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Generalised Point Interactions via Unitary Dilations

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Abstract

We present an inverse scattering construction of generalised point interactions (GPI) – point-like objects with non-trivial scattering behaviour. The construction is developed for single centre S-wave GPI models with rational S-matrices, and starts from an integral transform suggested by the scattering data. The theory of unitary dilations is then applied to construct a unitary mapping between Pontryagin spaces which extend the usual position and momentum Hilbert spaces. The GPI Hamiltonian is defined as a multiplication operator on the momentum Pontryagin space and its free parameters are fixed by a physical locality requirement. We determine the spectral properties and domain of the Hamiltonian in general, and construct the resolvent and Møller wave operators thus verifying that the Hamiltonian exhibits the required scattering behaviour. The physical Hilbert space is identified. The construction is illustrated by GPI models representing the effective range approximation. For negative effective range we recover a known class of GPI models, whilst the positive effective range models appear to be new. We discuss the interpretation of these models, along with possible extensions to our construction.

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1 Introduction and Main Ideas

Generalised point interactions (GPI) are solvable models in quantum mechanics representing point objects with non-trivial scattering behaviour. The prototype for such models is the class of point interactions (PI), introduced by Fermi [1] as (mathematically ill-defined) Hamiltonians of form $H = -\Delta + \lambda\delta(x)$ and rigorously defined as self-adjoint extensions of $-\Delta$ on the domain of smooth functions compactly supported away from the interaction centre [2]. This construction leads to 1-parameter families of PI Hamiltonians in dimensions 2 and 3 which provide the leading order (scattering length) approximation to the scattering behaviour of Schrödinger operators with short range potentials in the sector of zero angular momentum (see, for example [13]). We refer to [14] for an extensive bibliography on PI models.

GPI models are employed to treat more general scattering behaviour, such as higher order corrections to S-wave scattering, non-trivial scattering in non-zero angular momentum sectors or point objects in dimensions $d \geq 4$. In contrast to PI models, GPI Hamiltonians are not defined on the usual Hilbert space $L^2(\mathbb{R}^d)$, but on an extended space whose inner product may be indefinite (in which case one must identify a physical Hilbert space of states in order to recover the probability interpretation of quantum mechanics). Models of this type were first discussed by Shirokov [3], and given a mathematical foundation by Pavlov [4, 5, 6] and Shondin [7, 8] (see also [9]).

There are two principal constructions for GPI models in the literature, which we call the *auxiliary space* and *distributional* methods. The auxiliary space method starts with a given extended inner product space and then seeks the GPI Hamiltonians which 'live' on this space using generalisations of Krein's formula [5], or the von Neumann theory of deficiency indices [6]. Alternatively, for a restricted class of scattering data, one can write down a candidate resolvent whose free parameters are fixed by requiring that the characteristic properties of resolvents be satisfied [7].

On the other hand, the distributional method [8, 9] aims to make rigorous sense of the heuristic Hamiltonian $H = -\Delta + \omega$ for some distribution ω. Krein's formula [22] suggests that one define $(H - z)^{-1}$ as a perturbation of the free resolvent $R_0(z)$ of form $R_0(z) \mid \omega\rangle\langle\omega \mid R_0(z)$. In dimensions $d = 2, 3$, if ω is the δ-function, this yields the usual class of PI models, because the 'defect element' determined by the formal expression $\chi = R_0(z) \mid \omega\rangle$ is in $L^2(\mathbb{R}^d)$; however, in general one must extend the Hilbert space to include χ, or, more generally, $N \geq 1$ defect elements arising from N independent distributions. It turns out that $2N$ 'extra dimensions' are required, and that the extended inner product is indefinite, with rank of indefiniteness N. The inner product space is therefore a *Pontryagin space* (see Section 2) on which the GPI Hamiltonian is defined using Krein's formula.

There are, however, many circumstances under which one knows neither what the appropriate auxiliary space is, nor what the distributional description of the required interaction should be. It is therefore important to have available an inverse scattering construction for GPI models. In this paper, we present such a method, and develop it in

detail for single centre GPI models with non-trivial S-wave scattering. It is currently an open problem to extend this construction to higher angular momenta and dimensions $d \geq 4$; we discuss this further in the Conclusion.

The essence of the construction is as follows: the scattering data naturally defines an integral transform $\mathcal{T}$ between $\mathcal{H}_r = L^2((0,\infty), dr)$ and $\mathcal{H}_k = L^2((0,\infty), dk)$, i.e., the position and momentum Hilbert spaces. In general $\mathcal{T}$ is not unitary, the departure from unitarity being measured by $M_1 = \mathbf{I} - \mathcal{T}\mathcal{T}^*$ and $M_2 = \mathbf{I} - \mathcal{T}^*\mathcal{T}$, and the closures $\mathcal{M}_1$ and $\mathcal{M}_2$ of their respective ranges. Using the theory of *unitary dilations* (due in origin to Sz.-Nagy [20] and extended by Davis [21]) we may construct indefinite inner products on the $\mathcal{M}_i$ and hence enlarged inner product spaces $\mathcal{H}_r \oplus \mathcal{M}_1$ and $\mathcal{H}_k \oplus \mathcal{M}_2$ along with an operator $\hat{\mathcal{T}} : \mathcal{H}_r \oplus \mathcal{M}_1 \to \mathcal{H}_k \oplus \mathcal{M}_2$ which is unitary with respect to the relevant inner products and satisfies $P_{\mathcal{H}_k}\hat{\mathcal{T}}|_{\mathcal{H}_r} = \mathcal{T}$, where $P_{\mathcal{H}_k}$ is the orthoprojector onto $\mathcal{H}_k$. $\hat{\mathcal{T}}$ is said to be a unitary dilation[1] of $\mathcal{T}$. The construction of $\hat{\mathcal{T}}$ and the enlarged inner product spaces requires no information beyond that encoded in $\mathcal{T}$. We then define the GPI Hamiltonian h_{gpi} to act by multiplication on $\mathcal{H}_k \oplus \mathcal{M}_2$ (restricting to multiplication by k^2 on $\mathcal{H}_k$). The free parameters in h_{gpi} are fixed by a locality requirement described below. In this way, we not only construct the Hamiltonian, but also its spectral representation.

The plan and principal results of the paper are as follows. In Section 2, we briefly describe some features of analysis in spaces with indefinite inner product, and also discuss the construction of unitary dilations, essentially following Davis [21]. In addition, we sketch our construction in a general setting. Next, in Section 3, we consider the class of scattering data specified by S-wave partial waveshifts $\delta_0(k)$ of form

$$\cot \delta_0(k) = kr(k^2), \tag{1.1}$$

where $r(z)$ is a rational function with real coefficients. Shondin [7] refers to this class of data as the 'R class': it corresponds exactly with the scattering data of rational S-wave S-matrices satisfying the usual analytic continuation property $S(k) = S^*(-k)$ [15]. In particular, this class contains truncated low energy expansions of form

$$\cot \delta_0(k) = -\frac{1}{kL} + kr_0 + k^3 r_1 + \cdots + k^{2n+1} r_n, \tag{1.2}$$

for low energy parameters $L, r_0, r_1, \ldots, r_n$ and any $n \geq 0$, and thus furnishes approximations to the low energy S-wave behaviour of Schrödinger operators with short range potentials to arbitrary order. In [7], auxiliary space methods are employed to construct GPI models for the subclass of the R class in which $r(z)$ has negative imaginary part in the upper half plane. This is a somewhat restrictive class: for example, scattering data of form (1.2) is possible only with $r_1, \ldots, r_n = 0$ and $r_0 < 0$. In contrast, the method presented here allows one to treat the full R class.

The scattering data (1.1) naïvely suggests generalised continuum eigenfunctions of

[1] See Section 2 for a note on the nomenclature.

form $u_k(r) = (2/\pi)^{1/2} \sin(kr + \delta_0(k))$; accordingly, we define an integral transform $\mathcal{T}$ by

$$(\mathcal{T}\psi)(k) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \sin(kr + \delta_0(k))\psi(r)dr. \tag{1.3}$$

We explicitly construct the operators M_1 and M_2 (which are of finite rank) for a generic subclass of the R class – those whose scattering amplitudes exhibit only simple poles on the physical sheet. Hence the enlarged inner product spaces $\Pi_r = \mathcal{H}_r \oplus \mathcal{M}_1$ and $\Pi_k = \mathcal{H}_k \oplus \mathcal{M}_2$ are (generally) Pontryagin spaces. We determine the rank and signature of the M_i in terms of indices reminiscent of Levinson's theorem [15].

In Section 4, we define the GPI Hamiltonian as an operator on Π_r by

$$h_{\text{gpi}} = \hat{\mathcal{T}}^\dagger \begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{1.4}$$

where the dagger denotes the Pontryagin space adjoint, and we have used an obvious block matrix notation. We show that Λ is completely determined by imposing a physical locality condition: that the 'interaction' be localised at the origin. Mathematically, this is expressed by requiring $h_{\text{gpi}}(\psi, 0)^T = (-\psi'', 0)^T$ if $\psi \in C_0^\infty(0,\infty)$. Under this condition, the eigenvalues of h_{gpi} occur precisely at those energies for which the scattering amplitude derived from (1.1) exhibits poles on the physical sheet, as is the case for ordinary scattering from 'nice' potentials. We proceed to construct the eigenfunctions of h_{gpi}, thereby isolating the physical Hilbert space. We also determine the domain and resolvent of h_{gpi}, and explicitly construct its Møller wave operators in a two-space setting, verifying that they yield the required scattering theory.

In Section 5, we illustrate our procedure by constructing GPI models with scattering behaviour $\cot \delta_0(k) = -1/(kL) + kM$, representing the effective range approximation of low energy scattering theory [15]. For $M < 0$, $\mathcal{H}_r$ and $\mathcal{H}_k$ are extended to larger Hilbert spaces; this case has been treated previously using auxiliary space methods in [7] as models of type 'B_2' and arises as a special case of the construction in [4]. The case $M > 0$, for which Pontryagin spaces are required, appears to be new. Our methods allow the entire class of GPI Hamiltonians to be constructed, along with their spectral representations. A particularly interesting subclass of the models constructed correspond to the case $L = \infty$, with scattering theory $\cot \delta_0(k) = kM$. Such models reproduce the leading order behaviour of non-point interactions exhibiting a zero energy resonance. We refer to these models as *resonance point interactions* (RPI).

We also discuss how these GPI models may be used as models for Schrödinger operators with spherically symmetric potentials of compact support. To do this, we employ a general methodology for discussing the 'large scale effects of small objects' developed by Kay and the author [13]. In particular, we develop *fitting formulae* (analogous to those given in [13]) for matching a given potential $V(r)$ to the 'best fit' GPI model. Finally, in Section 6, we conclude by discussing various extensions to our method. An Appendix contains an algebraic result required in the body of the paper.

The motivation for the present work arose in a consideration of the scattering of charged particles off magnetic flux tubes of small radius [11], in which it was found that the scattering lengths for spin-$\frac{1}{2}$ particles generically take the values 0 or ∞ in certain angular momentum sectors. In consequence, the analogue of PI models representing dynamics in the background of an infinitesimally thin wire of flux fails to describe the leading order scattering theory in these sectors, and should be replaced by models analogous to the RPI models mentioned above. The special nature of this system can be attributed to the fact that it is an example of supersymmetric quantum mechanics. Elsewhere [12], we will construct the appropriate class of RPI for this system.

