Resonance Point Interactions

C.J. Fewster

Department of Applied Mathematics and Theoretical Physics,
University of Cambridge,
Silver Street, Cambridge CB3 9EW, U.K.

February 10, 2022

Abstract

A new construction is presented for point interactions (PI) and generalised point interactions (GPI). The construction is an inverse scattering procedure, using integral transforms suggested by the required scattering theory. The usual class of PI in 3 dimensions (i.e. the self adjoint extensions of the Laplacian on the domain of smooth functions compactly supported away from the origin) is reconstructed. In addition a 1-parameter family of GPI models termed resonance point interactions (RPI) is constructed, labelled by $M$. The case $M < 0$ coincides with a special case of a known GPI model; the case $M > 0$ appears to be new. In both cases, the Hilbert space of states must be extended, for $M < 0$, a larger Hilbert space is required, whilst for $M > 0$, the Hilbert space is extended to a Pontryagin space. In the latter case, the space of physical states is identified as a positive definite invariant subspace. Complete Møller wave operators are constructed for the models considered, using a two space formalism where necessary, which confirm that the PI and RPI models exhibit the required scattering theory. The physical interpretation of RPI as models for quantum mechanical systems exhibiting zero energy resonances is described.

*E-mail address: C.J.Fewster@amtp.cam.ac.uk
1 Introduction and Main Ideas

Point interactions (PI) have long been of interest as solvable models in quantum mechanics (see [13] for an extensive bibliography). Heuristically, they represent Hamiltonians with $\delta$-function potentials “$H = -\Delta + \lambda \delta(x)$”, although it is well known that such Hamiltonians fail to make rigorous sense in dimensions $d \geq 2$. Instead, a point interaction situated at the origin is rigorously defined as one of the self-adjoint extensions of the Laplacian on $C_0^\infty(\mathbb{R}^d \setminus \{0\})$, i.e. smooth functions compactly supported away from the origin. One of the most useful features of PI is that they represent a leading order approximation to the scattering theory of non-point interactions. For example, in 3 dimensions, the low energy expansion of the $S$-wave partial wave shift $\delta_0(k)$ [14] is

$$\cot \delta_0(k) = -\frac{1}{kL} + r_0k + O(k^3), \quad (1.1)$$

where $L$ and $r_0$ are the $S$-wave scattering length and effective range respectively, and the expansion is valid for spherically symmetric potentials decaying at least exponentially at infinity, and for $L \neq 0, \infty$. In $d = 3$, there is a 1-parameter family of PI, which may be labelled $\{H_L \mid L \in \mathbb{R} \cup \{\infty\}\}$, whose scattering theory is non-trivial only in the $S$-wave, where it is given by

$$\cot \delta_0(k) = -\frac{1}{kL}; \quad (1.2)$$

thus approximating (1.1) at leading order.

The PI described so far suffer from various limitations. Firstly, as noted for example by Grossmann and Wu [8], they are restricted only to dimensions $d \leq 3$, because $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d \setminus \{0\})$ in dimensions 4 and higher. Secondly, for $d = 2, 3$, they yield non-trivial scattering only in the sector of zero angular momentum. Thirdly, they give at best only the leading order approximation to the scattering theory, and in the special cases $L = 0, \infty$ fail to do even that, for the phase shift for a potential with scattering length $L = 0, \infty$ does not obey $\cot \delta_0(k) = O(k^{-1})$ at leading order, but rather

$$\cot \delta_0(k) = pk^{-3} + O(k^{-1}) \quad (1.3)$$

for $L = 0$, and

$$\cot \delta_0(k) = qk + O(k^3) \quad (1.4)$$

for $L = \infty$. To remove these limitations on PI, various generalised point interactions (GPI) have been proposed, which correspond heuristically to Hamiltonians with $\delta$-derivative and more general distributional potentials. Models of this type were first discussed by Shirokov [1] and were given a mathematical foundation by Pavlov [2, 3, 4] and Shondin [5, 6] (see also [7]). GPI are not defined on the usual Hilbert space $L^2(\mathbb{R}^3)$, but on a larger space: either an extended Hilbert space $L^2(\mathbb{R}^3) \oplus C^m \oplus C^m \oplus C^m \oplus C^m$, or a Pontryagin space $\Pi = L^2(\mathbb{R}^3) \oplus C^m \oplus C^m \oplus C^m \oplus C^m$. Due to the presence of negative and

\[1\]A Pontryagin space $\Pi$ is an inner product space which admits a direct orthogonal decomposition $\Pi = \mathcal{H}_+ \oplus \mathcal{H}_-$ into a Hilbert space $\mathcal{H}_+$ with positive definite inner product, and a finite dimensional
zero normed states, Pontryagin spaces do not immediately admit the usual probability interpretation of quantum mechanics. However, for GPI models it is often the case that there is a positive definite subspace $H^+_\Pi$ of $\Pi$ which is invariant under the unitary evolution generated by the GPI Hamiltonian and therefore has a natural interpretation as the space of physical states.

In conventional treatments of GPI, one decides at the outset how the Hilbert space is to be extended, and then constructs the class of GPI which ‘live’ on this space, either by a generalisation of the von Neumann theory of deficiency indices \cite{4}, or by constructing separable perturbations of the free Laplacian in accordance with a generalised version of Krein’s formula \cite{6, 7, 3}. In this paper, we present a new construction of point and generalised point interactions, which removes the necessity to determine the underlying inner product structure in advance. Rather, the appropriate extension to the initial space $L^2(\mathbb{R}^3)$ emerges naturally in the course of the construction.

Our construction depends on the observation that for a point-like ‘potential’, the scattering phase shifts completely determine the generalised eigenfunctions of the continuum spectrum. To see this, note that for a potential compactly supported within radius $a$ of the origin, the phase shifts determine the eigenfunctions (up to normalisation) for $r > a$, and therefore if $a \to 0$, the phase shift in a given angular momentum sector determines the continuum eigenfunctions in that sector for all values of the radial coordinate\footnote{In contrast to the usual treatments of GPI’s on Pontryagin spaces, we neglect the possibility of distributional contributions at the origin. See the discussion in Section 7.}. Thus, for example, in the $S$-wave, we have the radial eigenfunctions $u_k(r)$ at wavenumber $k$

\begin{equation}
    u_k(r) = \left(\frac{2}{\pi}\right)^{1/2} \sin(kr + \delta_0(k)).
\end{equation}

We introduce the notation $\mathcal{H}_r = L^2((0, \infty), dr)$ and $\mathcal{H}_k = L^2((0, \infty), dk)$ for Hilbert spaces of square integrable functions on position and momentum spaces respectively. Armed with the generalised eigenfunctions $u_k$, one can define an integral transform $U : \mathcal{H}_r \to \mathcal{H}_k$ so that

\begin{equation}
    f(r) = (U^{-1} \tilde{f})(r) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \sin(kr + \delta_0(k)) \tilde{f}(k) dk.
\end{equation}

If $U$ were unitary, then one could immediately define a self-adjoint operator $H = U^*k^2U$ for which the $u_k(r)$ would constitute a complete set of generalised eigenfunctions: one would thereby have constructed the spectral representation of $H$. In general, the mapping $U$ is not unitary and so one cannot proceed in this way. For relatively simple functions $\delta_0(k)$, it is, however, possible to determine exactly how $U$ fails to be unitary. One can then extend either $\mathcal{H}_r$ or $\mathcal{H}_k$ (or both) in such a way that $U$ may be extended to a unitary mapping $\hat{U}$. Thus a self-adjoint operator $H = \hat{U}^*k^2\hat{U}$ may be constructed, whose generalised continuum eigenfunctions (projected onto the original position Hilbert space $\mathcal{H}_r$) coincide with the $u_k(r)$.

\footnote{Hilbert space $\mathcal{H}_{-}$ with negative definite inner product. The dimension of $\mathcal{H}_{-}$ is called the rank of indefiniteness. See \cite{18}.}
In particular, in the cases studied, it is easy to determine how the Hilbert space should be extended. There is a certain amount of ambiguity in our procedure (as in other constructions of GPI); however, with the additional requirement of locality, it is possible to make natural choices for the various free parameters occurring. We also emphasise that our aim is not to construct the most general possible class of GPI, but rather to construct at least one GPI with the required scattering behaviour.

