
$$= \frac{1}{2\pi i}\int_0^\infty \left(\mathrm{Tr}(S(\lambda)^*S'(\lambda)) - c_3(6,V)\lambda - c_2(6,V)\right)\,\mathrm{d}\lambda + \frac{c_1(6,V)}{4(2\pi i)}$$
$$- 2\left(\frac{c_1(6,V)}{8(2\pi i)} + \frac{1}{2}\beta_6(V)\right),$$

which completes the proof. □

Unfortunately due to the large number of terms involved, a general argument showing that in higher even dimensions the "integral of one form" contributions and the η contributions combine to give the correct statement of Levinson's theorem is not given.

Appendix A

Computations of coefficients

In this appendix we provide some detailed computations of the coefficients appearing in Levinson's theorem. In particular in Section A.1 we provide the proof of Lemma 6.4.20 for the terms appearing in the integral of a one form contribution to the spectral flow in dimension $n = 6$.

A.1 Proof of Lemma 6.4.20

In this section we provide a proof of Lemma 6.4.20 for the contributions to the integral of a one form term to spectral flow in dimension $n = 6$.

Lemma A.1.1. *Let $n = 6$ and suppose V satisfies Assumption 6.2.1. Then*

$$\begin{aligned}&\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(V(\mathrm{Id}+H_t(0)^2)^{-s})\,\mathrm{d}t\right)\\&=\frac{\mathrm{Vol}(\mathbb{S}^5)}{12(2\pi)^6}\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x+\frac{\mathrm{Vol}(\mathbb{S}^5)}{24(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x-\frac{\mathrm{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6} V(x)\,\mathrm{d}x.\end{aligned}$$

Proof. We have $J_0(6) = \{(0,0)\}$, $J_1(6) = \{(0,0),(0,1),(1,1),(0,2),(1,2),(2,2)\}$ and $J_2(6) = \{((0,0),(2,2))\}$. For $\ell \geq 3$ we have $J_\ell(6) = \emptyset$. So there are eight terms to consider.

We write $X = X_0 + X_1 + X_2$, where

$$X_0 = t^2V^2 + t(\Delta V), \quad X_1 = -2t\sum_{j=1}^{6}\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j} \quad \text{and} \quad X_2 = 2tVH_0.$$

We begin with the case $\ell = 0, k = 0, p = 0$. Observe that $\int_0^1 \mathrm{d}t = 1$, $Y_0(0,\frac{1}{2}) = 1$,

$\operatorname*{Res}_{s=\frac{1}{2}}\left(\Gamma\left(s-\frac{3}{2}\right)\right)=-1$ and $\Gamma\left(\frac{3}{2}\right)=\frac{1}{2}\Gamma\left(\frac{1}{2}\right)$. So we find So we compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\int_0^1 \operatorname{Tr}(V(\mathrm{Id}+H_0^2)^{-s})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)(2\pi)^{-6}\left(\int_{\mathbb{R}^6}V(x)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}(1+|\xi|^4)^{-s}\,\mathrm{d}\xi\right)\right)\\
&=\frac{\operatorname{Vol}(\mathbb{S}^5)}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\left(\int_{\mathbb{R}^6}V(x)\,\mathrm{d}x\right)\left(\int_0^\infty r^{6-1}(1+r^4)^{-s}\,\mathrm{d}r\right)\right)\\
&=\frac{\operatorname{Vol}(\mathbb{S}^5)}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_0(0,s)\left(\int_{\mathbb{R}^6}V(x)\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{6}{4}\right)\Gamma\left(s-\frac{6}{4}\right)}{4\Gamma(s)}\right)\right)\\
&=-\frac{\operatorname{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6}V(x)\,\mathrm{d}x.
\end{aligned}$$