2 Preliminaries

2.1 Unitary Dilations

We begin by describing the unitary dilation theory required in the sequel. Let $\mathcal{H}_1, \ldots, \mathcal{H}_4$ be Hilbert spaces and $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. Then $\hat{T} \in \mathcal{L}(\mathcal{H}_1 \oplus \mathcal{H}_3, \mathcal{H}_2 \oplus \mathcal{H}_4)$ is called a *dilation* of T if $T = P_{\mathcal{H}_2}\hat{T}|_{\mathcal{H}_1}$ where $P_{\mathcal{H}_2}$ is the orthogonal projector onto $\mathcal{H}_2$. In block matrix form, $\hat{T}$ takes form

$$\hat{T} = \begin{pmatrix} T & P \\ Q & R \end{pmatrix}. \tag{2.1}$$

Our nomenclature follows that of Halmos [19]. Elsewhere (e.g., in the work of Davis [21]), the term 'dilation' (or 'dilatation') often means that $\hat{T}^n$ is a dilation of T^n and $(\hat{T}^*)^n$ is a dilation of $(T^*)^n$ for each $n = 1, 2, \ldots$ (in addition, $\mathcal{H}_1 = \mathcal{H}_2$, and $\mathcal{H}_3 = \mathcal{H}_4$). We refer to such operators as *power dilations*: in the block form (2.1), this requires $PR^nQ = 0$ for each $n = 0, 1, 2, \ldots$.

According to a result of Sz.-Nagy [20], any contraction T from one Hilbert space to another (i.e., a bounded operator satisfying $\|T\| \leq 1$) has a unitary dilation between larger Hilbert spaces. Subsequently, Davis [21] extended this result to arbitrary closed densely defined operators at the cost of introducing indefinite inner product spaces. (It is clear that if $\|T\| > 1$, no Hilbert space unitary dilation is possible.) In fact, Davis' construction yields a unitary *power* dilation of the original operator. This has no physical relevance in our construction, and so we use a more economical 'cut-down' version of Davis' result, described below. First, we briefly review the salient features of analysis in indefinite inner product spaces. Full treatments can be found in the monographs of Bognár [23] and Azizov and Iokhvidov [24].

We employ a particular class of indefinite inner product spaces known as *J-spaces*. Let $\mathcal{H}$ be a Hilbert space with (positive definite) inner product $\langle \cdot \mid \cdot \rangle$, equipped with a unitary involution, J. We define a non-degenerate indefinite inner product $[\cdot, \cdot]$ on $\mathcal{H}$ by

$$[x, y] = \langle x \mid Jy \rangle, \tag{2.2}$$

which we call the *J-inner product*. $\mathcal{H}$ equipped with the J-inner product is called a J-space. $\mathcal{H}$ admits decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- = \mathcal{H}_+[+]\mathcal{H}_-$ into the eigenspaces $\mathcal{H}_\pm$ of J with eigenvalue ± 1, where $[+]$ denotes the orthogonal direct sum in the J-inner product. If at least one of the $\mathcal{H}_\pm$ is finite dimensional, then $\mathcal{H}$ is a *Pontryagin space* with respect to $[\cdot, \cdot]$.

The topology of a J-space is determined by the Hilbert space norm; however, operator adjoints and the notion of unitarity are defined relative to the J-inner product. Thus if $\mathcal{H}_i$ $(i = 1, 2)$ are J_i-spaces, and $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$, the (J_1, J_2)-*adjoint* $T^\dagger$ of T is defined in terms of the Hilbert space adjoint T^* by

$$T^\dagger = J_1 T^* J_2. \tag{2.3}$$

Equivalently, $[T^\dagger x, y]_{\mathcal{H}_1} = [x, Ty]_{\mathcal{H}_2}$ for all $x \in \mathcal{H}_2$, $y \in \mathcal{H}_1$. If $[Ux, Uy]_{\mathcal{H}_2} = [x, y]_{\mathcal{H}_1}$ for all $x, y \in \mathcal{D} \subset \mathcal{H}_1$, U is said to be (J_1, J_2)-*isometric*; if in addition U is a linear isomorphism of $\mathcal{H}_1$ and $\mathcal{H}_2$, and $\mathcal{D} = \mathcal{H}_1$, U is said to be (J_1, J_2)-*unitary*. Equivalently, $UU^\dagger = \mathbf{I}_{\mathcal{H}_1}$ and $U^\dagger U = \mathbf{I}_{\mathcal{H}_2}$. If $\mathcal{H}_1 = \mathcal{H}_2$ with $J_1 = J_2 = J$, terms such as (J_1, J_2)-isometric are abbreviated to J-isometric etc.

We now show that any bounded operator between Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ has a unitary dilation between J-spaces. The proof is essentially due to Davis [21].

Theorem 2.1 *Let $\mathcal{H}_i$ $(i = 1, 2)$ be Hilbert spaces, and $T \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$. Define $M_1 = \mathbf{I} - TT^*$, $M_2 = \mathbf{I} - T^*T$ and $\mathcal{M}_i = \overline{\mathrm{Ran}\, M_i}$. Write $\mathcal{K}_i = \mathcal{H}_i \oplus \mathcal{M}_i$, and define $J_i = \mathbf{I} \oplus \mathrm{sgn}\,(M_i)$. Then $\mathcal{K}_i$ is a J_i-space and $\hat{T} : \mathcal{K}_1 \to \mathcal{K}_2$ defined by*

$$\hat{T} = \begin{pmatrix} T & -\mathrm{sgn}\,(M_1)|M_1|^{1/2} \\ |M_2|^{1/2} & T^*|_{\mathcal{M}_1} \end{pmatrix} \tag{2.4}$$

is a (J_1, J_2)-unitary dilation of T.

Proof: Note first that $\mathcal{M}_i$ is a $\mathrm{sgn}\,(M_i)$-space. For $\mathcal{M}_i$ is a Hilbert space, $\mathrm{sgn}\,(M_i)$ is self-adjoint, and because (in $\mathcal{H}_i$) $\overline{\mathrm{Ran}\, M_i} = (\ker M_i)^\perp$, $\mathrm{sgn}\,(M_i)$ is involutive on $\mathcal{M}_i$, and hence unitary. Thus the $\mathcal{K}_i$ are J_i-spaces. Now for any continuous Borel function f, we have the intertwining relations $Tf(T^*T) = f(TT^*)T$ and $T^*f(TT^*) = f(T^*T)T^*$. In particular, $TM_2 = M_1T$ and $T^*M_1 = M_2T^*$, which entail that $T|_{\mathcal{M}_2} : \mathcal{M}_2 \to \mathcal{M}_1$, and $T^*|_{\mathcal{M}_1} : \mathcal{M}_1 \to \mathcal{M}_2$. Thus $(T^*|_{\mathcal{M}_1})^* = T|_{\mathcal{M}_2}$. The (J_1, J_2)-adjoint $\hat{T}^\dagger$ of $\hat{T}$ may be written using the intertwining relations as

$$\hat{T}^\dagger = J_1 \hat{T}^* J_2 = \begin{pmatrix} T^* & \mathrm{sgn}\,(M_2)|M_2|^{1/2} \\ -|M_1|^{1/2} & T|_{\mathcal{M}_2} \end{pmatrix}. \tag{2.5}$$

Further application of these relations allows direct computation of $\hat{T}^\dagger\hat{T}$ and $\hat{T}\hat{T}^\dagger$ to verify unitarity. ■

In our application, M_1 and M_2 are finite rank, and so the J-spaces constructed above are Pontryagin spaces. Moreover, the rank of indefiniteness of the J_i-inner product is equal to $\frac{1}{2}(r_i - s_i)$, where r_i and s_i are the rank and signature of M_i.

We briefly consider the uniqueness of the unitary dilations constructed above. For technical reasons, we restrict to the case where the M_i are finite rank. Suppose $\mathcal{N}_i$ are J_i spaces ($i = 1, 2$) and that $\tilde{T} : \mathcal{H}_1 \oplus \mathcal{N}_1 \to \mathcal{H}_2 \oplus \mathcal{N}_2$ is a unitary dilation of T with matrix form (2.1). Unitarity of $\tilde{T}$ entails *inter alia* the three relations

$$Q^\dagger Q = M_2, \qquad PP^\dagger = M_1 \qquad QT^* + RP^\dagger = 0. \tag{2.6}$$

The first two entail the existence of isometries $U : \operatorname{Ran}|M_2|^{1/2} \to \operatorname{Ran} Q$ and $V : \operatorname{Ran}|M_1|^{1/2} \to \operatorname{Ran} P^\dagger$ such that $Q = U|M_2|^{1/2}$ and $P = -\operatorname{sgn} M_1 |M_1|^{1/2} V^\dagger$. Because the $\mathcal{M}_i$ are finite dimensional, $\operatorname{Ran} Q$ and $\operatorname{Ran} P^\dagger$ are closed and U is therefore a unitary operator from $\mathcal{M}_2$ to $\operatorname{Ran} Q$, and V is unitary from $\mathcal{M}_1$ to $\operatorname{Ran} P^\dagger$. The third relation entails that $R = UT^*|_{\mathcal{M}_1} V^\dagger$ on $\operatorname{Ran} P^\dagger$. Finally, because $\operatorname{Ran} Q$ is the unitary image of a finite dimensional J-space it is orthocomplemented and there exists an orthogonal projection $P_{\mathcal{H}_2 \oplus \operatorname{Ran} Q}$ onto $\mathcal{H}_2 \oplus \operatorname{Ran} Q$ in $\mathcal{H}_2 \oplus \mathcal{N}_2$. We then obtain

$$P_{\mathcal{H}_2 \oplus \operatorname{Ran} Q} \tilde{T}|_{\mathcal{H}_1 \oplus \operatorname{Ran} P^\dagger} = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & U \end{pmatrix} \hat{T} \begin{pmatrix} \mathbf{I} & 0 \\ 0 & V \end{pmatrix}. \tag{2.7}$$

Thus $\hat{T}$ is unique up to further dilation and unitary equivalence of the above form. If the M_i are not of finite rank, this statement also holds if the M_i are strictly positive. More generally, it is not clear whether $\overline{\operatorname{Ran} Q}$ is necessarily orthocomplemented; in addition, J-isometries are not necessarily bounded and cannot always be extended from a domain to its closure (see Section 5 of Chapter 2 in [24]).

2.2 Abstract Setting

In this section, we sketch our construction in a general setting, which makes clear how it may be extended. In particular, we show how the domain and action of the Hamiltonian is determined.

Let $\mathcal{H}_i$ ($i = 1, 2$) be Hilbert spaces and let A be a densely defined symmetric operator with domain $\mathcal{D} \subset \mathcal{H}_1$. Suppose that A possesses two self-adjoint extensions $A_\pm$ such that

$$A_\pm = \mathcal{T}_\pm^* \tilde{A} \mathcal{T}_\pm \tag{2.8}$$

where $\tilde{A}$ is a self-adjoint multiplication operator on $\mathcal{H}_2$ with $(\tilde{A} + \omega)^{-1}$ bounded for some $\omega \in \mathbb{R}$, and $\mathcal{T}_\pm$ are unitary operators $\mathcal{T}_\pm : \mathcal{H}_1 \to \mathcal{H}_2$. Let C and S be bounded multiplication operators on $\mathcal{H}_2$ and define

$$\mathcal{T} = C\mathcal{T}_+ + S\mathcal{T}_-. \tag{2.9}$$

In our application, C and S are determined by the scattering data. We define M_1 and M_2 as above, for simplicity assuming that they are finite rank (as they are in our application). The unitary dilation $\hat{\mathcal{T}}$ derived above is then used to define a self-adjoint operator B on the Pontryagin space $\Pi_1 = \mathcal{H}_1 \oplus \mathcal{M}_1$ by

$$B = \hat{\mathcal{T}}^\dagger \begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{2.10}$$

where Λ is a self-adjoint operator on $\mathcal{M}_2$ (with respect to its inner product). Thus

$$B \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} \mathcal{T}^* \tilde{A}(\mathcal{T}\varphi - \Theta) + \operatorname{sgn} M_2 |M_2|^{1/2} \Lambda(|M_2|^{1/2}\varphi + \mathcal{T}^*|_{\mathcal{M}_1}\Phi) \\ -|M_1|^{1/2}\tilde{A}(\mathcal{T}\varphi - \Theta) + \mathcal{T}|_{\mathcal{M}_2}\Lambda(|M_2|^{1/2}\varphi + \mathcal{T}^*|_{\mathcal{M}_1}\Phi) \end{pmatrix}, \tag{2.11}$$

where $\Theta = \operatorname{sgn} M_1 |M_1|^{1/2}\Phi$, and B has domain

$$D(B) = \{(\varphi, \Phi)^T \mid \mathcal{T}\varphi - \Theta \in D(\tilde{A})\}. \tag{2.12}$$