Although certain GPI models have previously been constructed by inverse methods [5] the analysis usually proceeds immediately from the $T$-matrix to the discussion of a candidate resolvent $R(z)$ whose free parameters are then constrained by the requirement that $R(z)$ actually be the resolvent of a self-adjoint operator on the pre-determined inner product space. In contrast, the present treatment focusses on integral transforms suggested by the scattering data.

After some preliminaries in Section 2, we illustrate our construction in two cases. Firstly, in Section 3, we construct the class of point interactions $H_L$ with scattering theory given by (1.2) thereby reconstructing the self-adjoint extensions of $-\Delta$ on $C_0^\infty(\mathbb{R}^3\setminus\{0\})$, as expected. As is well known, for $L > 0$, the self-adjoint extension $H_L$ possesses a single bound state: in the context of our construction, this is manifested in the need to extend $\mathcal{H}_k$. For $L < 0$, there is no bound state, and neither $\mathcal{H}_r$ nor $\mathcal{H}_k$ need be extended.

Secondly, in Section 4, we study the class of point interactions on $\mathbb{R}^3$ modelling potentials exhibiting zero energy resonances (infinite scattering length). As noted above, the leading order scattering behaviour of such systems (1.4) is not well-approximated by any of the usual PI. Instead, we construct generalised point interactions $H_{res}^M$ ($M \in \mathbb{R} \cup \{\infty\}$) with scattering theory

$$\cot \delta_0(k) = kM$$

(1.7)

in the $S$-wave, and trivial scattering for higher angular momenta. We refer to this class of GPI as resonance point interactions (RPI). The special cases $M = 0, \infty$ are identified with the PI $H^\infty, H^0$ respectively. Apart from this, there are two cases: $M > 0$ and $M < 0$. For $M < 0$, we find that $\mathcal{H}_r$ is extended to $L^2((0, \infty), dr) \oplus \mathbb{C}$, although the momentum Hilbert space is unchanged. This case represents a subset of the models of type $B_2$ discussed by Shondin [4]. For $M > 0$, both $\mathcal{H}_r$ and $\mathcal{H}_k$ are extended to Pontryagin spaces of form $L^2(0, \infty) \ominus \mathbb{C}$. This model appears to be new: moreover, it is not presently clear how the usual GPI constructions could be used to reproduce this model.

In Section 5, we verify that the PI and RPI models exhibit the required scattering theory by explicitly constructing the Møller wave operators (in a two space setting, where necessary). In Section 6, we consider the physical interpretation of RPI models. To do this, we employ a general methodology for discussing the ‘large scale effects of small objects’ developed by Kay and the author [12]. In particular, we develop a fitting formula (analogous to those given in [12]) for matching a given potential $V(r)$ with a zero energy resonance to the ‘best fit’ RPI. This leads to a natural interpretation of the
'extra dimension' in the extended Hilbert space of the $M < 0$ RPI models as representing a meta-stable state: part of a wavepacket incident on such an RPI disappears from the Hilbert space $L^2(\mathbb{R}^3)$ and the ‘missing’ probability is stored in the extra dimension before being slowly released with a $O(t^{-1/2})$ time dependence.

It might be objected that neither case $L = 0$, $\infty$ is generic, and that, to all intents and purposes, the usual PI suffice to describe the leading order behaviour. However, the motivation for the present work arose in a consideration of the scattering of charged particles off magnetic flux tubes of small radius \( [9] \), in which it was found that the scattering lengths for spin-$\frac{1}{2}$ particles generically take the values 0 or $\infty$ in certain angular momentum sectors. In consequence, the conventional point interactions (in this case the self-adjoint extensions of the operator describing the dynamics in the background of an infinitesimally thin wire of flux) fail to describe the leading order scattering theory in these sectors. The special nature of this system can be attributed to the fact that it is an example of supersymmetric quantum mechanics (see, for example \([10] \)). Elsewhere \([11] \), we will construct the appropriate class of RPI for this system.

2 Preliminaries

We develop various standard properties of the sine and cosine transforms $S$ and $C$ and also demonstrate density of certain subspaces which will be needed in the sequel. $S$ and $C$ are defined by

$$(Sf)(k) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} dr \sin kr f(r) \quad (Cf)(k) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} dr \cos kr f(r)$$

(2.1)

(the integrals are intended in the sense of ‘limit in the mean’). Both are unitary maps from $H_r$ to $H_k$, with inverses

$$(S^{-1}f)(r) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} dk \sin kr f(k) \quad (C^{-1}f)(r) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} dk \cos kr f(k).$$

(2.2)

Define the operators $E_\pm : L^2(0, \infty) \rightarrow L^2(\mathbb{R})$ by

$$(E_\pm \varphi)(x) = \begin{cases} \varphi(x) & x > 0 \\ \pm \varphi(x) & x < 0. \end{cases}$$

(2.3)

$E_\pm \varphi$ are the even and odd continuations of $\varphi$ respectively. For clarity, we also define the restriction operator $J : L^2(\mathbb{R}) \rightarrow L^2(0, \infty)$ by $(J \varphi)(x) = \varphi(x)$ for all $x \geq 0$. We also define Fourier transformation, $F$ by

$$(Ff)(k) = \int_{-\infty}^{\infty} \frac{dr}{\sqrt{2\pi}} e^{ikr} f(r).$$

(2.4)

These operators allow us to express $S$ and $C$ in terms of $F$:

$$(Cf)(k) = (JF E_+ f)(k) \quad (E_+ C f)(k) = (FE_+ f)(k)$$

$$(Sf)(k) = (JF E_- f)(k) \quad (E_- S f)(k) = (FE_- f)(k).$$

(2.5)
These relationships entail that $S$ and $C$ possess many properties inherited from Fourier transformation. The following is a simple corollary of the Paley-Wiener theorem.

**Proposition 2.1** Let $f \in C_0^\infty(0, \infty) \subset \mathcal{H}_r$. Then $(Cf)(k)$ ($(Sf)(k)$) is an even (odd), entire analytic function of $k$, whose restriction to the real axis decreases faster than polynomially at infinity. If $g \in C_0^\infty(0, \infty) \subset \mathcal{H}_k$, then $(C^{-1}g)(r)$ ($(S^{-1}g)(r)$) is an even (odd), entire analytic function of $r$, whose restriction to the real axis decreases faster than polynomially at infinity.

Next, we define the subspace $D^L$ of $L^2(\mathbb{R}, dk)$ for $L \in \mathbb{R}\setminus\{0\}$ by

$$D^L = \{(1 + (kL)^2)^{1/2} f \mid f \in C_0^\infty(\mathbb{R}\setminus\{0\})\} \quad (2.6)$$

and the normalised vector $\psi_L \in \mathcal{H}$ by

$$\psi_L(k) = \left(\frac{2|L|}{\pi}\right)^{1/2} (1 + (kL)^2)^{-1/2}. \quad (2.7)$$

We then prove the following:

**Lemma 2.2** $D^L \oplus \{\lambda E_+ \psi_L \mid \lambda \in \mathbb{C}\}$ is dense in $L^2(\mathbb{R}, dk)$ for any $L \in \mathbb{R}\setminus\{0\}$.

**Proof:** Suppose $\varphi \in L^2(\mathbb{R})$ is orthogonal to $D$. Then $(1 + (kL)^2)^{1/2} \varphi$ is the Fourier transform of a distribution supported at the origin. Hence

$$\varphi = \sum_{\alpha < n} \frac{a_\alpha k^\alpha}{(1 + (kL)^2)^{1/2}} \quad (2.8)$$

for some $a_\alpha, n$. Square integrability then forces $\varphi$ to be a multiple of $E_+ \psi_M$. ■

We now define the subspaces $D^L_\pm$ of $\mathcal{H}_k$ by

$$D^L_+ = \{(1 + (kL)^2)^{1/2} C f \mid f \in C_0^\infty(0, \infty)\}$$

$$D^L_- = \{(1 + (kL)^2)^{1/2} S f \mid f \in C_0^\infty(0, \infty)\} \quad (2.9)$$

**Proposition 2.3** $D^L_+ \oplus \{\lambda \psi_L \mid \lambda \in \mathbb{C}\}$ and $D^L_-$ are each dense in $\mathcal{H}_k$.