The next case is $\ell=1,k=0,p=0$. Observe that $\int_0^1 t^2\,\mathrm{d}t=\frac{1}{3}$, $\int_0^1 t\,\mathrm{d}t=\frac{1}{2}$, $Y_1(0,\frac{1}{2})=-\frac{1}{2}$ and $\operatorname*{Res}_{s=\frac{1}{2}}\left(\Gamma\left(s-\frac{1}{2}\right)\right)=1$. For clarity, we introduce the notation (ΔV) for the action of H_0 on V. We compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 \operatorname{Tr}(VX_0(\mathrm{Id}+H_0^2)^{-s-1})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1\left(t^2\operatorname{Tr}(V^3(\mathrm{Id}+H_0^2)^{-s-1})+t\operatorname{Tr}(V(\Delta V)(\mathrm{Id}+H_0^2)^{-s-1})\right)\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\frac{1}{3}\operatorname{Tr}(V^3(\mathrm{Id}+H_0^2)^{-s-1})+\frac{1}{2}\operatorname{Tr}(V(\Delta V)(\mathrm{Id}+H_0^2)^{-s-1})\right)\right)\\
&=(2\pi)^{-6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^6}\left(\frac{1}{3}V(x)^3+\frac{1}{2}V(x)[\Delta V](x)\right)\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}(1+|\xi|^4)^{-s-1}\,\mathrm{d}\xi\right)\right)\\
&=\frac{\operatorname{Vol}(\mathbb{S}^5)}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^6}\left(\frac{1}{3}V(x)^3+\frac{1}{2}V(x)[\Delta V](x)\right)\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{6}{4}\right)\Gamma\left(s+1-\frac{6}{4}\right)}{4\Gamma(s+1)}\right)\right)\\
&=-\frac{\operatorname{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6}\left(\frac{1}{3}V(x)^3+\frac{1}{2}|[\nabla V](x)|^2\right)\,\mathrm{d}x.
\end{aligned}$$

We move on to the case $\ell=1,k=0,p=1$. Observe that $\int_0^1(-2t)\,\mathrm{d}t=-1$. Then we find

$$
\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 \operatorname{Tr}(VX_1(\mathrm{Id}+H_0^2)^{-s-1})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 (-2t)\sum_{k=1}^{6}\operatorname{Tr}\left(V\frac{\partial V}{\partial x_k}\frac{\partial}{\partial x_k}(\mathrm{Id}+H_0^2)^{-s-1}\right)\,\mathrm{d}t\right)\\
&=i(2\pi)^{-6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6} V(x)\frac{\partial V}{\partial x_k}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_k(1+|\xi|^4)^{-s}\,\mathrm{d}\xi\right)\right)\\
&=0,
\end{aligned}
$$

since the ξ integral contains the integral of an odd function over a symmetric region.

The next term is $\ell=1, k=1, p=1$. Observe that $Y_1(1,\frac{1}{2})=\frac{3}{8}$, $\int_0^1(8t)\,\mathrm{d}t=4$ and $\operatorname*{Res}_{s=\frac{1}{2}}\left(\Gamma\left(s-\frac{1}{2}\right)\right)=1$. We write $X_1^{(1)}=[H_0^2,X_1]=H_0[H_0,X_1]+[H_0,X_1]H_0$. Note that $X_1^{(1)}$ is an order 4 operator and we can write $X_1^{(1)}=\sum_{j=0}^4 G_j$, with each G_j an order j operator. The operator $VG_j(\mathrm{Id}+H_0^2)^{-s-2}$ has order $j-4s-8$ and so gives a contribution which is holomorphic at $s=\frac{1}{2}$ when $j<4$. Thus only the operator G_4 can contribute a non-zero residue. We compute the commutator

$$
\begin{aligned}
&[H_0,X_1]\\
&=-2t\left(-\sum_{k=1}^{6}\frac{\partial^2}{\partial x_k^2}\left(\sum_{j=1}^{6}\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j}\right)-\sum_{j=1}^{6}\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j}H_0\right)\\
&=-2t\left(-\sum_{j,k=1}^{6}\left(\frac{\partial^3 V}{\partial x_k^2\partial x_j}\frac{\partial}{\partial x_j}+2\frac{\partial^2 V}{\partial x_k\partial x_j}\frac{\partial^2}{\partial x_k\partial x_j}+\frac{\partial V}{\partial x_j}\frac{\partial^3}{\partial x_k^2\partial x_j}\right)-\sum_{j=1}^{6}\frac{\partial V}{\partial x_j}\frac{\partial}{\partial x_j}H_0\right)\\
&=2t\sum_{j,k=1}^{6}\left(\frac{\partial^3 V}{\partial x_k^2\partial x_j}\frac{\partial}{\partial x_j}+2\frac{\partial^2 V}{\partial x_k\partial x_j}\frac{\partial^2}{\partial x_k\partial x_j}\right).
\end{aligned}
$$

