Contact interactions in quantum physics.

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Contents

Symmetric operators and self adjoint extensions

Let A be an (linear) operator on an infinite dimensional separable Hilbert space $\mathcal{H}$, with dense domain $\mathcal{D}(A)$. In order to define its adjoint, let us define the following domain:

$$\mathcal{D}^\dagger := \{\psi \in \mathcal{H} \ , \ \exists\, \phi \in \mathcal{H} \ \text{such that} \ \langle \psi | A\varphi \rangle = \langle \phi | \varphi \rangle \, , \ \forall\, \varphi \in \mathcal{D}(A)\} \tag{1}$$

This ϕ is unique, so that one may define one (linear) operator $A^\dagger$ with domain $\mathcal{D}^\dagger$, such that

$$A^\dagger \psi = \phi \, , \qquad \forall\, \psi \in \mathcal{D}^\dagger \, . \tag{2}$$

The operator $A^\dagger$ is well defined and linear on $\mathcal{D}^\dagger$, due to the denseness of $\mathcal{D}(A)$. Note that $\mathcal{D}^\dagger \equiv \mathcal{D}(A^\dagger)$.

Let A and B two operators with respective (dense) domains $\mathcal{D}(A)$ and $\mathcal{D}(B)$. We say that B extends A, $A \prec B$, if

$$\mathcal{D}(A) \subset \mathcal{D}(B) \quad \text{and} \quad A\psi = B\psi\,, \forall\, \psi \in \mathcal{D}(A)\,. \tag{3}$$

A symmetric operator on an infinite dimensional separable Hilbert space $\mathcal{H}$, A with dense domain $\mathcal{D}(A)$ is defined as

$$\langle \psi | A\varphi \rangle = \langle A\psi | \varphi \rangle\,. \tag{4}$$

Note that if A is symmetric, then, $A \prec A^\dagger$.

A symmetric operator A is self adjoint if $A \equiv A^\dagger$. In this case, $\mathcal{D}(A) \equiv \mathcal{D}(A^\dagger)$.

For an operator A with domain $\mathcal{D}(A)$, we define its kernel $\mathcal{N}(A)$ as

$$\mathcal{N}(A) := \{\psi \in \mathcal{D}(A)\,, \ \ A\psi = \mathbf{0}\}\,. \tag{5}$$

On the von Neumann Theorem.

A symmetric operator may or may not have self adjoint extensions. The criteria are the following (I is the identity operator $I\psi = \psi$, $\forall\, \psi \in H$). Let A a be a symmetric operator. Then,

1.- A is essentially self adjoint if it has a unique self adjoint extension. In particular, a self adjoint operator is essentially self adjoint. The symmetric operator A is essentially self adjoint if and only if

$$\dim \mathcal{N}(A^\dagger \pm iI) = 0\,. \tag{6}$$

2.- The symmetric operator A has an infinite number of (non unitarily equivalent) self adjoint extensions if and only if

$$\dim \mathcal{N}(A^\dagger + iI) = \dim \mathcal{N}(A^\dagger - iI) \neq 0\,. \tag{7}$$

3.- The symmetric operator A does not have self adjoint extensions if and only if

$$\dim \mathcal{N}(A^\dagger + iI) \neq \dim \mathcal{N}(A^\dagger - iI)\,. \tag{8}$$

Theorem (von Neumann).- Let A be a symmetric operator. The domain of its adjoint is

$$\mathcal{D}(A^\dagger) = \mathcal{D}(A) \dot{+} \mathcal{N}(A^\dagger - iI) \dot{+} \mathcal{N}(A^\dagger + iI)\,. \tag{9}$$

If condition (7) is fulfilled, the self adjoint extensions of A is in one-to-one correspondence with the set of unitary operators

$$U : \mathcal{N}(A^\dagger - iI) \longmapsto \mathcal{N}(A^\dagger + iI)\,. \tag{10}$$

Let us call A_U the extension corresponding to the unitary mapping U as above.