**Proof:** Note that $C_0^\infty(\mathbb{R}\setminus\{0\}) = E_+ C_0^\infty(0, \infty) \oplus E_- C_0^\infty(0, \infty)$ and hence that $D^L = E_+ D^L_+ \oplus E_- D^L_-$. By Lemma 2.2, $D^L \oplus \{\lambda E_+ \psi_M \mid \lambda \in \mathbb{C}\}$ is a dense subspace of $L^2(\mathbb{R}, dk)$ and admits an orthogonal decomposition into a subspace of even functions and a subspace of odd functions. It is trivial to show that the restrictions of these subspaces to $\mathbb{R}^+$ must therefore be individually dense in $\mathcal{H}_k$, and the result follows. ■

Finally, the following well known identities are valid for all $f \in C_0^\infty(0, \infty)$

$$k(Sf)(k) = \left(C \frac{d}{dr} f\right)(k); \quad k(Cf)(k) = -\left(S \frac{d}{dr} f\right)(k) \quad (2.10)$$

For $f \in C_0^\infty(0, \infty)$, we have

$$(S^{-1}kf)(r) = -\frac{d}{dr}(C^{-1}f)(r); \quad (C^{-1}kf)(r) = \frac{d}{dr}(S^{-1}f)(r) \quad (2.11)$$
3 Point Interactions

In this section, we put into practice the construction sketched in Section 1 by recon-
structing the familiar class of PI in 3 dimensions. Our starting point is the scattering
theory described by (1.2) in the $S$-wave for some $L \in \mathbb{R} \cup \{\infty\}$, and $\delta_{\ell}(k) = 0$ for all $k$ and all $\ell \geq 1$. We therefore restrict attention to the $S$-wave and attempt to make rig-
orous the heuristic spectral representation given by (1.6), extending the various Hilbert
spaces involved if necessary.

In terms of $S$ and $C$, we define the bounded mapping $F_L : \mathcal{H}_r \rightarrow \mathcal{H}_k$ by

$$F_L = (1 + (kL)^2)^{-1/2}S - kL(1 + (kL)^2)^{-1/2}C$$

in terms of which equation (1.4) may be re-written as

$$f(r) = (F_L^* \tilde{f})(r).$$

In the special cases $L = 0, \infty$, $F_L$ reduces to $S$ and $C$ respectively. Restricting to
$L \neq 0, \infty$, we now compute $F_L^*F_L$. We have

$$F_L^*F_L = I - C^{-1} \frac{1}{1 + (kL)^2}C - S^{-1} \frac{1}{1 + (kL)^2}S \quad \text{for } L > 0,$$

$$F_L^*F_L = I - C^{-1} \frac{kL}{1 + (kL)^2}C - S^{-1} \frac{kL}{1 + (kL)^2}S \quad \text{for } L < 0.$$
We now consider $F_L^*F_L$ and find

$$F_L^*F_L = I - \frac{1}{(1 + (kL)^2)^{1/2}} SC^{-1} \frac{kL}{(1 + (kL)^2)^{1/2}} - \frac{kL}{(1 + (kL)^2)^{1/2}} CS^{-1} \frac{1}{(1 + (kL)^2)^{1/2}}.$$ 

(3.9)

On the domain $D^L$ defined in (2.9), the last term may be re-written:

$$\frac{kL}{(1 + (kL)^2)^{1/2}} CS^{-1} \frac{1}{(1 + (kL)^2)^{1/2}} = \frac{L}{(1 + (kL)^2)^{1/2}} S dS^{-1} \frac{1}{(1 + (kL)^2)^{1/2}} = \frac{1}{(1 + (kL)^2)^{1/2}} SC^{-1} \frac{kL}{(1 + (kL)^2)^{1/2}}$$

(3.10)

using the identities (2.10) and (2.11). Thus we have $F_L^*F_L = I$ on $D^L$, which is dense by Proposition 2.3. Hence

$$F_L^*F_L = I.$$ 

(3.11)

Including the special cases $L = 0, \infty$, we have thus proved

**Proposition 3.1** For $L \leq 0$ or $L = \infty$, $F_L$ is a unitary mapping from $\mathcal{H}_r$ to $\mathcal{H}_k$.

In the case $L > 0$, $F_L$ fails to be unitary, as it has non-trivial kernel: $F_L | \chi_L = 0$. Note that this deficiency is restricted to a 1-dimensional subspace. We can compensate for the ‘missing probability’ by extending $\mathcal{H}_k$ to $\mathcal{H}_k \oplus \mathbb{C}$ (with inner product $\langle f \oplus \alpha \mid g \oplus \beta \rangle = \langle f \mid g \rangle_{L^2} + \alpha \beta$) and then defining the mapping $\hat{F}_L$ by

$$\hat{F}_L = [F_L, \langle \chi_L \mid ] : \mathcal{H}_r \rightarrow \mathcal{H}_k \oplus \mathbb{C}$$

$$f \rightarrow F_L f \oplus \langle \chi_L \mid f \rangle$$

(3.12)

We then have

**Proposition 3.2** For $L > 0$, $\hat{F}_L$ is a unitary mapping from $\mathcal{H}_r$ to $\mathcal{H}_k \oplus \mathbb{C}$, with inverse

$$\hat{F}_L^{-1}(f \oplus \alpha) = F_L^*f + \alpha \mid \chi_L \rangle.$$ 

(3.13)

**Proof:** Note that $F_L$ is a surjection onto $\mathcal{H}_k$ as a consequence of (3.11). The result then follows immediately from the definition of $\hat{F}_L$ and (3.8). 

Our extension to the momentum Hilbert space will, of course, carry the interpretation of a bound state with normalised eigenfunction $\chi_L(r) \in \mathcal{H}_r$. Note that the mapping $\hat{F}_L$ is just one of a 1-parameter family of physically equivalent possible mappings $\hat{F}_L^\delta = [F_L, e^{i\delta} \langle \chi_L \mid ]$ corresponding to re-phasing $\chi_L$. 

7
We may now proceed to define the point interaction Hamiltonians. In the case $L < 0$, and also in the special cases $L = 0, \infty$ we have seen that the mapping $\mathcal{F}_L$ is unitary, and so we may immediately define a self-adjoint operator by

$$h^L = \mathcal{F}_L^* k^2 \mathcal{F}_L$$

(3.14)

with domain $D(h^L) = \mathcal{F}_L^* D(k^2)$. In the case $L > 0$, however we must use the unitary mapping $\hat{\mathcal{F}}_L$, defining

$$h^L = \hat{\mathcal{F}}_L^{-1} (k^2 \oplus E_L) \hat{\mathcal{F}}_L$$

(3.15)

with domain $D(h^L) = \hat{\mathcal{F}}_L^{-1}(D(k^2) \oplus \mathbb{C})$, where $E_L \in \mathbb{R}$ is arbitrary. We have restricted our operator to be diagonal in the momentum representation in order to ensure that the continuum eigenfunctions are still given by the $u_k(r)$. Note that our construction does not uniquely determine the energy $E_L$ of the bound state – any $E_L$ results in an unbounded self-adjoint operator whose continuum eigenfunctions have the required form. In order to remove this ambiguity, we impose the additional requirement of locality, in the form of a requirement that $h^L$ should agree with $-d^2/dr^2$ on $C_0^\infty(0, \infty)$. Clearly this will automatically restrict us to self-adjoint extensions of $-d^2/dr^2$ on this domain.

**Proposition 3.3** $E_L = -|L|^{-2}$ is the unique value for which $h^L$ is local.

**Proof:** From Proposition 2.1, it follows that $\mathcal{F}_L C_0^\infty(0, \infty) \subset D(k^2)$ and hence $C_0^\infty(0, \infty) \subset D(h^L)$. For $f \in C_0^\infty(0, \infty)$, we compute

$$h^L f = \mathcal{F}_L^* k^2 \mathcal{F}_L f + E_L \langle \chi_L | f \rangle$$

$$= -\mathcal{F}_L^* \mathcal{F}_L f'' + E_L \langle \chi_L | f \rangle$$

$$= -f'' + \langle \chi_L | E_L \langle \chi_L | f \rangle - \langle \chi_L | f'' \rangle \rangle$$

$$= -f'' + (E_L + |L|^{-2}) \langle \chi_L | \chi_L \rangle$$

(3.16)

where we have used the fact that $k^2 \mathcal{F}_L f = -\mathcal{F}_L f''$ for $f \in C_0^\infty(0, \infty)$ and also that $(-d^2/dr^2|_{C_0^\infty(0, \infty)})^* \chi_L = -|L|^{-2} \chi_L$. The result follows immediately.