From this we immediately obtain the highest order component G_4 of $X_1^{(1)}$ as

$$
G_4=8t\sum_{j,k=1}^{6}\frac{\partial^2 V}{\partial x_k\partial x_j}\frac{\partial^2}{\partial x_k\partial x_j}H_0.
$$

So we compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 \operatorname{Tr}(VX_1^{(1)}(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 \operatorname{Tr}(VG_4(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=4\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{j,k=1}^{6}\operatorname{Tr}\left(\frac{\partial^2 V}{\partial x_k\partial x_j}\frac{\partial^2}{\partial x_k\partial x_j}H_0(\mathrm{Id}+H_0^2)^{-s-2}\right)\right)\\
&=i^2\frac{4}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{j,k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k\partial x_j}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_k\xi_j|\xi|^2(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right).
\end{aligned}$$

The terms in the sum with $j\neq k$ vanish, since the ξ integral contains the integral of an odd function over a symmetric interval. So we obtain

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 \operatorname{Tr}(VX_1^{(1)}(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=i^2\frac{4}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_k^2|\xi|^2(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right)\\
&=-\frac{4}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}|\xi|^4(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right)\\
&=-\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_0^\infty r^{10-1}(1+r^4)^{-s-2}\,\mathrm{d}r\right)\right)\\
&=-\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{10}{4}\right)\Gamma\left(s+2-\frac{10}{4}\right)}{4\Gamma(s+2)}\right)\right)\\
&=-\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\left(\frac{3}{8}\right)\left(\frac{1}{4}\right)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6}\int_{\mathbb{R}^6}V(x)[\Delta V](x)\,\mathrm{d}x\\
&=\frac{\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x.
\end{aligned}$$

Next we consider the term $\ell=1,k=0,p=2$. Observe that $Y_1(0,\frac{1}{2})=-\frac{1}{2}$ and

$\int_0^1 (2t)\,\mathrm{d}t = 1$. Then we find

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 \mathrm{Tr}(VX_2(\mathrm{Id}+H_0^2)^{-s-1})\,\mathrm{d}t\right)\\
&= \operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\int_0^1 2t\mathrm{Tr}(V^2H_0(\mathrm{Id}+H_0^2)^{-s-1})\,\mathrm{d}t\right)\\
&= (2\pi)^{-6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^6} V(x)^2\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}|\xi|^2(1+|\xi|^4)^{-s-1}\,\mathrm{d}\xi\right)\right)\\
&= \frac{\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^6} V(x)^2\,\mathrm{d}x\right)\left(\int_0^\infty r^{8-1}(1+r^4)^{-s-1}\,\mathrm{d}r\right)\right)\\
&= \frac{\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(0,s)\left(\int_{\mathbb{R}^6} V(x)^2\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{8}{4}\right)\Gamma\left(s+1-\frac{8}{4}\right)}{4\Gamma(s+1)}\right)\right)\\
&= 0,
\end{aligned}$$

since the final expression is holomorphic at $s=\frac{1}{2}$.

We next move to the $\ell = 1, k = 1, p = 2$ term. Observe that $Y_1(1,\frac{1}{2}) = \frac{3}{8}$, $\int_0^1(-8t)\,\mathrm{d}t = -4$, $\int_0^1(4t)\,\mathrm{d}t = 2$, $\int_0^1(8t)\,\mathrm{d}t = 4$ and $\operatorname*{Res}_{s=\frac{1}{2}}\left(\Gamma\left(s-\frac{1}{2}\right)\right) = 1$. Note that the operator $X_2^{(1)}$ is an order 5 operator and thus we can write $X_2^{(1)} = \sum_{j=0}^5 G_j$, where the operator G_j has order j. We determine that the operator $VG_j(\mathrm{Id}+H_0^2)^{-s-2}$ has order $j-4s-8$ and sogives a contribution which is holomorphic at $s=\frac{1}{2}$ if $j<4$. So only the operators G_4 and G_5 can give a non-zero residue. We compute that

$$[H_0^2, X_2] = 2t[H_0^2, VH_0] = 2t[H_0^2, V]H_0 = 2tH_0[H_0,V]H_0 + 2t[H_0,V]H_0^2.$$