Then,

$$\mathcal{D}(A_U) = \{\phi \in \mathcal{H}\,, \quad \phi = \psi + \varphi + U\varphi\}\,, \tag{11}$$

with

$$\psi \in \mathcal{D}(A)\,, \quad \varphi \in \mathcal{N}(A^\dagger - iI)\,. \tag{12}$$

and for all $\phi \in \mathcal{D}(A_U)$ as above

$$A_U\phi = A\psi + i\varphi - iU\varphi\,. \tag{13}$$

Theorem.- A symmetric operator A is essentially self adjoint if and only if $\mathrm{Ran}\,(A \pm iI)$ is dense in $\mathcal{H}$, or equivalently if and only if $\mathcal{N}(A^\dagger \pm iI) \equiv \{0\}$.

Examples

1.- Let $\mathcal{S}$ be the Schwartz space of all functions $f(x) : \mathbb{R} \longmapsto \mathbb{C}$ such that

i.) Are indefinitely differentiable at all points.

ii.) They verify that

$$\lim_{|x|\to\infty} x^n D^m f(x) = 0\,, \qquad n, m = 01, 2, \dots . \tag{14}$$

Then, $\mathcal{S} \subset L^2(\mathbb{R})$ with denseness. Define the operators Q and P on $\mathcal{S}$ as

$$[Qf](x) := x\, f(x)\,, \qquad [Pf](x) := -if'(x)\,, \qquad \forall\, f(x) \in \mathcal{S}\,. \tag{15}$$

Both are symmetric.

To see that Q is essentially self adjoint on $\mathcal{S}$, let us consider an arbitrary $f(x) \in \mathcal{S}$ and define

$$g_\pm(x) := \frac{f(x)}{x \pm i} \in \mathcal{S} \,. \tag{16}$$

Then,

$$(Q \pm iI) g_\pm(x) = f(x) \,. \tag{17}$$

Since $f(x)$ runs out all of $\mathcal{S}$, it results that $\mathrm{Ran}\,(Q \pm iI)$ is the whole $\mathcal{S}$ and is, therefore, dense in $L^2(\mathbb{R})$.

Due to the properties of the Fourier transform, $\mathrm{Ran}\,(P \pm iI)$ is also $\mathcal{S}$.

2.- Let us consider the Hilbert space $L^2[0,1]$. On this space, we may define $[Qf](x) := xf(x)$, for all $f(x) \in L^2[0,1]$. Then, Q is symmetric and bounded. Therefore, it is self adjoint.

Another story is P, defined as above: $[Pf](x) := -if'(x)$ with domain

$$\mathcal{D}(P) := \{f(x) \in C^1[0,1]\,, \quad f(0) = f(1) = 0\}\,. \tag{18}$$

Here, P is symmetric. However, let us calculate $\mathcal{N}(P^\dagger \pm iI)$. Since $P = -id/dx$, and $P^\dagger$ extends P, then, $P^\dagger = -id/dx$.

The deficiency indices for some symmetric operator are

$$n_\pm := \dim \mathcal{N}(A^\dagger \pm iI)\,. \tag{19}$$

In order to calculate them for P, we have:

$$(P^\dagger \pm iI)f(x) = 0 \Longrightarrow -if'(x) \pm f(x) = 0\,. \tag{20}$$

This gives the following pair of differential equations:

$$-if'(x) + f(x) = 0 \Longrightarrow f'(x) + if(x) = 0 \Longrightarrow f(x) = A\,e^{-x}\,, \tag{21}$$

$$-if'(x) - f(x) = 0 \Longrightarrow f'(x) - if(x) = 0 \Longrightarrow f(x) = B\,e^{x}\,. \tag{22}$$

Both functions $e^{-x}, e^{x} \in L^2[0,1]$, and therefore, $n_+ = n_- = 1$.

Thus, $\dim \mathcal{N}(P^\dagger \pm iI) = 1$. There is only one possibility for U and is $U = e^{i\alpha}$, with $\alpha \in [0, 2\pi)$. There are an infinite number of (non-equivalent) self adjoint extensions labelled by $\alpha \in [0, 2\pi)$.