To gain a more explicit description of $D(B)$, we impose the requirement that B be a self-adjoint extension of the non-densely defined operator $A \oplus 0$ on $\mathcal{D} \oplus 0 \subset \Pi_1$, i.e., $B(\varphi, 0)^T = (A\varphi, 0)^T$ for all $\varphi \in \mathcal{D}$. Later this will carry the physical interpretation of a locality condition. Because $\tilde{A}\mathcal{T}\varphi = \mathcal{T}A\varphi$ for such φ, this is equivalent to the requirement $|M_2|^{1/2}A\varphi = \Lambda|M_2|^{1/2}\varphi$ for all $\varphi \in \mathcal{D}$, which is satisfied if and only if $\mathcal{M}_2$ is invariant under A^* and

$$\Lambda = (|M_2|^{-1/2}A^*|_{\mathcal{M}_2}|M_2|^{1/2})^*. \tag{2.13}$$

As a consequence of locality, we note that if $(\varphi, \Phi)^T \in D(B)$ with $B(\varphi, \Phi)^T = (\tilde{\varphi}, \tilde{\Phi})^T$, then $\varphi \in D(A^*)$, and $\tilde{\varphi} = A^*\varphi$. For take any $\psi \in \mathcal{D}$. Then

$$\langle \tilde{\varphi} \mid \psi \rangle_{\mathcal{H}_1} = \left[\begin{pmatrix} \tilde{\varphi} \\ \tilde{\Phi} \end{pmatrix}, \begin{pmatrix} \psi \\ 0 \end{pmatrix} \right]_{\Pi_1} = \left[\begin{pmatrix} \varphi \\ \Phi \end{pmatrix}, B \begin{pmatrix} \psi \\ 0 \end{pmatrix} \right]_{\Pi_1} = \langle \varphi \mid A\psi \rangle_{\mathcal{H}_1}. \tag{2.14}$$

We may therefore re-write (2.12) as

$$D(B) = \left\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi \in D(A^*), \quad C\mathcal{T}_+\chi_+ + S\mathcal{T}_-\chi_- + \Theta \in D(\tilde{A}) \right\} \tag{2.15}$$

where we have written $\chi_\pm = (A_\pm + \omega)^{-1}(A^* + \omega)\varphi - \varphi$. The advantage of this expression is that $\chi_\pm$ is the unique element[2] of $\ker(A^* + \omega)$ such that $\varphi + \chi_\pm \in D(A_\pm)$. In our application, $\chi_\pm$ may be expressed in terms of the value of φ and its first derivative at the origin.

To determine the action of B more explicitly, we use the fact that the upper component of the right-hand side of (2.11) is equal to $A^*\varphi$ in order to compute $\tilde{\Theta} = \operatorname{sgn} M_1 |M_1|^{1/2}\tilde{\Phi}$. We obtain

$$\tilde{\Theta} = -M_1\tilde{A}(\mathcal{T}\varphi - \Theta) + \mathcal{T}(A^*\varphi - \mathcal{T}^*\tilde{A}(\mathcal{T}\varphi - \Theta)) = \mathcal{T}A^*\varphi - \tilde{A}(\mathcal{T}\varphi - \Theta) \tag{2.16}$$

Setting $\Theta = \Theta_1 - (C\mathcal{T}_+\chi_+ + S\mathcal{T}_-\chi_-)$, with $\Theta_1 \in D(\tilde{A})$, this becomes

$$\tilde{\Theta} = \tilde{A}\Theta_1 + \omega(\Theta_1 - \Theta) + \mathcal{T}(A^* + \omega)\varphi - (\tilde{A} + \omega)(\mathcal{T}\varphi + \Theta_1 - \Theta). \tag{2.17}$$

The last two terms cancel by definition of $\chi_\pm$ and we conclude that

$$B \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} A^*\varphi \\ (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1}\tilde{\Theta} \end{pmatrix} \tag{2.18}$$

where $\tilde{\Theta} = \tilde{A}(C\mathcal{T}_+\chi_+ + S\mathcal{T}_-\chi_- + \Theta) + \omega(C\mathcal{T}_+\chi_+ + S\mathcal{T}_-\chi_-)$.

[2] The $\chi_\pm$ are orthogonal to $\operatorname{Ran} A + \omega$; moreover, non-uniqueness would imply that $\ker(A^* + \omega) \cap D(A_\pm)$ is non-trivial, leading to a contradiction because $A_\pm + \omega$ has trivial kernel and A^* agrees with $A_\pm$ on $D(A_\pm)$.

3 Determination of M_1 and M_2

In this section, we determine the operators $M_1 = \mathbf{I} - \mathcal{T}\mathcal{T}^*$ and $M_2 = \mathbf{I} - \mathcal{T}^*\mathcal{T}$, where $\mathcal{T}$ is an integral transformation arising from the scattering data in the Shondin R class [7] given by

$$\cot\delta_0(k) = k^{-1}\frac{p(k^2)}{q(k^2)}, \qquad \delta_\ell(k) \equiv 0 \quad \text{for } \ell \geq 1, \tag{3.1}$$

where $p(z)$ and $q(z)$ are coprime polynomials in $\mathbb{R}[z]$, the ring of polynomials with real coefficients. In particular, we will show how the rank and signature of the M_i are determined by two 'Levinson indices' defined below.

The scattering amplitude corresponding to $\delta_0(k)$ is

$$f_0(k) = \frac{1}{k}e^{i\delta_0(k)}\sin\delta_0(k) = \frac{q(k^2)}{p(k^2) - ikq(k^2)}. \tag{3.2}$$

Defining the polynomial $W(z)$ by

$$W(z) = \begin{cases} p(-z^2) - zq(-z^2) & p(0) \neq 0 \\ p(-z^2)/z - q(-z^2) & p(0) = 0, \end{cases} \tag{3.3}$$

we note that $f_0(k)$ exhibits poles where $W(ik) = 0$. The set Ω of zeros of $W(z)$ in the left-hand half-plane $\operatorname{Re} z < 0$ corresponds to poles of $f_0(k)$ such that k^2 lies on the physical sheet. We refer to the situation where these poles (and hence the corresponding zeros of $W(z)$) are simple as the *generic case*. In Theorem 4.1, we will show that the discrete spectrum of the GPI Hamiltonian is precisely $\{E = -\omega^2 \mid \omega \in \Omega\}$ under the requirement of locality.[3]

The qualitative features of the scattering data (3.1) are described by the degrees of p and q, two indices $I_L^\pm$ defined below, and the asymptotic behaviour of $\cot\delta_0(k)$ given by

$$\sigma_0 = \operatorname{sgn}\lim_{k\to 0^+}\cot\delta(k) \qquad \text{and} \qquad \sigma_\infty = \operatorname{sgn}\lim_{k\to\infty}\cot\delta(k), \tag{3.4}$$

where the limits are allowed to be $\pm\infty$. The indices $I_L^\pm$ are defined by

$$I_L^+ = \frac{\delta_0(0) - \delta_0(\infty)}{\pi} \qquad \text{and} \qquad I_L^- = \frac{\zeta(0) - \zeta(\infty)}{\pi}, \tag{3.5}$$

where the auxiliary scattering data $\zeta(k)$ is defined by

$$\cot\zeta(k) = -k^{-1}\frac{p(-k^2)}{q(-k^2)}. \tag{3.6}$$

We refer to $I_L^\pm$ as the Levinson indices (although Levinson's theorem [15] will not hold in its usual form).

[3] These eigenvalues can be complex: we will return to this point in section 5.3.

We now define the integral transform $\mathcal{T} = \cos\delta_0(k)\mathcal{S} + \sin\delta_0(k)\mathcal{C}$, which is suggested by the naïve generalised eigenfunctions $u_k(r) = (2/\pi)^{1/2}\sin(kr + \delta_0(k))$. Here, $\mathcal{S}$ and $\mathcal{C}$ are the sine and cosine transforms, defined by

$$(\mathcal{S}\psi)(k) = \sqrt{\frac{2}{\pi}}\int_0^\infty dr \sin kr\psi(r) \quad \text{and} \quad (\mathcal{C}\psi)(k) = \sqrt{\frac{2}{\pi}}\int_0^\infty dr \cos kr\psi(r) \tag{3.7}$$

(the integrals are intended as limits in L^2-norm). Both are unitary maps from $\mathcal{H}_r$ to $\mathcal{H}_k$; their inverses have the same form, with r and k exchanged. Thus $\mathcal{T}$ is given explicitly by

$$\mathcal{T} = \frac{p(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{S} + \frac{kq(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{C}. \tag{3.8}$$

Because $\mathcal{S}$ and $\mathcal{C}$ furnish the spectral representations of $-d^2/dr^2$ with Dirichlet and Neumann boundary conditions respectively, we are in the general situation of Section 2.2.

We now restrict to the generic case and explicitly construct the M_i and compute their rank and signature. M_2 is given by the following proposition, whose proof is given later in this section.

Proposition 3.1 *In the generic case,*

$$M_2 = \sum_{\omega\in\Omega}\alpha_\omega \mid \xi_\omega\rangle\langle\xi_{\bar\omega}\mid, \tag{3.9}$$

where $\xi_\omega(r) = e^{\omega r}$, and α_ω is the residue

$$\alpha_\omega = \operatorname{Res}_\omega 2zf_0(-iz). \tag{3.10}$$

In addition, $\operatorname{Ran} M_2 = \operatorname{span}\{\xi_\omega \mid \omega \in \Omega\}$, *and*

$$\operatorname{rank} M_2 = \frac{1}{2}\deg W + I_L^+ \tag{3.11}$$

$$\operatorname{sig} M_2 = \frac{1}{2}\left(\sigma_0^2 - \sigma_\infty^2\right) - I_L^-. \tag{3.12}$$

Next, define $\mathcal{M}_1$ to be the space of all L^2-vectors of form $Q(k^2)k(p(k^2)^2+k^2q(k^2)^2)^{-1/2}$, such that $Q(z) \in \mathbb{C}[z]$ is a polynomial with complex coefficients. Thus

$$\mathcal{M}_1 = (p(k^2)^2 + k^2q(k^2)^2)^{-1/2}k\mathbb{C}_{\mathfrak{U}-1}[k^2] \tag{3.13}$$

where $\mathbb{C}_r[z]$ is the $r+1$-dimensional complex vector space of polynomials with complex coefficients and degree at most r, and $\mathfrak{U} = \dim\mathcal{M}_1$ is given by

$$\mathfrak{U} = \frac{1}{2}\deg W + \frac{1}{2}(\sigma_\infty^2 - \sigma_0^2) = \max\{\deg p, \deg q\} \tag{3.14}$$

M_1 is described by

Proposition 3.2 *In the generic case, M_1 vanishes on ${\mathcal{M}_1}^\perp$, and its action on $\mathcal{M}_1$ is given by $M_1 Q(k^2)k(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2} = \tilde{Q}(k^2)k(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2}$, where*

$$\tilde{Q}(k^2) = Q(k^2) + \sum_{\omega\in\Omega} \frac{Q(-\omega^2)\alpha_\omega}{q(-\omega^2)} \frac{p(k^2) - \omega q(k^2)}{\omega^2 + k^2}. \tag{3.15}$$

Moreover, $\operatorname{Ran} M_1 = \mathcal{M}_1$ *and*

$$\begin{aligned} \operatorname{rank} M_1 &= \frac{1}{2}\deg W + \frac{1}{2}(\sigma_\infty^2 - \sigma_0^2) && (3.16)\\ \operatorname{sig} M_1 &= -(I_L^+ + I_L^-). && (3.17) \end{aligned}$$

We now prove the above propositions.