We have also the relation

$$[H_0, V] = (\Delta V) - 2\sum_{k=1}^6 \frac{\partial V}{\partial x_k}\frac{\partial}{\partial x_k}.$$

The highest order term of $X_2^{(1)}$ can be read off directly as

$$G_5 = -8t\sum_{k=1}^6 \frac{\partial V}{\partial x_k}\frac{\partial}{\partial x_k}H_0^2.$$

A more involved calculation shows that

$$G_4 = 4t(\Delta V)H_0^2 + 8t\sum_{j,k=1}^6 \frac{\partial^2 V}{\partial x_j\partial x_k}\frac{\partial^2}{\partial x_j\partial x_k}H_0.$$

For ease of exposition we write $G_4 = G_{4,1} + G_{4,2}$ where where

$$G_{4,1} = 4t(\Delta V)H_0^2, \qquad \text{and} \qquad G_{4,2} = 8t \sum_{j,k=1}^{6} \frac{\partial^2 V}{\partial x_j \partial x_k} \frac{\partial^2}{\partial x_j \partial x_k}.$$

So we compute that

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \int_0^1 \mathrm{Tr}(V G_5 (\mathrm{Id} + H_0^2)^{-s-2}) \, \mathrm{d}t \right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \int_0^1 (-8t) \sum_{k=1}^{6} \mathrm{Tr} \left(V \left(\frac{\partial V}{\partial x_k} \frac{\partial}{\partial x_k} \right) H_0^2 (\mathrm{Id} + H_0^2)^{-s-2} \right) \, \mathrm{d}t \right) \\
&= i \frac{4}{(2\pi)^6} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \sum_{k=1}^{6} \left(\int_{\mathbb{R}^6} V(x) \frac{\partial V}{\partial x_k} \, \mathrm{d}x \right) \left(\int_{\mathbb{R}^6} \xi_k |\xi|^4 (1 + |\xi|^4)^{-s-2} \, \mathrm{d}\xi \right) \right) \\
&= 0,
\end{aligned}$$

since the ξ integral contains the integral of an odd function over a symmetric region. The $G_{4,1}$ contribution can be determined as

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \int_0^1 \mathrm{Tr}(V G_{4,1} (\mathrm{Id} + H_0^2)^{-s-2}) \, \mathrm{d}t \right) \\
&= \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \int_0^1 4t \mathrm{Tr} \left(V(\Delta V) H_0^2 (\mathrm{Id} + H_0^2)^{-s-2} \right) \, \mathrm{d}t \right) \\
&= \frac{2}{(2\pi)^6} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \left(\int_{\mathbb{R}^6} V(x) [\Delta V](x) \, \mathrm{d}x \right) \left(\int_{\mathbb{R}^6} |\xi|^4 (1 + |\xi|^4)^{-s-2} \, \mathrm{d}\xi \right) \right) \\
&= \frac{2\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \left(\int_{\mathbb{R}^6} V(x) [\Delta V](x) \, \mathrm{d}x \right) \left(\int_0^\infty r^{10-1} (1 + r^4)^{-s-2} \, \mathrm{d}r \right) \right) \\
&= \frac{2\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6} \operatorname*{Res}_{s=\frac{1}{2}} \left(Y_1(1,s) \left(\int_{\mathbb{R}^6} |[\nabla V](x)|^2 \, \mathrm{d}x \right) \left(\frac{\Gamma\left(\frac{10}{4}\right) \Gamma\left(s + 2 - \frac{10}{4}\right)}{4\Gamma(s+2)} \right) \right) \\
&= \frac{2\mathrm{Vol}(\mathbb{S}^5)}{(2\pi)^6} \left(\frac{3}{8} \right) \left(\frac{1}{4} \right) \int_{\mathbb{R}^6} |[\nabla V](x)|^2 \, \mathrm{d}x \\
&= \frac{3\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6} \int_{\mathbb{R}^6} |[\nabla V](x)|^2 \, \mathrm{d}x.
\end{aligned}$$