We now determine the domain of $h^L$ explicitly. This is, of course, well known; we discuss it here only to show how it may be derived within the terms of our construction.

**Theorem 3.4** $h^L$ has domain

$$D(h^L) = \{ \varphi \mid \varphi, \varphi' \in AC_{loc}(0, \infty); \varphi'' \in L^2(0, \infty); \varphi(0) + L \varphi'(0) = 0 \}$$

(3.17)

where the boundary condition $\varphi(0) + L \varphi'(0) = 0$ is to be interpreted as $\varphi(0) = 0$ for $L = 0$, and $\varphi'(0) = 0$ for $L = \infty$.

**Proof:** We give details for the case $L < 0$ and indicate how the proof is modified for the remaining cases. Note that $C_0^\infty(0, \infty) \subset \mathcal{H}_k$ is a core for $k^2$, and hence $\mathcal{D} = \mathcal{F}_L^* C_0^\infty(0, \infty)$ is a core for $h^L$. Any $f \in \mathcal{D}$ may be written

$$f = (S^{-1} - C^{-1} k L) \varphi$$

(3.18)
where \( \varphi = (1 + (kL)^2)^{-1/2}F_L f \in C^\infty_0(0, \infty) \). By Proposition 2.1 and identities of the sine and cosine transforms, we find that \( f(r) = g(r) - Lg'(r) \), where \( g(r) = S^{-1}\varphi \) is odd, entire analytic, and decreasing faster than polynomially as \( r \to \infty \). In particular, \( f(0) + LF'(0) = 0 \) for all \( f \in D \). Moreover, there is at least one \( f_0 \in D \) for which \( f_0(0) \neq 0 \), for otherwise we would have \( C^{-1}k(1 + (kL)^2)^{-1/2}\eta(0) = 0 \) for all \( \eta \) in the dense set \( C^\infty_0(0, \infty) \), obtaining a contradiction. Now \( h^L \) agrees with \( -d^2/dr^2 \) (acting in the sense of distributions) on \( D \), and is symmetric on this domain. Thus

\[
D(h^L) = D((h^L|_D)^*) = \{ \varphi | \langle \varphi | f'' \rangle = \langle \varphi'' | f \rangle, \text{ for all } f \in D \} \tag{3.19}
\]

and the required result follows easily. The cases \( L = 0, \infty \) may be treated similarly, using \( S^{-1}C^\infty_0(0, \infty) \) and \( C^{-1}C^\infty_0(0, \infty) \) as cores. For \( L > 0 \), the appropriate core is \( D = F^*_L C^\infty_0(0, \infty) \oplus \{ \lambda \chi_L(r) | \lambda \in \mathbb{C} \} \).

We can assemble the full PI Hamiltonian acting on \( L^2(\mathbb{R}^3) \): with respect to the decomposition

\[
L^2(\mathbb{R}^3) = \bigoplus_{\ell=0}^{\infty} L^2(\mathbb{R}^+, r^2dr) \otimes K_\ell \tag{3.20}
\]

where \( K_\ell \) is the subspace of \( L^2(\mathbb{S}^2, d\Omega) \) spanned by \( Y_{\ell,-\ell}, \ldots, Y_{\ell,\ell} \), \( H^L \) is defined by

\[
H^L = U^*h^L U \otimes I \oplus \bigoplus_{\ell=1}^{\infty} U^*\bar{h}_\ell U \otimes I \tag{3.21}
\]

where \( U : L^2(\mathbb{R}^+, dr) \to L^2(\mathbb{R}^+, r^2dr) \) is the unitary operator \( (Uf)(r) = rf(r) \), and \( \bar{h}_\ell \) (\( \ell \geq 1 \)) is the unique self-adjoint extension of \( -d^2/dr^2 + \ell(\ell + 1)/r^2 \) on \( C^\infty_0(0, \infty) \subset \mathcal{H}_r \).

To summarise, we have seen how the usual class of point interactions may be constructed from a consideration of the required scattering theory.

## 4 Resonance Point Interactions

We now construct the class of RPI models by a similar method to that used in the previous section. In this case, the relevant heuristic spectral representation is again given by (L3), but with \( \delta_0(k) \) now specified by (L7) for some \( M \in \mathbb{R} \cup \{ \infty \} \). Accordingly, we consider the bounded mapping \( \mathcal{T}_M \) defined by

\[
\mathcal{T}_M = (1 + (kM)^2)^{-1/2}C + kM(1 + (kM)^2)^{-1/2}S. \tag{4.1}
\]

In the special cases \( M = 0, \infty \), \( \mathcal{T}_M \) reduces to \( C \) and \( S \) respectively. Hence in these cases, \( \mathcal{T}_M \) is unitary from \( \mathcal{H}_r \) to \( \mathcal{H}_k \) and the operators \( h^M_{\text{res}} = \mathcal{T}_M k^2 \mathcal{T}_M \) are well defined self-adjoint operators. Comparing with the previous section, we see that \( h^0_{\text{res}} = h^0 \), and \( h^\infty_{\text{res}} = h^\infty \).
We now consider the remaining cases. Firstly, we compute $T_M^*T_M$. We have

\[
T_M^*T_M = I + C^{-1} \frac{1}{1 + (kM)^2} C - S^{-1} \frac{1}{1 + (kM)^2} S
+ C^{-1} \frac{kM}{1 + (kM)^2} S + S^{-1} \frac{kM}{1 + (kM)^2} C
\]

(4.2)

and so, by the arguments used in the previous section,

\[
T_M^*T_M = \begin{cases} I + |\chi_M\rangle\langle\chi_M| & M > 0 \\ I & M < 0 \end{cases}
\]

(4.3)

which should be compared with equation (3.8).

Computing $T_M^*T_M$,

\[
T_M^*T_M = I + \frac{1}{(1 + (kM)^2)^{1/2}} C S^{-1} \frac{kM}{1 + (kM)^2} (1 + (kM)^2)^{1/2}
+ \frac{kM}{(1 + (kM)^2)^{1/2}} C S^{-1} \frac{1}{1 + (kM)^2} (1 + (kM)^2)^{1/2}
\]

(4.4)

On the domain $D_M^+$ defined in (2.9), the last term may be re-written:

\[
\frac{kM}{(1 + (kM)^2)^{1/2}} S C^{-1} \frac{1}{(1 + (kM)^2)^{1/2}} = \frac{M}{(1 + (kM)^2)^{1/2}} C \frac{d}{dr} C^{-1} \frac{1}{(1 + (kM)^2)^{1/2}}
\]

\[
= \frac{-M}{(1 + (kM)^2)^{1/2}} C S^{-1} \frac{k}{(1 + (kM)^2)^{1/2}}
\]

(4.5)

Proposition 2.3 shows that $D_+ \oplus \{\lambda \psi_M | \lambda \in \mathbb{C}\}$ is dense in $H_k$, so we require the action of $T_M^*T_M$ on $\psi_M$. Explicit computation using the standard results

\[
(C \chi_M)(k) = \left(\frac{4|M|}{\pi}\right)^{1/2} \frac{1}{1 + (kM)^2}, \quad (S \chi_M)(k) = \left(\frac{4|M|}{\pi}\right)^{1/2} \frac{k|M|}{1 + (kM)^2}
\]

(4.6)

yields

\[
(T_M \chi_M)(k) = \begin{cases} \sqrt{2} \psi_M(k) \frac{1 - (kM)^2}{1 + (kM)^2} & M < 0 \\ \sqrt{2} \psi_M(k) & M > 0 \end{cases}
\]

(4.7)

and

\[
(T_M^* \psi_M)(r) = \frac{1}{\sqrt{2}}(1 + \text{sgn} M) \chi_M(r).
\]

(4.8)

from which we obtain

\[
T_M^*T_M \psi_M = \begin{cases} 2 \psi_M & M > 0 \\ 0 & M < 0 \end{cases}
\]