Proof of Proposition 3.1: M_2 may be written in two equivalent forms:

$$\begin{aligned} M_2 &= \mathcal{S}^{-1}\sin^2\delta_0(k)\mathcal{S} - \mathcal{C}^{-1}\sin^2\delta_0(k)\mathcal{C} \\ &\quad -\mathcal{C}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{S} - \mathcal{S}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{C} && (3.18)\\ &= \mathcal{C}^{-1}\cos^2\delta_0(k)\mathcal{C} - \mathcal{S}^{-1}\cos^2\delta_0(k)\mathcal{S} \\ &\quad -\mathcal{C}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{S} - \mathcal{S}^{-1}\sin\delta_0(k)\cos\delta_0(k)\mathcal{C}. && (3.19) \end{aligned}$$

To convert this into an integral kernel we use the following Lemma, which may be proved by standard means (cf. Theorem IX.29 in [17]). Here, $v(x)$ and $w(x)$ stand for either $\sin x$ or $\cos x$, and $\mathcal{V}$ and $\mathcal{W}$ are the corresponding integral transforms from $\mathcal{H}_r$ to $\mathcal{H}_k$.

Lemma 3.3 *Let $g(k) \in L^2(\mathbb{R}^+) \cap L^\infty(\mathbb{R}^+)$ and define $G = \mathcal{V}^{-1}g(k)\mathcal{W}$. Then G has integral kernel*

$$G(r,r') = \frac{2}{\pi}\int_0^\infty v(kr)w(kr')g(k)dk, \tag{3.20}$$

(where the integral is a limit in L^2-norm).

In the case $\deg p > \deg q$, $\sin^2\delta_0(k)$ and $\sin\delta_0(k)\cos\delta_0(k)$ are $L^2 \cap L^\infty$ and so, applying Lemma 3.3 to (3.18) and combining terms, M_2 has integral kernel

$$M_2(r,r') = \frac{i}{\pi}\int_{-\infty}^\infty e^{i\delta_0(k)}\sin\delta_0(k)e^{ik(r+r')}dk = \frac{1}{\pi}\int_{-\infty}^\infty \frac{ikq(k^2)e^{ik(r+r')}}{p(k^2) - ikq(k^2)}dk. \tag{3.21}$$

Making the substitution $z = ik$ and closing the contour in the left-hand half-plane, the integrand has a simple pole at each $\omega \in \Omega$ and (3.9) follows. If $\deg q \geq \deg p$, $\cos^2\delta_0(k)$ and $\sin\delta_0(k)\cos\delta_0(k)$ are $L^2 \cap L^\infty$, and we use (3.19) to obtain

$$M_2(r,r') = \frac{1}{\pi}\int_{-\infty}^\infty e^{i\delta_0(k)}\cos\delta_0(k)e^{ik(r+r')}dk, \tag{3.22}$$

which yields the same result as before, because $e^{i\delta_0(k)}\cos\delta_0(k)$ and $ie^{i\delta_0(k)}\sin\delta_0(k)$ have identical poles and residues (their difference is unity).

By linear independence of the ξ_ω and non-vanishing of the α_ω, it follows that $\operatorname{Ran} M_2 = \mathcal{M}_2 = \operatorname{span}\{\xi_\omega \mid \omega \in \Omega\}$, so $\operatorname{rank} M_2 = |\Omega|$, the cardinality of Ω. Using residue calculus, $|\Omega|$ is given by

$$|\Omega| = \lim_{R\to\infty}\frac{1}{2\pi i}\int_{C_R\cup\Gamma_R}\frac{W'(z)}{W(z)}dz, \tag{3.23}$$

where C_R is a semicircle of radius R, centre the origin, lying in the left-hand half-plane, and Γ_R is the portion of the imaginary axis between $-iR$ and $+iR$. The contour is described anticlockwise, and it follows that

$$|\Omega| = \frac{1}{2}\deg W + \frac{1}{2\pi}\int_{-\infty}^\infty \frac{W'(ik)}{W(ik)}dk. \tag{3.24}$$

In the case $p(0) \neq 0$, the second term may be rearranged to give

$$\frac{1}{\pi}\int_0^\infty \frac{2k^2q(k^2)p'(k^2) - p(k^2)(q(k^2) + 2k^2q'(k^2))}{p(k^2)^2 + k^2q(k^2)^2}dk = \frac{\delta_0(0) - \delta_0(\infty)}{\pi}, \tag{3.25}$$

where the final step follows from the observation that the integrand on the left hand side equals $\sin^2\delta_0(k)d/dk\cot\delta_0(k) = -\delta_0'(k)$. Hence $|\Omega| = \frac{1}{2}\deg W + I_L^+$ and (3.11) follows. A similar argument is used when $p(0) = 0$.

To compute $\operatorname{sig} M_2$, we define the hermitian form $m_2(\varphi,\psi) : \mathcal{M}_2 \times \mathcal{M}_2 \to \mathbf{C}$ by $m_2(\varphi,\psi) = \langle\varphi \mid M_2\psi\rangle$. Labelling the elements of Ω as $\omega_1,\ldots,\omega_{|\Omega|}$, and writing $\psi = \sum_i c_i\xi_{\omega_i}$, we have

$$m_2(\psi,\psi) = \sum_{i,j,k}\overline{c_i}\langle\xi_{\omega_i} \mid \xi_{\omega_j}\rangle\alpha_j\langle\xi_{\overline{\omega_j}} \mid \xi_{\omega_k}\rangle c_k = c^\dagger\Xi^\dagger A\Xi c, \tag{3.26}$$

where A and Ξ are hermitian. Ξ has components $\Xi_{ij} = \langle\xi_{\omega_i} \mid \xi_{\omega_j}\rangle$, and is non-singular by linear independence of the ξ_ω. By Sylvester's Law of Inertia [25], the signature of M_2 equals that of A, which has components

$$A_{ij} = \begin{cases} \alpha_{\omega_i} & \omega_i = \overline{\omega_j} \\ 0 & \text{otherwise.} \end{cases} \tag{3.27}$$

A may easily be diagonalised with eigenvalues $\{\alpha_\omega \mid \omega \in \mathbb{R}\} \cup \{\pm|\alpha_\omega| \mid \omega \notin \mathbb{R}\}$. Labelling the ω_i so that $\omega_1,\ldots,\omega_r$ are the real elements of Ω, we therefore have $\operatorname{sig} M_2 = \operatorname{sig}\operatorname{diag}(\alpha_{\omega_1}\ldots,\alpha_{\omega_r})$. (We have used the fact that $\alpha_{\overline{\omega}} = \overline{\alpha_\omega}$, and in particular that $\omega_r \in \mathbb{R}$ implies $\alpha_r \in \mathbb{R}$.) Defining $\zeta(k)$ by (3.6), it is easy to show that $\cot\zeta(-\omega) = 1$ for $\omega \in \Omega$, and that

$$\alpha_\omega = 2\lim_{z\to-\omega}\frac{z+\omega}{1-\cot\zeta(z)} = \frac{1}{\zeta'(-\omega)}. \tag{3.28}$$

Thus $\operatorname{sig}\operatorname{diag}(\alpha_1,\ldots,\alpha_r)$ is equal to the number of times that $\zeta(k) \equiv \pi/4 \pmod{\pi}$ as k traverses $\mathbb{R}^+$, counted according to the sign of $\zeta'(k)$ at such points. This is related to the Levinson index I_L^- by (3.12). ∎

Proof of Proposition 3.2: We compute

$$M_1 = -\frac{p(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\mathcal{S}\mathcal{C}^{-1}\frac{kq(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}} - \frac{kq(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\mathcal{C}\mathcal{S}^{-1}\frac{p(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}. \tag{3.29}$$

Now let $\psi \in C_0^\infty(0,\infty)$. The identity $p(k^2)\mathcal{S}\mathcal{C}^{-1}kq(k^2)\mathcal{S}\psi = -kq(k^2)\mathcal{C}\mathcal{S}^{-1}p(k^2)\mathcal{S}\psi$ follows from elementary properties of the sine and cosine transforms, and entails that M_1 vanishes identically on the closure of $\mathcal{D} = (p(k^2)^2+k^2q(k^2))^{1/2}\mathcal{S}C_0^\infty(0,\infty)$. For any $\psi \perp \mathcal{D}$, $(p(k^2)^2+k^2q(k^2))^{1/2}\psi$ must be the sine transform of a distribution supported at the origin (cf. Theorem V.11 in [16]) and is therefore an odd polynomial. Thus $\overline{\mathcal{D}}^\perp$ is precisely the space $\mathcal{M}_1$ defined above; M_1 vanishes on $\mathcal{M}_1^\perp$ and $\operatorname{Ran} M_1 \subset \mathcal{M}_1$.

Next, we compute the action of M_1 on $\mathcal{M}_1$. By contour integration,

$$\mathcal{T}^*\frac{kQ(k^2)}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}} = -\left(\frac{\pi}{2}\right)^{1/2}\sum_{\omega\in\Omega}\frac{Q(-\omega^2)\alpha_\omega}{q(-\omega^2)}\xi_\omega(r), \tag{3.30}$$

for polynomials $Q(z)$ such that the operand is in L^2. The standard results

$$(\mathcal{C}\xi_\omega)(k) = -\left(\frac{2}{\pi}\right)^{1/2}\frac{\omega}{\omega^2+k^2}; \qquad (\mathcal{S}\xi_\omega)(k) = \left(\frac{2}{\pi}\right)^{1/2}\frac{k}{\omega^2+k^2} \tag{3.31}$$

entail

$$T\xi_\omega = \left(\frac{2}{\pi}\right)^{1/2}\frac{k}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\frac{p(k^2)-\omega q(k^2)}{\omega^2+k^2}, \tag{3.32}$$

which allows one to read off the action of M_1 as required.

To compute the rank and signature of M_1, we note that the intertwining relations $M_1\mathcal{T} = \mathcal{T}M_2$ and $M_2\mathcal{T}^* = \mathcal{T}^*M_1$ entail that M_1 and M_2 have common spectrum with identical multiplicities, except possibly for unit eigenvalues.[4] It follows that

$$\operatorname{rank} M_1 - \operatorname{rank} M_2 = \operatorname{sig} M_1 - \operatorname{sig} M_2 = \dim\ker\mathcal{T}^* - \dim\ker\mathcal{T}, \tag{3.33}$$

because $\ker\mathcal{T}^*$ and $\ker\mathcal{T}$ are the unit eigenspaces of M_1 and M_2 respectively. It therefore remains to determine the dimensions of the relevant kernels. Firstly, note that (from (3.30)) $\psi = Q(k^2)k(p(k^2)^2+k^2q(k^2)^2)^{-1/2} \in \ker\mathcal{T}^*$ if and only if $\psi \in \mathcal{M}_1$ and $Q(-\omega^2) = 0$ for each $\omega \in \Omega$ (because $\mathcal{M}_1^\perp \subset \ker M_1$, $\mathcal{T}^*$ cannot have kernel in $\mathcal{M}_1^\perp$). Thus $\prod_{\omega\in\Omega}(z+\omega^2)$ divides $Q(z)$ and so

$$\dim\ker\mathcal{T}^* = \min\{\mho - |\Omega|, 0\}. \tag{3.34}$$

Now consider $\ker\mathcal{T}$. We note that

$$q(-\omega_i^2)\mathcal{T}\xi_{\omega_i} = \left(\frac{2}{\pi}\right)^{1/2}\frac{k}{(p(k^2)^2+k^2q(k^2)^2)^{1/2}}\frac{p(k^2)q(-\omega_i^2)-p(-\omega_i^2)q(k^2)}{k^2+\omega_i^2}, \tag{3.35}$$

and apply the following abstract algebraic result, which is proved in the appendix.

[4] This can be viewed as an example of spectral supersymmetry – cf. Theorem 6.3 in [26]

Lemma 3.4 *Let $Q, R \in \mathbb{C}[z]$ be coprime with $\max\{\deg Q, \deg R\} = k \geq 0$, and let $\lambda_1, \ldots, \lambda_m$ be distinct elements of $\mathbb{C}$. Then the polynomials $P_1(z), \ldots P_m(z)$, defined by*

$$(z-\lambda_i)P_i(z) = R(\lambda_i)Q(z) - Q(\lambda_i)R(z) \tag{3.36}$$

span a $\min\{k,m\}$-dimensional subspace of $\mathbb{C}_{k-1}[z]$.