Next we determine the $G_{4,2}$ contribution as

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 \mathrm{Tr}(VG_{4,2}(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 8t\sum_{j,k=1}^{6}\mathrm{Tr}\left(V\frac{\partial^2 V}{\partial x_j\partial x_k}\frac{\partial^2}{\partial x_j\partial x_k}H_0(\mathrm{Id}+H_0^2)^{-s-2}\right)\mathrm{d}t\right)\\
&=i^2\frac{4}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{j,k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j\partial x_k}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_j\xi_k|\xi|^2(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right).
\end{aligned}$$

For $j\neq k$ the ξ integrals vanish since they are of an odd function. So we obtain

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\int_0^1 \mathrm{Tr}(VG_{4,2}(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=i^2\frac{4}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_k^2|\xi|^2(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right)\\
&=-\frac{4}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}|\xi|^4(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right)\\
&=-\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\int_0^\infty r^{10-1}(1+r^4)^{-s-2}\,\mathrm{d}r\right)\right)\\
&=-\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(1,s)\sum_{k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_k^2}\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{10}{4}\right)\Gamma\left(s+2-\frac{10}{4}\right)}{4\Gamma(s+2)}\right)\right)\\
&=\frac{4\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\left(\frac{3}{8}\right)\left(\frac{1}{4}\right)\left(\int_{\mathbb{R}^6}V(x)[\Delta V](x)\,\mathrm{d}x\right)\\
&=\frac{\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x.
\end{aligned}$$

Combining the $G_{4,1}$ and $G_{4,2}$ contributions we find

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(\int_0^1 \mathrm{Tr}(VX_2^{(1)}(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&=\frac{3\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x+\frac{\mathrm{Vol}(\mathbb{S}^5)}{16(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x\\
&=\frac{\mathrm{Vol}(\mathbb{S}^5)}{4(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x.
\end{aligned}$$

We now move to the $\ell=1,k=2,p=2$ term. Observe that $Y_1(s,\frac{1}{2})=-\frac{5}{16}$ and $\int_0^1(32t)\,\mathrm{d}t=16$. The operator $X_2^{(2)}$ is an order 8 operator and thus can be written as $X_2^{(2)}=\sum_{j=0}^{8}G_j$ where each operator G_j has order j. The operator $VG_j(\mathrm{Id}+H_0^2)^{-s-3}$ has order $j-4s-12$ and so gives a contribution which is holomorphic at $s=\frac{1}{2}$ if $j<8$.

Thus only the operator G_8 will contribute a non-zero residue. By writing

$$\begin{aligned} X_2^{(2)} &= 2t[H_0^2,[H_0^2,VH_0]] \\ &= 2tH_0^2[H_0,[H_0,V]]H_0 + 4tH_0[H_0,[H_0,V]]H_0^2 + 2t[H_0,[H_0,V]]H_0^3, \end{aligned}$$

we can compute directly the highest order component of $X_2^{(2)}$ as

$$G_8 = 32t\sum_{j,k=1}^{6}\frac{\partial^2 V}{\partial x_j\partial x_k}\frac{\partial^2}{\partial x_j\partial x_k}H_0^3.$$

So we find

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\int_0^1 \operatorname{Tr}(VX_2^{(2)}(\mathrm{Id}+H_0^2)^{-s-3})\,\mathrm{d}t\right) \\ &= \operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\int_0^1 32t\sum_{j=1}^{6}\operatorname{Tr}\left(V\frac{\partial^2 V}{\partial x_j^2}\frac{\partial^2}{\partial x_j}H_0^3(\mathrm{Id}+H_0^2)^{-s-3}\right)\,\mathrm{d}t\right) \\ &= i^2\frac{16}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\sum_{j,k=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j\partial x_k}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_j\xi_k|\xi|^6(1+|\xi|^4)^{-s-3}\,\mathrm{d}\xi\right)\right). \end{aligned}$$