(4.9)

Assembling our results, we have

\[
T_M^*T_M = \begin{cases} 1+ |\psi_M\rangle\langle\psi_M| & M > 0 \\ 1- |\psi_M\rangle\langle\psi_M| & M < 0 \end{cases}
\]

(4.10)
We now modify $\mathcal{T}_M$ in order to obtain a unitary operator. First note that the $M < 0$ case is analogous to the $L > 0$ case for $\mathcal{F}_L$, except that here, it is $\mathcal{T}_M\mathcal{T}_M^*$ rather than $\mathcal{F}_L^*\mathcal{F}_L$, which fails to be the identity. Accordingly, we extend the position Hilbert space to $\mathcal{H}_r \oplus \mathbb{C}$ (with the obvious inner product) and define the mapping $\hat{T}_M$ by

$$
\hat{T}_M : \mathcal{H}_r \oplus \mathbb{C} \rightarrow \mathcal{H}_k
f \oplus \alpha \rightarrow T_M f + \alpha | \psi_M \rangle.
$$

(4.11)

$\hat{T}_M$ is unique up to re-phasing of $\psi_M$. We then have

**Proposition 4.1** For $M < 0$, $\hat{T}_M$ is a unitary mapping from $\mathcal{H}_r \oplus \mathbb{C}$ to $\mathcal{H}_k$ with inverse

$$
\hat{T}_M^{-1} f = [T_M^*, \langle \psi_M | ] f = T_M^* f \oplus \langle \psi_M | f \rangle.
$$

(4.12)

We may therefore construct a self-adjoint operator $h^M_{\text{res}}$ on $\mathcal{H}_r \oplus \mathbb{C}$ by

$$
h^M_{\text{res}} = \hat{T}_M^{-1} k^2 \hat{T}_M
$$

(4.13)

with domain $D(h^M_{\text{res}}) = \hat{T}_M^{-1} D(k^2)$. We will return to the physical interpretation of the ‘extra dimension’ in Section 6.

We now examine the properties of $h^M_{\text{res}}$. By the same arguments as in the case of $L > 0$ PI, the domain of $h^M_{\text{res}}$ includes the (non-dense) subspace $\mathcal{D} = \{ \phi \oplus 0 \mid \phi \in C^\infty_0(0, \infty) \}$. Moreover, one can easily see that

$$
h^M_{\text{res}}(\phi \oplus 0) = \mathcal{T}_M^* k^2 \mathcal{T}_M \phi \oplus \langle \psi_M | k^2 \mathcal{T}_M \phi \rangle = -\mathcal{T}_M^* \mathcal{T}_M \phi'' \oplus \langle \psi_M | -\mathcal{T}_M \phi'' \rangle = -\phi'' \oplus 0
$$

(4.14)

for $\phi \in C^\infty_0(0, \infty)$ where we have used the fact that $\mathcal{T}_M^* \mathcal{T}_M = 0$ for $M < 0$. Hence, $h^M_{\text{res}}$ is a self-adjoint extension of the non-densely defined operator

$$
- \frac{d^2}{dr^2} \oplus 0 \quad \text{on} \quad \mathcal{D} \subset L^2((0, \infty), dr) \oplus \mathbb{C}
$$

(4.15)

The $h^M_{\text{res}}$ are therefore local, and belong to the class of models considered by Pavlov [4] and also by Shondin [5]. In the nomenclature of [5], the $h^M_{\text{res}}$ for $M < 0$ form a subset of models of ‘type $B_2$’.

To describe the domain of $h^M_{\text{res}}$ explicitly, we use a similar argument to that employed in the PI case, identifying $\mathcal{D} = \hat{T}_M^{-1} C^\infty_0(0, \infty)$ as a core for $h^M_{\text{res}}$. If $g(k) \in C^\infty_0(0, \infty)$, then $\langle \psi_M | g \rangle = |M|^{1/2}(\mathcal{T}_M^* g)(0)$, and so $\mathcal{D}$ may be written

$$
\mathcal{D} = \{ f \oplus |M|^{1/2} f(0) \mid f \in \mathcal{T}_M C^\infty_0(0, \infty) \}.
$$

(4.16)

Any function $f \in \mathcal{T}_M C^\infty_0(0, \infty)$ may be written $f(r) = g(r) - Mg'(r)$, where $g(r)$ is analytic, even, and decreasing faster than polynomially as $r \to 0$. As a consequence, $f'(0) = -Mf''(0)$. On $\mathcal{D}$, $h^M_{\text{res}}$ has action

$$
h^M_{\text{res}} f \oplus |M|^{1/2} f(0) = -f'' \oplus -|M|^{1/2} f''(0) = -f'' \oplus -|M|^{-1/2} f'(0)
$$

(4.17)
The domain of $h_{\text{res}}^M$ is equal to $D((h_{\text{res}}^M|D)^*)$. We have

$$
\langle \varphi \oplus \Phi_1 \mid h_{\text{res}}^M(f \oplus |M|^{1/2}f(0)) \rangle = (-\varphi'' | f) + \overline{\varphi(0)}f'(0) - \overline{\varphi'(0)}f(0)
- \overline{\Phi_1}|M|^{-1/2}f'(0)
$$

(4.18)

for any $\varphi$ such that $\varphi'' \in L^2(0, \infty)$ in the sense of distributions. Note that $-d^2/dr^2$ is not symmetric on $T^*_MC_\infty^\infty(0, \infty)$. Hence, if $\varphi \oplus \Phi_1 \in D(h_{\text{res}}^M)$, with $h_{\text{res}}^M \varphi \oplus \Phi_1 = -\varphi'' \oplus \Phi_2$, then

$$
\overline{\varphi'(0)}f(0) - \overline{\varphi(0)}f'(0) = \Phi_1|M|^{-1/2}f'(0) + \Phi_2|M|^{1/2}f(0).
$$

(4.19)

for all $f \in T^*_MC_\infty^\infty(0, \infty)$. Moreover, $f(0)$ and $f'(0)$ are independent on this domain. The following is then immediate.

**Theorem 4.2** The domain of $h_{\text{res}}^M$ is

$$
D(h_{\text{res}}^M) = \{ \varphi \oplus \Phi \mid \varphi, \varphi' \in AC_{\text{loc}}(0, \infty); \varphi'' \in L^2(0, \infty); \Phi = |M|^{1/2}\varphi(0) \}
$$

(4.20)

with action

$$
h_{\text{res}}^M(\varphi \oplus |M|^{1/2}\varphi(0)) = -\varphi'' \oplus -|M|^{-1/2}\varphi'(0).
$$

(4.21)

In contrast to the usual PI case, the boundary condition corresponding to (4.20) is energy dependent: the eigenfunction equation at energy $k^2$ is equivalent to the equation $-\varphi'' = k^2\varphi$, with boundary condition

$$
k^2M\varphi(0) = \varphi'(0)
$$

(4.22)

and the generalised eigenfunction at energy $k^2$ is therefore

$$
u_k = \left(\frac{2}{\pi}\right)^{1/2} \sin(kr + \delta_0(k)) \oplus |M|^{1/2}\sin\delta_0(k)
$$

(4.23)

with $\delta_0(k)$ given by (1.7).

As a result of our construction, the spectral properties of $h_{\text{res}}^M$ are easily identified: $h_{\text{res}}^M$ has purely absolutely continuous spectrum $\sigma(h_{\text{res}}^M) = \sigma_{\text{ac}}(h_{\text{res}}^M) = [0, \infty)$.