In our application, $m = |\Omega|$ with $\lambda_i = -\omega_i^2$ for each $i = 1, \ldots, m$ and $k = \max\{\deg p, \deg q\} = \mho$. Thus $\dim\mathcal{T}\operatorname{Ran} M_2 = \min\{|\Omega|, \mho\}$ and so

$$\dim\ker\mathcal{T} = \min\{|\Omega| - \mho, 0\}. \tag{3.37}$$

It follows that $\operatorname{rank} M_1 - \operatorname{rank} M_2 = \operatorname{sig} M_1 - \operatorname{sig} M_2 = \mho - |\Omega|$, from which (3.16) and (3.17) follow. ■

4 The GPI Hamiltonian

4.1 Locality and Spectral Properties

The results of the previous two sections allow the construction of a unitary dilation $\hat{\mathcal{T}}$ of the integral transform $\mathcal{T}$. Here, we employ $\hat{\mathcal{T}}$ to define a GPI Hamiltonian consistent with scattering theory (3.1). We denote $\Pi_r = \mathcal{H}_r \oplus \mathcal{M}_1$ and $\Pi_k = \mathcal{H}_k \oplus \mathcal{M}_2$ with J-inner products specified by $J_r = \mathbf{I}_{\mathcal{H}_r} \oplus \operatorname{sgn}(M_1)$, and $J_k = \mathbf{I}_{\mathcal{H}_k} \oplus \operatorname{sgn}(M_2)$. In terms of our general discussion in Section 2.2, we set $A = -d^2/dr^2$ on domain $C_0^\infty(0,\infty)$, and define $\mathcal{T}_+ = \mathcal{S}$, $\mathcal{T}_- = \mathcal{C}$, setting S and C to be multiplication by $\sin\delta_0(k)$ and $\cos\delta_0(k)$ respectively. Thus $A_+ = \mathcal{S}^*k^2\mathcal{S}$, the self-adjoint extension of A with Dirichlet boundary conditions, whilst $A_- = \mathcal{C}^*k^2\mathcal{C}$ is the extension with Neumann boundary conditions. The operators $A_\pm + 1$ both have bounded inverse.

The S-wave GPI Hamiltonian is defined by

$$h_{\text{gpi}} = \hat{\mathcal{T}}^\dagger\begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix}\hat{\mathcal{T}}, \tag{4.1}$$

where Λ is a $\operatorname{sgn}(M_2)$-self-adjoint operator $\Lambda^\dagger = \Lambda$ on $\mathcal{M}_2$. To fix Λ, we impose locality, i.e., that $h_{\text{gpi}}(\psi, 0)^T = (-\psi'', 0)^T$ for all $\psi \in C_0^\infty(0,\infty)$. From Section 2.2, this is possible because $\mathcal{M}_2$ is invariant under A^*: $(-d^2/dr^2|_{C_0^\infty(0,\infty)})^*\xi_\omega = -\omega^2\xi_\omega$. For general $\psi \in \mathcal{M}_2$, we have

$$A^*\psi = -\sum_{\omega\in\Omega}\alpha_\omega\omega^2 \mid \xi_\omega\rangle\langle\xi_{\overline{\omega}} \mid M_2^{-1}\psi\rangle, \tag{4.2}$$

for $\psi \in \mathcal{M}_2$ and it follows immediately from Section 2.2 that

Theorem 4.1 *In the generic case, the unique choice of Λ consistent with locality is*

$$\Lambda = -\left(\operatorname{sgn}(M_2)|M_2|^{1/2}\right)^{-1}\sum_{\omega\in\Omega}\alpha_\omega\omega^2 \mid \xi_\omega\rangle\langle\xi_{\overline{\omega}} \mid |M_2|^{-1/2}. \tag{4.3}$$

We proceed to determine the eigenvectors and eigenvalues of Λ. First note that $\langle \xi_{\overline{\omega_j}} \mid M_2^{-1}\xi_{\omega_i}\rangle = \alpha_{\omega_i}^{-1}\delta_{ij}$, which follows from the identity $\xi_{\omega_i} = \sum \alpha_\omega \mid \xi_\omega\rangle\langle\xi_{\overline{\omega}} \mid M_2^{-1}\xi_{\omega_i}\rangle$ using linear independence of the ξ_ω and non-vanishing of the α_ω. It is then a matter of computation to see that $\varphi_i = \left(\operatorname{sgn}(M_2)|M_2|^{1/2}\right)^{-1}\xi_{\omega_i}$ is an eigenvector of Λ with eigenvalue $-\omega_i^2$ for each $i = 1,\ldots,|\Omega|$. Because Λ has rank $|\Omega|$, this exhausts the discrete spectrum of h_{gpi}. The following is then immediate.

Theorem 4.2 *In the generic case, and with Λ is defined as above, h_{gpi} has the following spectral properties: $\sigma(h_{\text{gpi}}) = \sigma_{\text{ac}}(h_{\text{gpi}}) \cup \sigma_{\text{pp}}(h_{\text{gpi}})$ where $\sigma_{\text{ac}}(h_{\text{gpi}}) = \mathbb{R}^+$ and $\sigma_{\text{pp}}(h_{\text{gpi}})$ consists of the $|\Omega|$ eigenvalues $-\omega_i^2$, whose corresponding eigenvectors are*

$$\psi_i = \hat{\mathcal{T}}^\dagger\varphi_i = \begin{pmatrix} \xi_{\omega_i} \\ \mathcal{T}\left(\operatorname{sgn}(M_2)|M_2|^{1/2}\right)^{-1}\xi_{\omega_i} \end{pmatrix}. \tag{4.4}$$

The absolutely continuous subspace is the Hilbert space $\hat{\mathcal{T}}^\dagger\mathcal{H}_k$.

This bears out our earlier statement that the poles of the scattering amplitude on the physical sheet correspond to the discrete energy spectrum, if locality is imposed.

The physical Hilbert space is required to be a positive definite invariant subspace of Π_r relative to h_{gpi}.[5] In Π_k, we have the $[\cdot,\cdot]_{\Pi_k}$-orthogonal decomposition $\Pi_k = \mathcal{H}_k[+]\mathcal{M}_2$, where $\mathcal{M}_2$ is spanned by the eigenvectors φ_i of Λ. We compute

$$[\varphi_i,\varphi_j]_{\mathcal{M}_2} = \langle \xi_{\omega_i} \mid M_2^{-1}\xi_{\omega_j}\rangle = \begin{cases} 0 & \omega_i \neq \overline{\omega_j} \\ \alpha_{\omega_j}^{-1} & \omega_i = \overline{\omega_j}. \end{cases} \tag{4.5}$$

Hence Π_k is decomposable as $\Pi_k = \mathcal{H}_k[+]E_+[+]E_-[+]H$ where E_+ is the space spanned by the φ_i with $[\varphi_i,\varphi_i]_{\mathcal{M}_2} > 0$ ($\alpha_{\omega_i} > 0$), E_- that spanned by those with $[\varphi_i,\varphi_i]_{\mathcal{M}_2} < 0$ ($\alpha_{\omega_i} < 0$), and H is the *hyperbolic invariant subspace* spanned by those φ_i with $\omega_i \notin \mathbb{R}$. Moreover, this is a decomposition into invariant subspaces, because $D(k^2)$ is dense in $\mathcal{H}_k$. The physical Hilbert space $\mathcal{H}_{\text{phys}}$ is therefore defined by

$$\mathcal{H}_{\text{phys}} = \hat{\mathcal{T}}^\dagger(\mathcal{H}_k[+]E_+). \tag{4.6}$$

We briefly discuss the uniqueness of the GPI Hamiltonian constructed in this way. As noted in Section 2.1, $\hat{\mathcal{T}}$ is unique up to further unitary dilation and unitary equivalence because the M_i are of finite rank. Further dilation merely corresponds to the (trivial) freedom to form the direct sum of h_{gpi} with the Hamiltonian of an arbitrary independent system. On the other hand, replacing $\hat{\mathcal{T}}$ by $(\mathbf{I}\oplus U_2)\mathcal{T}(\mathbf{I}\oplus U_1)$ where U_i is a $\operatorname{sgn} M_i$-unitary operator on $\mathcal{M}_i$ for $i = 1,2$, it is easy to show that the local GPI Hamiltonian h'_{gpi} obtained is given by

$$h'_{\text{gpi}} = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & U_1 \end{pmatrix}^\dagger h_{\text{gpi}} \begin{pmatrix} \mathbf{I} & 0 \\ 0 & U_1 \end{pmatrix}. \tag{4.7}$$

[5] An invariant subspace $\mathcal{L}$ of a J-space $\mathcal{K}$ relative to a linear operator A on $\mathcal{K}$ is a subspace of $\mathcal{K}$ such that $\overline{D(A)\cap\mathcal{L}} = \mathcal{L}$ and $\operatorname{Ran} A|_{\mathcal{L}} \subset \mathcal{L}$, where the closure is taken in the norm topology of $\mathcal{K}$.

We have therefore constructed a family of unitarily equivalent GPI Hamiltonians on Π_r corresponding to the same scattering data. It is clearly sufficient to study h_{gpi} alone in order to determine the domain and scattering properties of h'_{gpi}.

4.2 Domain and Resolvent

We now determine the domain and explicit action of the operator h_{gpi} under the locality assumption. Our result is the following:

Theorem 4.3 *Let $\Theta_0 = (2/\pi)^{1/2}k^{2\mathfrak{U}-1}(p(k^2)^2+k^2q(k^2)^2)^{-1/2}$. Then in the generic case,*

$$\begin{aligned} D(h_{\text{gpi}}) \;=\; \Bigg\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi,\varphi' \in AC_{\text{loc}}(0,\infty);\quad \Phi \in \mathcal{M}_1, \\ \Phi = (\operatorname{sgn} M_1|M_1|^{1/2})^{-1}(\lambda[\varphi]\Theta_0 + \Theta_1), \\ \Theta_1 \in D(k^2)\cap\mathcal{M}_1 \Bigg\}, \end{aligned} \tag{4.8}$$

where

$$\lambda[\varphi] = \begin{cases} P\varphi(0) & \deg p > \deg q \\ P\varphi(0) - Q\varphi'(0) & \deg p = \deg q \\ -Q\varphi'(0) & \deg p < \deg q, \end{cases} \tag{4.9}$$

and P and Q are the leading coefficients of $p(z)$ and $q(z)$ respectively. (In the case $M_1 = 0$, $D(h_{\text{gpi}}) = \{\varphi \mid \varphi,\varphi' \in AC_{\text{loc}}(0,\infty),\ \lambda[\varphi] = 0\}$.) Moreover,

$$h_{\text{gpi}}\begin{pmatrix} \varphi \\ \Phi \end{pmatrix} = \begin{pmatrix} -\varphi'' \\ \tilde{\Phi} \end{pmatrix}, \tag{4.10}$$

where $\tilde{\Phi}$ is given in terms of $\tilde{\Theta} = \operatorname{sgn} M_1|M_1|^{1/2}\tilde{\Phi}$ by

$$\tilde{\Theta} = k^2\Theta_1 + \left(\frac{2}{\pi}\right)^{1/2}\frac{k(\lambda[\varphi]k^{2\mathfrak{U}} - \varphi(0)p(k^2) + \varphi'(0)q(k^2))}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}. \tag{4.11}$$

Proof: From the discussion in Section 2.2, $D(h_{\text{gpi}})$ consists of vectors $(\varphi,\Phi)^T$ with $\varphi \in D((-d^2/dr^2|_{C_0^\infty(0,\infty)})^*)$ and such that

$$\frac{p(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{S}\chi_+ + \frac{kq(k^2)}{(p(k^2)^2 + k^2q(k^2)^2)^{1/2}}\mathcal{C}\chi_- + \Theta \in D(k^2) \tag{4.12}$$

where $\Theta = \operatorname{sgn} M_1|M_1|^{1/2}\Phi$ and χ_+ (χ_-) is the unique element of $\ker(-d^2/dr^2|^*_{C_0^\infty(0,\infty)}+1)$ such that $\varphi+\chi_+$ ($\varphi+\chi_-$) is in the domain of the Laplacian with Dirichlet (Neumann) boundary conditions at the origin. φ and its first derivative are necessarily locally absolutely continuous and so $\chi_\pm$ are easily seen to be

$$\chi_+ = -\varphi(0)e^{-r} \qquad \chi_- = \varphi'(0)e^{-r}. \tag{4.13}$$

Taking sine and cosine transforms as appropriate, equation (4.12) may be re-written as

$$(p(k^2)^2 + k^2 q(k^2)^2)^{-1/2} k \frac{-p(k^2)\varphi(0) + q(k^2)\varphi'(0)}{1+k^2} + \Theta \in D(k^2). \tag{4.14}$$

Θ must therefore be chosen to cancel the leading order behaviour of the first term as $k \to \infty$. Because $\mathcal{M}_1 = \mathbb{C}\Theta_0 + (D(k^2) \cap \mathcal{M}_1)$, this fixes the coefficient of Θ_0 as $\lambda[\varphi]$. However, no other constraints are placed on Θ, and so $\Theta = \lambda[\varphi]\Theta_0 + \Theta_1$, where $\Theta_1 \in D(k^2) \cap \mathcal{M}_1$ (note that this space has dimension $\min\{\mho - 1, 0\}$ and can be trivial).