The domain of $P^\dagger$ is now,

$$\mathcal{D}(P^\dagger) \equiv C^1[0,1]\,. \tag{23}$$

Thus, the domain of each of the $P_U \equiv P_\alpha$ for fixed $\alpha \in [0, 2\pi)$ should be

$$\mathcal{D}(P_\alpha) = \{f(x) \in C^1[0,1]\,,\ \ f(0) = e^{i\alpha} f(1)\}\,, \tag{24}$$

with $P_\alpha f(x) := -if'(x)$.

3.- Take the Hilbert space $L^2[0,\infty)$. By performing exactly the same procedure, we note that $e^{-x} \in L^2[0,\infty)$ and $e^{x} \notin L^2[0,\infty)$, so that $n_+ = 1$ and $n_- = 0$. Both deficiency indices are different and P on $L^2[0,\infty)$ does not have self adjoint extensions.

A particularly interesting example

Let $L^2(\mathbb{R})$ be and

$$A := -\frac{d^2}{dx^2} \quad \text{on} \quad \mathcal{D}(A) := \{f(x) \in W_2^2(\mathbb{R})\,, \quad f(0) = f'(0) = 0\}\,. \tag{25}$$

The domain of the adjoint $A^\dagger$ is

$$\mathcal{D}(A^\dagger) \equiv W_2^2(\mathbb{R}/\{0\})\,. \tag{26}$$

Let us calculate the deficiency indices of A. For n_+:

$$x < 0\,, \quad -f''(x) + if(x) = 0\,, \implies \tag{27}$$

$$f_-(x) = C \exp\left\{\frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}\right\} x + D \exp\left\{-\frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}\right\} x\,, \tag{28}$$

anf $f_-(x) = 0$ for $x > 0$.

$$x > 0\,, \quad -f''(x) + if(x) = 0\,, \implies \tag{29}$$

$$f_+(x) = C\,\exp\left\{\frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}\right\}x + D\exp\left\{-\frac{\sqrt{2}}{2} + i\frac{\sqrt{2}}{2}\right\}x\,, \tag{30}$$

and $f_+(x) = 0$ for $x < 0$.

Therefore, $n_+ = 2$. Analogously, $n_- = 2$.

The set of all unitary operators

$$U : \mathcal{N}(A^\dagger - iI) \longmapsto \mathcal{N}(A^\dagger + iI)\,, \quad U = e^{i\varphi}\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{31}$$

depends of 4 real parameters ($\det U = 1$). Consequently, the set of all self adjoint extensions of A depends of 4 real parameters.

Matching conditions at the origin

There is another way to fix the self adjoint extensions by using matching conditions at the origin.

Let $\varphi(x), \psi(x) \in \mathcal{D}(A^\dagger)$. Then,

$$\begin{aligned}
\langle\varphi| - \psi''\rangle &= \int_{-\infty}^{0} \varphi(x)[-\psi''(x)]\,dx + \int_{0}^{\infty} \varphi(x)[-\psi''(x)]\,dx \\
&= \varphi(0-)[-\psi'(0-)] - \int_{-\infty}^{0} \varphi'(x)[-\psi'(x)]\,dx \\
&\quad -\varphi(0+)[-\psi'(0+)] - \int_{0}^{\infty} \varphi'(x)[-\psi'(x)]\,dx\,, \qquad (32)
\end{aligned}$$

which gives,

$$= \varphi(0-)[-\psi'(0-)] - \varphi(0+)[-\psi'(0+)]$$

$$-\varphi'(0-)[-\psi(0-)] + \varphi'(0+)[-\psi(0+)] + \langle -\varphi''|\psi\rangle \,. \tag{33}$$

Thus, domains for the self adjointness of the extensions of A are characterized by the following matching conditions at the origin:

$$\psi(0-)\varphi'(0-) - \psi'(0-)\varphi(0-) = \varphi(0+)\psi'(0+) - \varphi'(0+)\psi(0+)\,, \tag{34}$$

which in matrix form reads for any $\varphi(x) \in \mathcal{D}(A^\dagger)$:

$$\begin{pmatrix} \varphi(0+) \\ \varphi'(0+) \end{pmatrix} = e^{i\lambda} \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \varphi(0-) \\ \varphi'(0-) \end{pmatrix}, \tag{35}$$

where λ is real and A, B, C, D being real numbers with $AD - BC = 1$. In the sequel, we denote the matrix M as

$$M := \begin{pmatrix} A & B \\ C & D \end{pmatrix} . \tag{36}$$

This self adjoint extensions have been classified in: Kurasov P 1996 Distribution theory for discontinuous test functions and differential operators with generalized coefficients J. Math. Anal. Appl. **201**(1), 297-323.