Turning to the case $M > 0$, we note that our original choice of continuum eigenfunctions form an ‘over complete’ set. We can remedy this by extending to a Pontryagin space, the heuristic motivation being that this will allow us to subtract off the ‘excess probability’. It is only possible to construct unitary mappings between Pontryagin spaces with the same rank of indefiniteness, so we must extend both position and momentum spaces to Pontryagin spaces. As before, we find that the failure of unitarity is located in a one dimensional subspace, which suggests that we choose Pontryagin spaces of form $\Pi = L^2(0, \infty) \ominus C$, where the indefinite inner product is given by

$$
\langle f \ominus \alpha \mid g \ominus \beta \rangle_\Pi = \langle f \mid g \rangle_{L^2} - \overline{\alpha}\beta.
$$

(4.24)
We define the mapping $\hat{T}_M$, unique up to re-phasing of $\psi_M$ and $\chi_M$, by

$$\hat{T}_M : \mathcal{H}_r \oplus \mathbb{C} \rightarrow \mathcal{H}_k \oplus \mathbb{C}
\quad f \oplus \alpha \rightarrow (T_M f - \alpha | \psi_M) \oplus (-\langle \chi_M | f \rangle_{L^2} + \alpha \sqrt{2}).$$

(4.25)

A short computation proves

**Proposition 4.3** For $M > 0$, $\hat{T}_M$ is a unitary mapping from $\mathcal{H}_r \oplus \mathbb{C}$ to $\mathcal{H}_k \oplus \mathbb{C}$, with inverse

$$\hat{T}_M^{-1} : \mathcal{H}_k \oplus \mathbb{C} \rightarrow \mathcal{H}_r \oplus \mathbb{C}
\quad f \oplus \alpha \rightarrow (T_M^* f + \alpha | \chi_M) \oplus (\langle \psi_M | f \rangle_{L^2} + \alpha \sqrt{2})$$

(4.26)

Hence, we can construct the RPI Hamiltonian for $M > 0$ on $L^2((0, \infty), dr) \oplus \mathbb{C}$:

$$h^M_{\text{res}} = \hat{T}_M^{-1} \left( k^2 \oplus E_M \right) \hat{T}_M$$

(4.27)

(We have again chosen the Hamiltonian to be diagonalised by $\hat{T}_M$.) As in the case of PI for $L > 0$, a single free real parameter $E_M$ is introduced by our procedure. $E_M$ is interpreted as the energy of a negative-normed eigenstate $| \chi_M \rangle \oplus \sqrt{2}$. Such a state is undesirable in a quantum theory. Accordingly, we decompose the position Pontryagin space $\Pi_r$ into the orthogonal subspaces $\mathcal{H}_+$ and $\mathcal{L}$ (which are independent of the choice of $E_M$) given by

$$\Pi_r = \mathcal{H}_+ \hat{\oplus} \mathcal{L}
\mathcal{H}_+ = \hat{T}_M^{-1}(\mathcal{H}_k \ominus 0)
\mathcal{L} = \hat{T}_M^{-1}(0 \ominus \mathbb{C}) = \{ \lambda (| \chi_M \rangle \oplus \sqrt{2}) | \lambda \in \mathbb{C} \}$$

(4.28)

where we use the notation $\hat{\oplus}$ in contrast to the decomposition $\Pi_r = \mathcal{H}_r \ominus \mathbb{C}$.

Due to the diagonal structure of $h^M_{\text{res}}$ in the momentum representation, $h^M_{\text{res}}$ respects this decomposition

$$h^M_{\text{res}} = h^M_{\text{res},+} \hat{\oplus} E_M.$$  

(4.29)

Moreover, $\mathcal{H}_+$ is an intrinsically complete, positive definite subspace of $\Pi_r$ of unit codimension, orthogonal to the negative-normed eigenstate found above; it may therefore naturally be identified as the space of physical states. The operator $h^M_{\text{res},+}$ and the space $\mathcal{H}_+$ are independent of the value of $E_M$, so to some extent this parameter has no physical meaning. However, if one wishes the operator $h^M_{\text{res}}$ to be local on the Pontryagin space $\Pi_r$, one can identify the value $E_M = -|M|^{-2}$ as the unique value compatible with this requirement by similar arguments to those used in the PI case for $L > 0$.

We now describe the domain of $h^M_{\text{res},+}$ in more detail. We have $D(h^M_{\text{res},+}) = \hat{T}_M^{-1}(D(k^2) \ominus 0) \subset \mathcal{H}_+$. The domain $\mathcal{D} = \hat{T}_M^{-1}(C^\infty_0(0, \infty) \ominus 0)$ is a core for $h^M_{\text{res},+}$, and may be written

$$\mathcal{D} = \{ f | M |^{1/2} f(0) | f \in T_M^* C^\infty_0(0, \infty) \}.$$  

(4.30)
As before, we note that any function \( f \in T^* M_c\infty(0, \infty) \) may be written \( f(r) = g(r) - M g'(r) \), where \( g(r) \) is analytic, even, and decreasing faster than polynomially as \( r \to 0 \), and that \( f'(0) = -M f''(0) \) in consequence. The action of \( h^{M}_{\text{res,+}} \) on \( D \) is given by

\[
h^{M}_{\text{res,+}}(f \oplus |M|^{1/2} f(0)) = -f'' \oplus |M|^{-1/2} f'(0)
\]  

(4.31)

An exact analogue of the argument used in the \( M < 0 \) case then yields

**Theorem 4.4**  
The domain of \( h^{M}_{\text{res,+}} \) is given by

\[
D(h^{M}_{\text{res,+}}) = \{ \varphi \oplus \Phi \mid \varphi, \varphi' \in AC_{\text{loc}}(0, \infty); \varphi'' \in L^2(0, \infty); \Phi = |M|^{1/2} \varphi(0) \}
\]  

(4.32)

with action

\[
h^{M}_{\text{res,+}}(\varphi \oplus \Phi) = -\varphi'' \oplus |M|^{-1/2} \varphi'(0).
\]  

(4.33)

We therefore have the full domain \( D(h^{M}_{\text{res}}) = D(h^{M}_{\text{res,+}}) \otimes L \)

\[
D(h^{M}_{\text{res}}) = \{(\varphi \oplus \Phi) + \alpha(|\chi_M\rangle \oplus \sqrt{2}) \mid \varphi, \varphi' \in AC_{\text{loc}}(0, \infty); \varphi'' \in L^2(0, \infty); \Phi = |M|^{1/2} \varphi(0); \alpha \in \mathbb{C} \}
\]  

(4.34)

and action

\[
h^{M}_{\text{res}}(\varphi \oplus \Phi) + \alpha(|\chi_M\rangle \oplus \sqrt{2}) = -\varphi'' \oplus |M|^{-1/2} \varphi'(0) + \alpha E_M(|\chi_M\rangle \oplus \sqrt{2}).
\]  

(4.35)

As before, the \( h^{M}_{\text{res}} \) exhibit energy dependent boundary conditions: solving the eigenvalue equation at energy \( k^2 \) yields solutions obeying

\[
k^2 M \varphi(0) = \varphi'(0).
\]  

(4.36)

The spectral properties of \( h^{M}_{\text{res}} \) are as follows: \( \sigma(h^{M}_{\text{res}}) = \sigma_{pp}(h^{M}_{\text{res}}) \cup \sigma_{ac}(h^{M}_{\text{res}}) \), with \( \sigma_{pp}(h^{M}_{\text{res}}) = \{E_M\} \) and \( \sigma_{ac}(h^{M}_{\text{res}}) = [0, \infty) \).

We can assemble the full RPI models on \( \mathbb{R}^3 \) as before: defining \( H^{M}_{\text{res}} \) by

\[
H^{M}_{\text{res}} = \tilde{U}^* h^{M}_{\text{res}} \tilde{U} \otimes I \oplus \bigoplus_{\ell=1}^{\infty} \tilde{U}^* \tilde{h}_\ell U \otimes I
\]  

(4.37)

where, for \( M < 0 \), \( \tilde{U}(f \oplus \alpha) = rf(r) \oplus \alpha \), and for \( M > 0 \), \( \tilde{U}(f \oplus \alpha) = rf(r) \oplus \alpha \).

5 Scattering Theory

The original aim of our construction was to produce PI and GPI Hamiltonians with a given \( S \)-wave phase shift. It is therefore expedient to check that the models described above actually exhibit the required behaviour. The usual method of demonstrating the existence and completeness of Møller wave operators for PI and GPI models is to show
that their resolvents are trace class perturbations of that for the free Laplacian, and then to apply Kuroda-Birman theory \[16\]. Instead, we will use a method which builds on our construction and yields the Møller operators (and their completeness) directly.

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

\[
\Omega^\pm(A,B;J) = \lim_{t \to \mp \infty} e^{iA} J e^{-iB} P_{ac}(B) \tag{5.1}
\]

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

Our results in this section follow from

**Proposition 5.1** \(U_tC S^{-1} U_t \to \pm i1\) as \(t \to \mp \infty\), where \(U_t\) is multiplication by \(e^{-ik^2t}\) on \(\mathcal{H}_k\).