The statement concerning the action of $h_{\rm gpi}$ follows immediately from the discussion in Section 2.2, and some simple algebra. ∎

The resolvent of $h_{\rm gpi}$ may be written in the form of Krein's formula as

$$(h_{\rm gpi} - z)^{-1} = \begin{pmatrix} R_0(z) & 0 \\ 0 & R_1(z) \end{pmatrix} + \frac{q(z)}{p(z) + (-z)^{1/2} q(z)} F(z) F(\overline{z})^\dagger. \tag{4.15}$$

Here, $R_0(z) = \mathcal{S}^{-1}(k^2 - z)^{-1}\mathcal{S}$ is the free resolvent and the defect element $F(z) \in \Pi_r$ is given by

$$F(z) = \begin{pmatrix} e^{-(-z)^{1/2} r} \\ (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \Psi(z) \end{pmatrix}, \tag{4.16}$$

where $\Psi(z) \in \mathcal{M}_1$ is

$$\Psi(z) = \left(\frac{2}{\pi}\right)^{1/2} \frac{k(p(k^2)q(z) - p(z)q(k^2))}{(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}, \tag{4.17}$$

and the operator $R_1(z)$ is defined on $\mathcal{M}_1$ by

$$\begin{aligned} R_1(z)\Phi &= (\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \frac{1}{k^2 - z} \Big\{ \operatorname{sgn} M_1 |M_1|^{1/2} \Phi \\ &\quad + \left(\frac{2}{\pi}\right)^{1/2} \frac{kq(k^2)}{(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}} [(\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \Psi(\overline{z}), \Phi]_{\mathcal{M}_1} \Big\} \end{aligned} \tag{4.18}$$

Exploiting the decomposition $\mathcal{H}_r = \overline{\operatorname{Ran}(-d^2/dr^2 - z)|_{C_0^\infty(0,\infty)}} \oplus \mathbb{C} e^{-(-\overline{z})^{1/2} r}$, it is a matter of computation to show that (4.15) holds for vectors of form $(\varphi, 0)^T$ with $\varphi \in \mathcal{H}_r$. Next, for $\Phi \in \mathcal{M}_1$ such that

$$\Theta = \operatorname{sgn} M_1 |M_1|^{1/2} \Phi = \left(\frac{2}{\pi}\right)^{1/2} \frac{kQ(k^2)}{(p(k^2)^2 + k^2 q(k^2)^2)^{1/2}}, \tag{4.19}$$

we claim that $[(\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \Psi(\overline{z}), \Phi]_{\mathcal{M}_1} = -Q(z)/q(z)$. Comparing with Theorem 4.3, this entails that (4.15) holds for $(0, \Phi)^T$ if $Q(z) = 0$. Finally, one may verify that (4.15) holds in the case $Q(k^2) \equiv 1$, and therefore on the whole of Π_r. It remains to establish the formula $[(\operatorname{sgn} M_1 |M_1|^{1/2})^{-1} \Psi(\overline{z}), \Phi]_{\mathcal{M}_1} = -Q(z)/q(z)$ employed above.

The RHS is equal to $\langle \mathcal{T}^* q(\overline{z}) \Psi(\overline{z}) \mid M_2^{-1} \mathcal{T}^* \Theta \rangle + \langle q(\overline{z}) \Psi(\overline{z}) \mid \Theta \rangle$. Using the identity $\langle \xi_{\overline{\omega_j}} \mid M_2^{-1} \xi_{\omega_i} \rangle = \alpha_{\omega_i}^{-1} \delta_{ij}$ and the results of Section 3, the first term is

$$\langle \mathcal{T}^* q(\overline{z}) \Psi(\overline{z}) \mid M_2^{-1} \mathcal{T}^* \Theta \rangle = \sum_{\omega \in \Omega} \frac{p(z) - \omega q(z)}{q(-\omega^2)(\omega^2 + z)} Q(-\omega^2) \alpha_\omega. \tag{4.20}$$

Moreover, the second term may be written

$$\begin{aligned} \langle q(\overline{z}) \Psi(\overline{z}) \mid \Theta \rangle &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{ikQ(k^2)(p(z) - ikq(z))}{(k^2 - z)(p(k^2) - ikq(k^2))} \\ &= -Q(z) - \sum_{\omega \in \Omega} \frac{p(z) - \omega q(z)}{q(-\omega^2)(\omega^2 + z)} Q(-\omega^2) \alpha_\omega \end{aligned} \tag{4.21}$$

and the required result follows.

4.3 Scattering Theory

In this section, we construct Møller wave operators for $h_{\rm gpi}$ relative to the free Hamiltonian $h_0 = \mathcal{S} k^2 \mathcal{S}$ on $\mathcal{H}_r$ in order to check that $h_{\rm gpi}$ actually exhibits the required scattering behaviour. Because scattering is a function of the continuous spectrum only, our results in this section are actually independent of the precise form of Λ, and therefore of the locality requirement.

We work in the S-wave, and employ a two space setting: let B be self-adjoint on $\mathcal{H}_1$, A be self-adjoint on $\mathcal{H}_2$ and $\mathcal{J}$ be a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_2$. Then the Møller operators $\Omega^\pm(A, B; \mathcal{J})$ are defined by

$$\Omega^\pm(A, B; \mathcal{J}) = \lim_{t \to \mp\infty} e^{iAt} \mathcal{J} e^{-iBt} P_{\rm ac}(B), \tag{4.22}$$

and are said to be complete if the closure of $\operatorname{Ran}\Omega^\pm(A, B; \mathcal{J})$ is equal to $\operatorname{Ran} P_{\rm ac} A$.

In the following, $\mathcal{J}_r$ and $\mathcal{J}_k$ are the natural embeddings of $\mathcal{H}_r$ and $\mathcal{H}_k$ into Π_r and Π_k respectively.

Theorem 4.4 *Let $\mathcal{J} : \mathcal{H}_r \to \Pi_r$ be given by $\mathcal{J} = \hat{\mathcal{T}}^\dagger \mathcal{J}_k \mathcal{T}$. Then $\Omega^\pm(h_{\rm gpi}, h_0; \mathcal{J})$ exist, are complete, and given by*

$$\Omega^\pm(h_{\rm gpi}, h_0; \mathcal{J}) = \hat{\mathcal{T}}^\dagger \mathcal{J}_k e^{\pm i\delta_0(k)} \mathcal{S}, \tag{4.23}$$

where $\delta_0(k)$ is given by (3.1).

Proof: Writing U_t for multiplication by $e^{-ik^2 t}$ on $\mathcal{H}_k$, we have

$$\begin{aligned} e^{ih_{\rm gpi} t} \mathcal{J} e^{-ih_0 t} P_{\rm ac}(h_0) &= \hat{\mathcal{T}}^\dagger \begin{pmatrix} U_{-t} & 0 \\ 0 & \exp i\Lambda t \end{pmatrix} \hat{\mathcal{T}} \mathcal{J} \mathcal{S}^{-1} U_t \mathcal{S} \\ &= \hat{\mathcal{T}}^\dagger \mathcal{J}_k U_{-t} \mathcal{T} \mathcal{S}^{-1} U_t \mathcal{S}. \end{aligned} \tag{4.24}$$

Now, for any $u(k) \in C_0^\infty(0,\infty)$,

$$\begin{aligned} \|U_{-t}\mathcal{T}\mathcal{S}^{-1}U_t u(k) - e^{\pm i\delta_0(k)}u(k)\|^2 &= \|\sin\delta_0(k)\mathcal{C}(\mathcal{C}^{-1} \pm i\mathcal{S}^{-1})U_t u(k)\|^2 \\ &\leq \frac{2}{\pi}\int_0^\infty dr \left|\int_0^\infty dk e^{i(\pm kr - k^2 t)}u(k)\right|^2, \end{aligned} \tag{4.25}$$

which vanishes as $t \to \mp\infty$ by (non)-stationary phase arguments (see the Corollary to Theorem XI.14 in [18]) and we deduce that $U_{-t}\mathcal{T}\mathcal{S}^{-1}U_t \to e^{\pm i\delta_0(k)}$ in this limit. The existence and form of the Møller operators are then immediate. One easily checks that they are unitary maps from $\mathcal{H}_r$ to $P_{ac}(h_{gpi}) = \hat{\mathcal{T}}^\dagger \mathcal{J}_k \mathcal{H}_k$, thus verifying completeness. ■

We conclude that our construction does indeed yield the required scattering theory, and also that – as a by-product of the construction – complete Møller operators may easily and explicitly be determined.

5 Examples

As an application, we construct the class of GPI models with scattering data

$$\cot\delta_0(k) = -\frac{1}{kL} + kM, \tag{5.1}$$

where L the scattering length, and M is twice the effective range. These models therefore represent the effective range approximation to the behaviour of a non-point interaction in the S-wave. This class of models has been partially studied by Shondin [7], who considered the case $M < 0$ ('models of type B_2') using an auxiliary space method. This case appears as a special case of the models considered by Pavlov in [4]. (We also note that van Diejen and Tip [9] have constructed models of type $\cot\delta_0(k) = (ak+bk^3+ck^5)^{-1}$ using the distributional method.)

The case $M > 0$ does not appear to have been treated before. In fact, this case can be obtained by an *ad hoc* modification of the methods of [7], and it may therefore seem that the general methods described above do not add significantly to this model. However, our methods construct the Hamiltonian without the need to specify an auxiliary space *a priori*; in addition, we construct not just the Hamiltonian, but also its spectral representation as an eigenfunction expansion. Moreover, the spectral theory, scattering behaviour and domain can all be read off easily from the results of Section 4. We also note that the auxiliary space $\mathcal{M}_1$ is one dimensional, whereas the distributional method always results in an even dimensional auxiliary space; thus it is not immediately apparent how the models constructed here can arise in the distributional formalism.

The above class of GPI models contains two interesting sub-families: the ordinary point interactions ($M = 0$) and also the resonance point interactions arising formally by setting $L = \infty$, i.e. $\cot\delta_0(k) = kM$ with $M \in \mathbb{R} \cup \{\infty\}$. Such models are required in situations where the scattering length is generically forced to be infinite, e.g. in certain systems of supersymmetric quantum mechanics.

We begin by briefly treating the point interactions, both for completeness and also to demonstrate how this class arises in our formalism. We then turn to the general case, obtaining RPI models in the limit $L \to -\infty$.