For $j\neq k$ the ξ integral vanishes since it contains the integral of an odd function over a symmetric region. We thus compute

$$\begin{aligned} &\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\int_0^1 \operatorname{Tr}(VX_2^{(2)}(\mathrm{Id}+H_0^2)^{-s-3})\,\mathrm{d}t\right) \\ &= i^2\frac{16}{(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\sum_{j=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}\xi_j^2|\xi|^6(1+|\xi|^4)^{-s-3}\,\mathrm{d}\xi\right)\right) \\ &= -\frac{16}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\sum_{j=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j^2}\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}|\xi|^8(1+|\xi|^4)^{-s-3}\,\mathrm{d}\xi\right)\right) \\ &= -\frac{16\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\sum_{j=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j^2}\,\mathrm{d}x\right)\left(\int_0^\infty r^{14-1}(1+r^4)^{-s-3}\,\mathrm{d}r\right)\right) \\ &= -\frac{16\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_1(2,s)\sum_{j=1}^{6}\left(\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j^2}\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{14}{4}\right)\Gamma\left(s+3-\frac{14}{4}\right)}{4\Gamma(s+3)}\right)\right) \\ &= -\frac{16\mathrm{Vol}(\mathbb{S}^5)}{6(2\pi)^6}\left(-\frac{5}{16}\right)\left(\frac{1}{4}\right)\sum_{j=1}^{6}\int_{\mathbb{R}^6}V(x)\frac{\partial^2 V}{\partial x_j^2}\,\mathrm{d}x \\ &= -\frac{5\mathrm{Vol}(\mathbb{S}^5)}{24(2\pi)^6}\int_{\mathbb{R}^6}V(x)[\Delta V](x)\,\mathrm{d}x \\ &= -\frac{5\mathrm{Vol}(\mathbb{S}^5)}{24(2\pi)^6}\int_{\mathbb{R}^6}|[\nabla V](x)|^2\,\mathrm{d}x. \end{aligned}$$

Finally, we consider the $\ell = 2, k = (0,0), p = (2,2)$ term. Observe that $Y_2(0, \frac{1}{2}) = \frac{3}{8}$ and $\int_0^1 4t^2 \,\mathrm{d}t = \frac{4}{3}$. The operator X_2^2 is an order 4 operator and thus can be written as $X_2^2 = \sum_{j=0}^4 G_j$ with each operator G_j of order j. The operator $VG_j(\mathrm{Id} + H_0^2)^{-s-2}$ has order $j - 4s - 8$ and so gives a contribution which is holomorphic at $s = \frac{1}{2}$ if $j < 4$. Thus the only term which contributes a non-zero residue is G_4, which can be computed easily as

$$G_4 = 4t^2V^2H_0^2.$$

So we compute

$$\begin{aligned}
&\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_2(0,s)\int_0^1 \mathrm{Tr}(VX_2^2(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&= \operatorname*{Res}_{s=\frac{1}{2}}\left(Y_2(0,s)\int_0^1 4t^2\mathrm{Tr}(V^3H_0^2(\mathrm{Id}+H_0^2)^{-s-2})\,\mathrm{d}t\right)\\
&= \frac{4}{3(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_2(0,s)\left(\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x\right)\left(\int_{\mathbb{R}^6}|\xi|^4(1+|\xi|^4)^{-s-2}\,\mathrm{d}\xi\right)\right)\\
&= \frac{4\mathrm{Vol}(\mathbb{S}^5)}{3(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_2(0,s)\left(\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x\right)\left(\int_0^\infty r^{10-1}(1+r^4)^{-s-2}\,\mathrm{d}r\right)\right)\\
&= \frac{4\mathrm{Vol}(\mathbb{S}^5)}{3(2\pi)^6}\operatorname*{Res}_{s=\frac{1}{2}}\left(Y_2(0,s)\left(\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x\right)\left(\frac{\Gamma\left(\frac{10}{4}\right)\Gamma\left(s+2-\frac{10}{4}\right)}{4\Gamma(s+2)}\right)\right)\\
&= \frac{4\mathrm{Vol}(\mathbb{S}^5)}{3(2\pi)^6}\left(\frac{3}{8}\right)\left(\frac{1}{4}\right)\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x\\
&= \frac{\mathrm{Vol}(\mathbb{S}^5)}{8(2\pi)^6}\int_{\mathbb{R}^6} V(x)^3\,\mathrm{d}x. \qquad \square
\end{aligned}$$

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