**Proof:** For any \(u(k) \in C_0^\infty(0, \infty)\), we compute

\[
\|U_tC S^{-1} U_t u(k) \mp iu(k)\|^2 = \|(C^{-1} \pm iS^{-1}) U_t u(k)\|^2 = \frac{2}{\pi} \int_0^\infty dr \left| \int_0^\infty dke^{i(\pm kr - k^2t)} u(k) \right|^2 \tag{5.2}
\]

and note that the last expression vanishes if \(t \to \mp \infty\) by (non)-stationary phase arguments (see the Corollary to Theorem XI.14 in \[16\]).

Using this result, we see that if \(Q = \cos \delta_0(k) S + \sin \delta_0(k) C\), then

\[
U_t Q S^{-1} U_t \to e^{\pm i\delta_0(k)} \tag{5.3}
\]

as \(t \to \mp \infty\). It is then easy to construct the Møller wave operators for the PI and RPI models. For the PI case, we take \(\mathcal{H}_1 = \mathcal{H}_2\) and \(J\) to be the identity, writing \(\Omega^\pm(A,B)\) for the wave operators.

**Theorem 5.2** \(\Omega^\pm(h^L,h^0)\) exist, are complete, and given by

\[
\Omega^\pm(h^L,h^0) = F^* L e^{\pm i\delta_0(k)} S \tag{5.4}
\]

where \(\delta_0(k)\) is given by \(1.2\).

**Proof:** For \(L \leq 0, L = \infty\), the existence and form of the Møller operators is immediate from the above, and the definition of \(h^L\) as \(F^* k^2 F\). Completeness holds because all three factors in \(5.4\) are unitary, and hence \(\text{Ran} \Omega^\pm(h^L,h^0) = \mathcal{H} = \text{Ran} P_{ac} h^L\). For \(L > 0\), we have

\[
e^{ih^L t} e^{-ih^0 t} = F^* U_t F S^{-1} U_t S + e^{-i|L|^2 t} | \chi_L \rangle \langle \chi_L | S^{-1} U_t S \tag{5.5}
\]

The second term vanishes as \(|t| \to \infty\) by another non-stationary phase argument, and the required result follows because \(\text{Ran} F^* L = \text{Ran} P_{ac} h^L\). \(\blacksquare\)
Theorem 5.3 For $M < 0$, $\Omega^\pm(h_{\text{res}}^M, h^0; J)$ exist, are complete, and given by

$$\Omega^\pm(h_{\text{res}}^M, h^0) = \hat{T}_M^{-1} e^{\pm i\delta_0(k)} S$$

(5.6)

where $\delta_0(k)$ is given by (1.7), and $J : \mathcal{H}_r \to \mathcal{H}_r \oplus \mathbb{C}$ is defined by $Jf = f \oplus 0$.

Proof: The existence and form of the operators is due to Proposition 5.1 and the following observation along with the form of $T_M$ and the fact that $\mathcal{T}_M J = \mathcal{T}_M \oplus 0$. Completeness holds because $\operatorname{Ran} \hat{T}_M^{-1} = \mathcal{H}_r = \operatorname{Ran} P_{ac} h_{\text{res}}^M$.

For the case $M > 0$, our two spaces are $\mathcal{H}_+ = \mathcal{H}_+ \oplus \mathbb{C}$.

Theorem 5.4 For $M > 0$, $\Omega^\pm(h_{\text{res}}^M, h^0; J)$ exist, are complete, and given by

$$\Omega^\pm(h_{\text{res}}^M, h^0) = \hat{T}_M^{-1} e^{\pm i\delta_0(k)} S$$

(5.7)

where $\delta_0(k)$ is given by (1.7), and $J : \mathcal{H}_r \to \mathcal{H}_r \oplus \mathbb{C}$ is defined by $Jf = P_+(f \ominus 0)$, with $P_+$ the orthogonal projector onto $\mathcal{H}_+$.

Proof: The argument proceeds as before, completeness holding because the wave operators are isometries from $\mathcal{H}_r$ to $\mathcal{H}_+ = P_{ac} h_{\text{res}}^M$.

We conclude that our construction does indeed yield the required scattering theory, and also (because of the way in which the PI and RPI Hamiltonians were defined) that complete Møller operators may easily and explicitly be determined.

6 Physical Interpretation

In this section, we show how RPI models may be used to model Schrödinger operators $H = -\Delta + V$, where $V$ is smooth, spherically symmetric, compactly supported within radius $a$ of the origin, and exhibits a zero energy resonance. Our methodology is analogous to that developed in [12], in which the non-resonant case is discussed. Here, we develop a formalism (the fitting formula) for selecting the ‘best fit’ RPI for such operators. The range of energies for which the approximation is valid can be determined by a ‘believability’ analysis analogous to that developed in [12]. We will not do this here.

The $S$-wave wavefunction at wavenumber $k$ obeys

$$\left\{ -\frac{d^2}{dr^2} + V(r) \right\} u_k(r) = k^2 u_k(r),$$

(6.1)

where $u(r)$ obeys regular boundary conditions, i.e. $u(0) = 0$. Because $V$ is supported within radius $a$ of the origin, the phase shift is given by

$$\cot \delta_0(k) = \frac{ka \sin ka + D(k) \cos ka}{ka \cos ka - D(k) \sin ka},$$

(6.2)
where \(D(k) = au'_k(a)/u_k(a)\). Expanding \(D(k)\) in powers of \((ka)^2\), \(D(k) = D_0 + D_1(ka)^2 + O((ka)^4)\), and substituting in (6.2), we find
\[
\text{cot} \delta_0(k) = \frac{D_0 + (1 + D_1 - D_0)(ka)^2 + O((ka)^4)}{(1 - D_0)ka + O((ka)^3)}.
\] (6.3)

This then leads to the expression \(L = a(D_0 - 1)/D_0\) for the scattering length. Clearly, a zero energy resonance (infinite scattering length) occurs when \(D_0 = 0\). In this case, the leading order behaviour of \(\delta_0(k)\) is given by
\[
\text{cot} \delta_0(k) = (1 + D_1)ka + O((ka)^3).
\] (6.4)

Comparing with (1.7), we find that the leading order approximation to the dynamics is given by the RPI \(H_{res}^M\), with \(M = a(1 + D_1)\). Thus it suffices to compute \(D_1\) for the potential of interest. To do this, we use the well-known formula (see, e.g. [17], p.236)
\[
D(k_1) - D(k_2) = -((k_1a)^2 - (k_2a)^2)\int_0^a u_{k_1}(r)u_{k_2}(r)dr.
\] (6.5)

Using this to expand \(D(k)\) about \(k = 0\), we find
\[
D_1 = -a^{-1}\int_0^a u_0(r)^2dr
\] (6.6)
and thus arrive at the fitting formula (cf. [12])
\[
M = a\left(1 - \frac{a^{-1}\int_0^a u_0(r)^2dr}{u_0(a)^2}\right).
\] (6.7)

The best fit RPI can therefore be computed in terms of the zero energy solution to (6.1). In addition, the labelling parameter obeys the bound
\[
-\infty \leq M < a.
\] (6.8)

Moreover, this bound is best possible: for any \(M\) in the above range, one can clearly find a smooth function \(u_0(r)\) satisfying regular boundary conditions at the origin, \(u_0\) constant for \(r > a\) and such that (6.7) holds. Then the potential defined by \(V(r) = u_0'(r)/u_0(r)\) has infinite scattering length, and scattering theory approximated at leading order by \(H_{res}^M\).

It is interesting to note that the RPI models themselves obey (6.7) in the following sense: the zero energy generalised eigenfunction for \(M < 0\) is given by
\[
u_0 = 1 \oplus |M|^{1/2}.
\] (6.9)

Interpreting the integral in (6.7) for elements \(f \oplus \alpha\) of \(H_c \oplus \mathbb{C}\) as \(\int_0^a |f(r)|^2dr + |\alpha|^2\), the right hand side of equation (6.7) is then equal to \(M\). Similarly, for \(M > 0\), we interpret
the integral for $f \otimes \alpha \in \mathcal{H}_r \otimes \mathbb{C}$ as $\int_a^0 |f(r)|^2 dr - |\alpha|^2$ and use the generalised zero energy eigenfunction

$$u_0 = 1 \otimes |M|^{1/2} \quad (6.10)$$

to yield the value $M$.