5.1 Point Interactions

The required integral transform is

$$\mathcal{T} = (1+(kL)^2)^{-1/2}\mathcal{S} - kL(1+(kL)^2)^{-1/2}\mathcal{C}. \tag{5.2}$$

In the cases $L = 0, \infty$, $\mathcal{T}$ reduces to $\mathcal{S}$ and $\mathcal{C}$ respectively, and the Hamiltonian is given immediately by $\mathcal{T}^* k^2 \mathcal{T}$. We exclude these cases from the rest of our discussion.

We therefore apply the construction of Section 3, with $p(z) \equiv -L^{-1}$ and $q(z) \equiv 1$. We find that $\mho = 0$, so $M_1 = 0$ (i.e. $\mathcal{T}\mathcal{T}^* = \mathbf{I}$). Straightforward application of Proposition 3.1 yields

$$M_2 = \begin{cases} |\chi_L\rangle\langle\chi_L| & L > 0 \\ 0 & L < 0, \end{cases} \tag{5.3}$$

where $\chi_L(r) = (2/L)^{1/2}e^{-r/L}$ is normalised to unity. Hence if $L < 0$, $\mathcal{T}$ is unitary and the Hamiltonian is $h_L = \mathcal{T}^* k^2 \mathcal{T}$, with purely absolutely continuous spectrum $\mathbb{R}^+$. In the case $L > 0$, the momentum Hilbert space is extended to $\mathcal{H}_k \oplus \mathbf{C}$, representing a single bound state, and the unitary dilation $\hat{\mathcal{T}} : \mathcal{H}_r \to \mathcal{H}_k \oplus \mathbf{C}$ takes form

$$\hat{\mathcal{T}} = \begin{pmatrix} \mathcal{T} \\ \langle\chi_L| \end{pmatrix}; \qquad \hat{\mathcal{T}}^* = \begin{pmatrix} \mathcal{T}^* & |\chi_L\rangle \end{pmatrix}. \tag{5.4}$$

($\mathcal{H}_k \oplus \mathbf{C}$ has the obvious inner product.) The Hamiltonian is

$$h_L = \hat{\mathcal{T}}^{-1}\begin{pmatrix} k^2 & 0 \\ 0 & \lambda \end{pmatrix}\hat{\mathcal{T}} = \mathcal{T}^* k^2 \mathcal{T} + \lambda\,|\chi_L\rangle\langle\chi_L|, \tag{5.5}$$

and the locality requirement fixes $\lambda = -L^{-2}$, which is, of course, the usual value. Finally, the domain of h_L is given by Theorem 4.3 as the space of φ with $\varphi, \varphi' \in AC_{loc}(0,\infty)$ and $\lambda_{0,1}[\varphi] = 0$, i.e. the well known boundary condition

$$\varphi(0) + L\varphi'(0) = 0. \tag{5.6}$$

To summarise, all the well known properties of point interactions may be derived within our formalism.

5.2 Effective Range Approximation

In this section, we maintain $M \neq 0$, $L \neq 0$, setting $p(z) = -L^{-1} + zM$ and $q(z) \equiv 1$. We find

$$\mho = 1; \qquad |\Omega| = \begin{cases} 1 + \frac{1}{2}(\operatorname{sgn} M + \operatorname{sgn} L) & L \neq \infty \\ \frac{1}{2}(1 + \operatorname{sgn} M) & L = \infty. \end{cases} \tag{5.7}$$

Note that the $L = \infty$ case (RPI models) is included in the general formula if one regards this as the limit $L \to -\infty$. Writing $W(z) = -M(z-\omega_1)(z-\omega_2)$, Ω is the subset of $\{\omega_1, \omega_2\}$ lying in the left-hand half-plane, and we have $\omega_1+\omega_2 = -M^{-1}$, $\omega_1\omega_2 = (ML)^{-1}$. The residues α_ω are

$$\alpha_{\omega_1} = -\frac{2\omega_1}{M(\omega_1-\omega_2)}, \qquad \alpha_{\omega_2} = \frac{2\omega_2}{M(\omega_1-\omega_2)}. \tag{5.8}$$

The space $\mathcal{M}_1 = \operatorname{Ran} M_1$ is equal to $\mathbf{C} \mid \eta\rangle$, where

$$\eta(k) = \mathcal{N}\frac{k}{(k^2+(k^2M-L^{-1})^2)^{1/2}}, \tag{5.9}$$

and the normalisation constant is

$$\mathcal{N} = \begin{cases} (2|M|/\pi)^{1/2} & ML > 0 \\ (2|M|/\pi)^{1/2}(1-4ML^{-1})^{1/4} & ML < 0. \end{cases} \tag{5.10}$$

Using Proposition 3.2, we obtain

$$M_1 = \lambda \mid \eta\rangle\langle\eta \mid; \qquad \lambda = \begin{cases} +1 & M<0, L<0 \\ -\operatorname{sgn} M(1-4ML^{-1})^{-1/2} & ML<0 \\ -1 & M>0, L>0, \end{cases} \tag{5.11}$$

which reduces in the limit $L \to -\infty$ to $\lambda = -\operatorname{sgn} M$.

We now distinguish three cases, corresponding to $|\Omega| = 0, 1, 2$.

Case (i) $|\Omega| = 0$ $(L, M < 0)$.

We have $M_1 = \mid \eta\rangle\langle\eta \mid$ and $M_2 = 0$. Hence $\mathcal{H}_k$ is not extended, but $\mathcal{H}_r$ is extended to $\mathcal{H}_r \oplus \mathcal{M}_1$. Writing Φ for the component of η in $\mathcal{M}_1$, we regard this as $\mathcal{H}_r \oplus \mathbf{C}$ with inner product $\langle(\varphi,\Phi)^T \mid (\psi,\Psi)^T\rangle = \langle\varphi \mid \psi\rangle_{L^2} + \overline{\Phi}\Psi$. The dilation $\hat{\mathcal{T}}$ given by

$$\hat{\mathcal{T}} = \begin{pmatrix} \mathcal{T} & -\mid\eta\rangle \end{pmatrix}; \qquad \hat{\mathcal{T}}^* = \begin{pmatrix} \mathcal{T} \\ -\langle\eta\mid \end{pmatrix} \tag{5.12}$$

is a unitary $\hat{\mathcal{T}} : \mathcal{H}_r \oplus \mathbf{C} \to \mathcal{H}_k$, and the Hamiltonian is $h_{L,M} = \hat{\mathcal{T}}^* k^2 \hat{\mathcal{T}}$.

In the limit $L \to -\infty$, we arrive at the RPI models for $M < 0$, which take the above form with η replaced by its limit $\eta \to \psi_M(k) = (2|M|/\pi)^{1/2}(1+(kM)^2)^{-1/2}$. (This conclusion can also be reached by direct computation.)

Case (ii) $|\Omega| = 1$ $(\operatorname{sgn} L = -\operatorname{sgn} M)$.

Without loss, we take $\operatorname{Re}\omega_1 < 0$, so $\Omega = \{\omega_1\}$ and

$$\omega_1 = \frac{1+\operatorname{sgn} M(1-4ML^{-1})^{1/2}}{-2M}. \tag{5.13}$$

Because the eigenvalue of M_1 is not unity, M_2 must also have eigenvalue $-\operatorname{sgn} M(1-4ML^{-1})^{-1/2}$, with normalised eigenvector $\chi(r) = (-2\omega_1)^{-1/2}e^{\omega_1 r}$. Hence

$$M_2 = -\operatorname{sgn} M(1-4ML^{-1})^{-1/2} \mid \chi\rangle\langle\chi \mid . \tag{5.14}$$

The extended inner product spaces are $\mathcal{H}_r \oplus \mathbf{C}$ and $\mathcal{H}_k \oplus \mathbf{C}$, with J-inner product specified by $J_r = \mathbf{I}_{\mathcal{H}_r} \oplus (-\operatorname{sgn} M)$, $J_k = \mathbf{I}_{\mathcal{H}_k} \oplus (-\operatorname{sgn} M)$. (If $M < 0$, these are positive definite inner products). The unitary dilation has matrix form

$$\begin{aligned} \hat{\mathcal{T}} &= \begin{pmatrix} \mathcal{T} & \operatorname{sgn} M(1-4ML^{-1})^{-1/4} \mid \eta\rangle \\ (1-4ML^{-1})^{-1/4}\langle\chi \mid & (1+\operatorname{sgn} M(1-4ML^{-1})^{-1/2})^{1/2} \end{pmatrix} \\ \hat{\mathcal{T}}^\dagger &= \begin{pmatrix} \mathcal{T}^* & -\operatorname{sgn} M(1-4ML^{-1})^{-1/4} \mid \chi\rangle \\ -(1-4ML^{-1})^{-1/4}\langle\eta \mid & (1+\operatorname{sgn} M(1-4ML^{-1})^{-1/2})^{1/2} \end{pmatrix}, \end{aligned} \tag{5.15}$$

and the Hamiltonian is

$$h_{L,M} = \hat{\mathcal{T}}^\dagger \begin{pmatrix} k^2 & 0 \\ 0 & -\omega_1^2 \end{pmatrix} \hat{\mathcal{T}}, \tag{5.16}$$

where the eigenvalue has been fixed in accordance with locality.

In the limit $L \to -\infty$, we arrive at the RPI models for $M > 0$, which take the above form with η replaced by ψ_M, and χ replaced by χ_M. Again, this case can be computed directly.

Case (iii) $|\Omega| = 2$ $(M, L > 0)$.

In this case, either both ω_i are real and negative, or they form a complex conjugate pair with negative real part. Initially, we restrict to generic case, in which $\omega_1 \neq \omega_2$ (i.e., $L \neq 4M$). By Proposition 3.1,

$$M_2 = -\frac{2}{M(\omega_1-\omega_2)}\{\omega_1 \mid \xi_{\omega_1}\rangle\langle\xi_{\omega_1} \mid -\omega_2 \mid \xi_{\omega_2}\rangle\langle\xi_{\omega_2} \mid\}, \tag{5.17}$$

which has eigenvalues ± 1 with orthonormal eigenfunctions $\mid \chi_\pm\rangle$ given by

$$\mid \chi_+\rangle = \left(\frac{2}{L}\right)^{1/2} \frac{\mid \xi_{\omega_1}\rangle - \mid \xi_{\omega_2}\rangle}{\omega_1-\omega_2} \tag{5.18}$$

$$\mid \chi_-\rangle = \left(\frac{2}{M}\right)^{1/2} \frac{\omega_1 \mid \xi_{\omega_1}\rangle - \omega_2 \mid \xi_{\omega_2}\rangle}{\omega_1-\omega_2}. \tag{5.19}$$

Using $\chi_\pm$ as a basis for $\mathcal{M}_2$, we write $(\Phi_+, \Phi_-)^T$ for $\Phi = \Phi_+ \mid \chi_+\rangle + \Phi_- \mid \chi_-\rangle \in \mathcal{M}_2$. The extended momentum inner product space is $\Pi_k = \mathcal{H}_k \oplus \mathbf{C}^2$, with inner product $[(\varphi,\Phi)^T, (\psi,\Psi)^T] = \langle\varphi \mid \psi\rangle_{L^2} + \overline{\Phi_+}\Psi_+ - \overline{\Phi_-}\Psi_-$.

$\mathcal{H}_r$ is extended to $\mathcal{H}_r \oplus \mathbf{C}$ with J-inner product given by $\mathbf{I}_{\mathcal{H}_r} \oplus -1$. The unitary dilation $\hat{\mathcal{T}} : \mathcal{H}_r \oplus \mathbf{C} \to \mathcal{H}_k \oplus \mathbf{C}^2$ is

$$\hat{\mathcal{T}} = \begin{pmatrix} T & \mid\eta\rangle \\ \langle\chi_+\mid & 0 \\ \langle\chi_-\mid & \sqrt{2} \end{pmatrix}; \qquad \hat{\mathcal{T}}^\dagger = \begin{pmatrix} T^* & \mid\chi_+\rangle & -\mid\chi_-\rangle \\ -\langle\eta\mid & 0 & \sqrt{2} \end{pmatrix}. \tag{5.20}$$

Finally, the Hamiltonian is

$$h_{L,M} = \hat{\mathcal{T}}^{\dagger} \begin{pmatrix} k^2 & 0 \\ 0 & \Lambda \end{pmatrix} \hat{\mathcal{T}}, \tag{5.21}$$

where Λ is a 2×2 matrix. Locality requires

$$\Lambda = \begin{pmatrix} (ML)^{-1} & M^{-3/2}L^{-1/2} \\ -M^{-3/2}L^{-1/2} & M^{-1}(L^{-1} - M^{-1}) \end{pmatrix}, \tag{5.22}$$

as may be shown by a short computation.