We briefly consider the interpretation of the extension to the Hilbert space $\mathcal{H}_r$ in the case $M < 0$. From the fitting formula, it is clear that $M$ is negative if and only if the mean square value of $u_0(r)$ within $r < a$ exceeds $u_0(a)^2$. Hence this case is used to model Schrödinger operators whose zero energy generalised eigenfunctions are peaked inside the interaction region. This is characteristic of resonant behaviour and corresponds to a physical picture of a particle being detained inside the region, before being gradually released. If the radius of support is shrunk to a point, the particle must be completely removed from the space in order to model this process. It is therefore natural that the Hilbert space be extended in this case.

One may study the time behaviour of the proportion of a wavepacket in the extra dimension. Starting with a normalised vector $0 \oplus 1$, the evolved packet is given by $\mathcal{T}^{-1}_M e^{-ik^2t} \psi_M$. The proportion remaining in the initial state at time $t$ is

$$\varphi(t) = \langle \psi_M | e^{-ik^2t} \psi_M \rangle = \frac{2|M|}{\pi} \int_0^\infty dk \frac{e^{-ik^2t}}{1 + (kM)^2} \quad (6.11)$$

which may be approximated using the method of stationary phase to give

$$\varphi(t) \sim \frac{2|M|}{\sqrt{\pi t}} e^{-i\pi/4} + O(t^{-1}) \quad (6.12)$$

as $t \to \infty$. It is interesting that the decay is not exponential. The $M > 0$ case does not admit such a simple interpretation due to the redefinition of the space of physical states.

As a simple example of the use of the fitting formula, we consider the example of a square well with a zero energy resonance. Setting $V(r) = -((n+\frac{1}{2})\pi/a)^2$ ($n = 0, 1, 2, \ldots$) for $r < a$ and $V(r) = 0$ for $r > a$, we find $u_0(r) = \sin(n + \frac{1}{2})\pi r/a$. Equation (6.7) then yields $M = a/2$ for any value of $n$.

## 7 Conclusion

We have seen how PI and GPI models may be constructed and studied using integral transforms suggested by the scattering data. In addition, we have constructed a new class of RPI models (the case $M > 0$). The RPI models obey energy dependent boundary conditions and are defined on a Hilbert or Pontryagin space which extends the usual space of states. In the Pontryagin case a positive definite invariant subspace may be constructed which may be interpreted as the physical state space.
It is instructive to compare our methods with those usual in constructions of GPI models on Pontryagin spaces \([6]\). One starts with the desire to include wavefunctions with distributional terms in the space of states. Accordingly, choosing a dense subspace \(\mathcal{D} \subset \mathcal{H}_r\) and an anti-linear functional \(\omega\) (more generally \(m\) such functionals) on \(\mathcal{D}\) \((\omega \not\in \mathcal{H}_r)\) one constructs a linear space \(\mathcal{H}\) generated by elements

\[
\psi = \psi_0 + \lambda \omega
\]

with \(\psi_0 \in \mathcal{D}, \lambda \in \mathbb{C}\). The next step is to extend the Hilbert space inner product \(\langle \cdot | \cdot \rangle\) from \(\mathcal{D}\) to a sesquilinear form \((\cdot, \cdot)\) on \(\mathcal{H}\) by defining

\[
(\psi_0, \varphi_0) = \langle \psi_0 | \varphi_0 \rangle \quad \psi_0, \varphi_0 \in \mathcal{D}
\]

\[
(\psi_0, \omega) = \omega(\psi_0) \quad \psi_0 \in \mathcal{D}
\]

(recall that \(\omega\) is anti-linear). This leaves \((\omega, \omega)\) as a free parameter which is usually fixed on the basis of a physically inspired renormalisation of certain divergent integrals. The form \((\cdot, \cdot)\) is in general indefinite; however, there is a closely related positive definite inner product which is used to form the completion \(\mathcal{H}\) of \(\mathcal{H}\). With respect to \((\cdot, \cdot)\), \(\mathcal{H}\) is a Pontryagin space \(\mathcal{H}_r \oplus \mathbb{C} \ominus \mathbb{C}\). One can then seek the GPI models which ‘live’ on \(\mathcal{H}\).

The present treatment has various advantages over this procedure. Firstly, one need not determine the distribution \(\omega\) in advance; moreover the form of the Pontryagin space is suggested naturally by the over completeness of the generalised eigenfunctions \((1.5)\). Indeed, distributions need never explicitly occur in our construction; although it is clear (e.g. from the domain of definition of \(h_{\text{res}}^M\)) that the component of the wavefunction in the ‘extra dimension’ carries a distributional interpretation. Finally, it is not clear that the usual procedure can encompass the \(M > 0\) RPI models without modification, as the natural Pontryagin space is \(\mathcal{H}_r \oplus \mathbb{C}\) rather than \(\mathcal{H}_r \oplus \mathbb{C} \ominus \mathbb{C}\). It is possible that these models are restrictions of GPI models in the larger space; however, it seems more likely to us that a better starting point would be to choose a non-dense test space \(\mathcal{D}\) consisting of vectors orthogonal to a 1-dimensional subspace. It is not presently clear exactly how this would be implemented, nor what the appropriate distribution \(\omega\) would be.

The construction presented here has so far only been employed for interactions whose scattering is non-trivial only in the \(S\)-wave. One of the great strengths of the usual constructions is that the generalisation to higher angular momenta is relatively straightforward. It would be interesting to extend the present treatment to this case.

Finally, it is of interest to understand whether RPI models can arise as limits of sequences of Schrödinger operators with potentials of compact support decreasing to the origin, e.g. in the spirit of \([12]\) in which the usual class of PI is exhibited as strong resolvent limits of such sequences (see \([13]\) for a treatment using sequences of scaled potentials in the norm resolvent topology). We hope to address these issues elsewhere.

Acknowledgements: The notions of fitting formulae and the general methodology of Section 6 are due in origin to Bernard Kay \([12]\). I also thank Bernard for useful conversations and encouragement, and Churchill College, Cambridge, for financial support under a Gateway Studentship.
References

[1] Yu.M. Shirokov, Theor. Math. Phys. 46 191 (1981) and other papers in the same issue

[2] B.S. Pavlov, Theor. Math. Phys. 59 544 (1984)

[3] B.S. Pavlov, Russian Math. Surveys 42 127 (1987)

[4] B.S. Pavlov and A.A. Shushkov, Math. USSR. Sbornik 65 147 (1990)

[5] Yu.G. Shondin, Theor. Math. Phys. 64 937 (1985)

[6] Yu.G. Shondin, Theor. Math. Phys. 74 220 (1988)

[7] J.F. van Diejen and A. Tip, J. Math. Phys. 32 630 (1991)

[8] A. Grossmann and T.T. Wu, J. Math. Phys. 25 1742 (1984)

[9] C.J. Fewster and B.S. Kay, Low Energy Quantum Dynamics in Magnetic Fields of Small Support in preparation

[10] B. Thaller, The Dirac Equation (Springer-Verlag 1992)

[11] C.J. Fewster, Thin Wire Idealisations of the Dirac Equation in the Presence of a Flux Tube in preparation

[12] B.S. Kay and C.J. Fewster, When Can A Small Object Have A Big Effect At Large Scales? in preparation

[13] S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden, Solvable Models in Quantum Mechanics (Springer-Verlag, New York, 1988)

[14] R.G. Newton, Scattering Theory of Waves and Particles (McGraw-Hill, New York, 1966)

[15] M. Reed and B. Simon, Methods of Modern Mathematical Physics Vol II: Fourier Analysis, Self-Adjointness (Academic Press, New York, 1975)

[16] M. Reed and B. Simon, Methods of Modern Mathematical Physics Vol III: Scattering Theory (Academic Press, New York, 1979)

[17] E. Merzbacher, Quantum Mechanics 2nd ed. (Wiley, New York, 1970)

[18] J. Bognár, Indefinite Inner Product Spaces (Springer Verlag, Berlin, 1974)