Turning briefly to the degenerate case where $L = 4M > 0$, it is easy to see that M_1 and M_2 change continuously as L and M vary (maintaining $L, M > 0$). The degenerate case can then be obtained as a limit, with $\chi_{\pm}$ taking their limiting forms

$$\chi_+(r) = \left(\frac{2}{L}\right)^{1/2} r e^{-r/2M}; \qquad \chi_-(r) = \left(\frac{2}{M}\right)^{1/2} \left(1 - \frac{r}{2M}\right) e^{-r/2M}. \tag{5.23}$$

In all generic cases, the domain of $h_{L,M}$ may be read off from Theorem 4.3:

$$D(h_{L,M}) = \left\{ \begin{pmatrix} \varphi \\ \Phi \end{pmatrix} \mid \varphi, \varphi' \in AC_{\mathrm{loc}}(0,\infty), \quad \Phi = -|M|^{1/2}\varphi(0) \right\}, \tag{5.24}$$

and the action is given by

$$h_{L,M} \begin{pmatrix} \varphi \\ -|M|^{1/2}\varphi(0) \end{pmatrix} = \begin{pmatrix} -\varphi'' \\ -\operatorname{sgn} M |M|^{-1/2}(\varphi'(0) + L^{-1}\varphi(0)) \end{pmatrix}. \tag{5.25}$$

The domain and action of RPI models correspond to the $L \to -\infty$ limit of the above, and the non-generic case by taking the limit $L \to 4M$.

5.3 Physical Interpretation

In this section, we discuss how the effective range models constructed above may be used to model Schrödinger operators $H = -\Delta + V$, where V is smooth, spherically symmetric and compactly supported within radius a of the origin. Our methodology is analagous to that developed in [13], in which the scattering length approximation is discussed. Namely, we give *fitting formulae* for selecting the 'best fit' model for a given Hamiltonian. The range of energies for which the approximation is valid can be determined by a 'believability' analysis analagous to that developed in [13]. We will not do this here.

The fitting formulae are based on the following idea: given a potential $V(r)$ supported within radius a of the origin, one solves the zero energy Schrödinger equation $-u_0'' + Vu_0 = 0$ with regular boundary conditions at the origin. The low energy parameters L and M are given in terms of $u_0(r)$ (using the arguments of Section 11.2 of [15]) by

$$L = a - \left.\frac{u_0}{u_0'}\right|_{r=a}, \tag{5.26}$$

and

$$M = a\left\{1 - \frac{a}{L} + \frac{1}{3}\left(\frac{a}{L}\right)^2 - \left(1 - \frac{a}{L}\right)^2 \frac{\int_0^a |u_0(r)|^2 dr}{a|u_0(a)|^2}\right\}. \tag{5.27}$$

Thus the scattering behaviour is $\cot\delta_0(k) = -(kL)^{-1} + kM + O(k^3)$ and the best fit GPI model in our class is $h_{L,M}$. Equations (5.26) and (5.27) are called the fitting formulae; (5.26) is the fitting formula used in [13].

Note that M obeys the bound

$$-\infty \le M < a\left\{1 - \frac{a}{L} + \frac{1}{3}\left(\frac{a}{L}\right)^2\right\}. \tag{5.28}$$

Moreover, this bound is best possible: for any $L \in \mathbb{R} \cup \{\infty\}$ and any M in the above range, one can clearly find a smooth function $u_0(r)$ satisfying regular boundary conditions at the origin, $u_0 \propto (1 - r/L)$ for $r > a$ and such that (5.27) holds. Then the potential defined by $V(r) = u_0''(r)/u_0(r)$ has S-wave scattering behaviour approximated at second order by $h_{L,M}$. The contribution to the total scattering cross section from the effective range term generally outweighs that from higher angular momenta, so the S-wave GPI model provides a second order approximation to the full scattering behaviour.

We note that M becomes increasingly negative as u_0 becomes more strongly peaked within the region $r < a$. Intuitively, it is this peaking which corresponds to the 'extra probability' stored in the Hilbert space extension to $\mathcal{H}_r$ in the case $M < 0$. On the other hand, if one interprets $h_{L,M}$ as corresponding to a zero radius potential, for $M > 0$, we would require $\int_0^a |u_0(r)|^2 dr < 0$, so the introduction of negative normed states is quite natural. Heuristically, therefore, one can understand why different parameter ranges for M require dilations to Hilbert or Pontryagin spaces.

Finally, we discuss the interpretation of the discrete spectrum of $h_{L,M}$. We have constructed $h_{L,M}$ so that its scattering behaviour matches that of a given Schrödinger operator at low energies. At higher energies, the approximation breaks down – in the language of [13], we say that it is no longer 'believable'. Thus, deeply bound states are unlikely to be believable. In particular, for $0 < L < 4M$, $h_{L,M}$ exhibits a complex conjugate pair of eigenvalues, which can never be believable.[6] Such phenomena are artifacts of the idealisation process, due to the truncation of the low energy expansion. The issue of believability is discussed in more detail in [13]; similar comments are made in [9].

[6] These are not eigenvalues of $h_{L,M}$ restricted to the physical Hilbert space. However, they persist as poles in the scattering amplitude and our remarks still apply: $h_{L,M}$ does not give a reliable approximation to the scattering theory at those scales.

6 Conclusion

We begin by discussing various generalisations of our method. There are many situations in which the analysis of Section 2.2 may be applied. In two dimensions, for example, one can consider radial GPI Hamiltonians which agree with

$$h = -\frac{1}{r}\frac{d}{dr}r\frac{d}{dr} + \frac{\nu^2}{r^2} \tag{6.1}$$

away from the origin, as models for an infinitesimal 'dot' of magnetic flux ν, with $|\nu| < 1$. For $\nu \neq 0$, naïve generalised eigenfunctions may be constructed from a given scattering behaviour as linear combinations of Bessel functions J_ν and $J_{-\nu}$ (or J_0 and N_0 if $\nu = 0$) and the linear transformation $\mathcal{T}$ is expressed in terms of the corresponding Hankel transforms. In [12] we pursue this line in order to construct RPI type models for the Dirac equation in the presence of an infinitesimal line of flux. These models yield the leading order approximation to the scattering in this case.

Our method could also be applied to S-wave GPI models with a Coulombic tail. In this case, the appropriate integral transforms would be based upon Whittaker functions and the scattering data would be specified in terms of Coulomb-modified partial wave shifts. In this case, the dimension of $\mathcal{M}_2$ would be countably infinite, due to the countable discrete spectrum of such models. However, one would expect $\mathcal{M}_1$ to remain finite dimensional for simple models.

Secondly, it is of interest to generalise the unitary dilation method to sectors of higher angular momentum with $\ell \geq 1$ (and the corresponding analogues for magnetic flux dots - i.e. $|\nu| \geq 1$ - and Coulombic GPI for $\ell \geq 1$). This is more problematic, because the radial Hamiltonian $-d^2/dr^2 + \ell(\ell+1)/r^2$ is essentially self-adjoint on $C_0^\infty(0,\infty)$ and so the method of Section 2.2 does not apply. Put another way, the spherical Bessel functions $n_\ell(x)$ are too singular at $x = 0$ to form the kernel of a unitary integral transform for $\ell \geq 1$. However, by subtracting functions whose small x divergences cancel those of $n_\ell(x)$, but which decay sufficiently fast at large x (e.g. exponentially) to leave the asymptotic behaviour of the generalised eigenfunctions unaltered, it may be possible to define a 'mutilated' Hankel transform to which our method might be applied. The grounds for our optimism are as follows: it is usual for GPI Hamiltonians to admit eigenfunction expansion, and one can regard the mapping to this spectral representation as a unitary dilation of its 'compression' to a mapping from $\mathcal{H}_r$ to $\mathcal{H}_k$. Thus the fact that the distributional method can generate GPI models for $\ell \geq 1$ suggests that unitary dilation methods can also be applied in this context. It is hoped to return to this elsewhere.

Finally, we consider applications to the definition of arrays of point scatterers. Here, the most likely use of our methods is to generate the 'monomer' by inverse scattering. By passing to the resolvent written in the form of Krein's formula, one can isolate the appropriate 'defect element' and proceed to form the array by methods discussed in [9], which generalise the procedure for arrays of PI developed in [27].

To summarise, we have introduced an inverse scattering construction for GPI models using the theory of unitary dilations, and developed the method in detail for the

class of single centre S-wave GPI models with rational S-matrices. A physical locality requirement completes the specification of the Hamiltonian, whose scattering, spectral and domain properties are explicitly determined from our results.

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Appendix

The following abstract result appears to be new. Although we prove it for polynomials over $\mathbb{C}$, the statement and proof generalise immediately to any field F. I thank Clive Wells for useful discussions concerning this result and for supplying an alternative proof.

Lemma 3.4 *Let $Q, R \in \mathbb{C}[z]$ be coprime with $\max\{\deg Q, \deg R\} = k \geq 0$, and let $\lambda_1, \ldots, \lambda_m$ be distinct elements of $\mathbb{C}$. Then the polynomials $P_1(z), \ldots P_m(z)$, defined by*

$$(z - \lambda_i)P_i(z) = R(\lambda_i)Q(z) - Q(\lambda_i)R(z) \tag{A.1}$$

span a $\min\{k, m\}$-dimensional subspace of $\mathbb{C}_{k-1}[z]$.

Proof: First consider the case where Q and R are coprime. Clearly the P_i span a subspace of $\mathbb{C}_{k-1}[z]$ of dimension at most $n = \min\{k, m\}$. It is enough to show that $P_1, \ldots, P_n$ are linearly independent. Assuming without loss of generality that $\deg Q = k$, we define $\tilde{Q}_i(z) = (Q(z) - Q(\lambda_i))/(z - \lambda_i)$ and $\tilde{R}_i(z) = (R(z) - R(\lambda_i))/(z - \lambda_i)$. By determining the coefficients of P in terms of those of Q and the λ_i, one may easily check that $\sum_{i=1}^n \alpha_i \tilde{Q}_i(z) = 0$ for some $\underline{\alpha} = (\alpha_1, \ldots, \alpha_n)^T \in \mathbb{C}^n$ if and only if $V\underline{\alpha} = 0$, where V is the $n \times n$ Vandermonde matrix [25] with components $V_{ij} = \lambda_j^{i-1}$. But V is non-singular, because the λ_i are distinct. Thus $\tilde{Q}_1(z), \ldots, \tilde{Q}_n(z)$ are linearly independent over $\mathbb{C}$.

Now note that $P_i(z) = R(z)\tilde{Q}_i(z) - Q(z)\tilde{R}_i(z)$. If the $P_1, \ldots, P_n$ are linearly dependent, there exists $0 \neq \underline{\alpha} = (\alpha_1, \ldots, \alpha_n)^T \in \mathbb{C}^n$ such that $R(z)S(z) = Q(z)T(z)$ where $S(z) = \sum_i \alpha_i \tilde{Q}_i(z)$ and $T(z) = \sum_i \alpha_i \tilde{R}_i(z)$. $S(z) \not\equiv 0$ because the $\tilde{Q}_i(z)$ are linearly independent. Hence Q and R possess a common factor (for Q does not divide S, nor does R divide T, because $\deg S < \deg Q$ and $\deg T < \deg R$) and we obtain a contradiction. Hence $P_1, \ldots, P_n$ are linearly independent over $\mathbb{C}$. ∎

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