One may also define domains for A, for which its functions show similar jumps on a finite set of real numbers $\{x_1, x_2, \ldots, x_N\}$. A self adjoint extension of A would be fixed by giving a relation like (35) at each of the points $\{x_1, x_2, \ldots, x_N\}$.

Particular cases of interest

One dimensional Dirac delta interaction at the origin. The Schrödinger equation is (assume that $\psi(x)$ is continuous at the origin)

$$-\psi''(x) + \alpha\,\delta(x)\,\psi(x) = E\psi(x)\,. \tag{37}$$

Then, let us integrate

$$-\int_{-\varepsilon}^{\varepsilon} \psi''(x)\,dx + \alpha \int_{-\varepsilon}^{\varepsilon} \delta(x)\,\psi(x)\,dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x)\,dx\,, \tag{38}$$

which gives

$$-[\psi'(\varepsilon) - \psi'(-\varepsilon)] + \alpha\,\psi(0) = E[\Phi(\varepsilon) - \Phi(-\varepsilon)]\,. \tag{39}$$

Taking limits as $\varepsilon \longmapsto 0$, one has

$$-\psi'(0+) + \psi'(0-) + \alpha\,\psi(0) = 0\,. \tag{40}$$

In matrix form,

$$\begin{pmatrix} \psi(0+) \\ \psi'(0+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \psi'(0-) \end{pmatrix}, \tag{41}$$

which obeys to the form (35). The consequence is that the Dirac delta potential emerges after the choice of a suitable selfadjoint extension of the symmetric operator A.

A similar expression can be obtained if the delta would be centered in another point different from the origin. If the Schrödinger equation as in (36) were of the form

$$-\psi''(x) + \sum_{n=1}^{N} \alpha_n \, \delta(x - x_i) \, \psi(x) = E \, \psi(x) \,, \tag{42}$$

then, the Dirac delta interaction at each of the points x_i, $i = 1, 2, \ldots, N$ is defined by a matching condition similar to (41).

Let us call $\Omega := \{x_1, x_2, \dots, x_N\}$ a set of N points in the real axis. Let $\mathcal{D}_\Omega$ be the space of all compact support functions, which are indefinitely differentiable, except at the points of Ω at which these functions and their first derivatives may have a finite jump.

For each $\psi(x) \in \mathcal{D}_\Omega$ and x an arbitrary real number, one defines:

$$\tilde{\delta}_x(\psi) := \frac{\psi(x-) + \psi(x+)}{2}\,, \quad \tilde{\delta}'_x(\psi) := -\frac{\psi'(x-) + \psi'(x+)}{2}\,. \tag{43}$$

The second derivative of any function $\psi(x) \in \mathcal{D}_\Omega$ in the distributional sense is

$$\frac{d^2\psi(x)}{dx^2} = \left[\frac{d^2\psi(x)}{dx^2}\right] + \sum_{n=1}^{N} \left([\psi']_{x_n}\delta(x - x_n) + [\psi]_{x_n}\delta'(x - x_n)\right), \tag{44}$$

$$[\psi]_{x_n} := \psi(x_n+) - \psi(x_n-)\,, \quad n = 1, 2, \dots, N\,. \tag{45}$$

Then, one defines the following distributional products ($\psi(x) \in \mathcal{D}_\Omega$):

$$\psi(x)\,\delta(x-x_n) = \tilde{\delta}_{x_n}(\psi)\,\delta(x-x_n)\,, \tag{46}$$

$$\psi(x)\,\delta'(x-x_n) = \tilde{\delta}_{x_n}(\psi)\,\delta'(x-x_n) + \tilde{\delta}'_{x_n}(\psi)\,\delta(x-x_n)\,. \tag{47}$$

Consider now the following Hamiltonian:

$$H := -\frac{d^2}{dx^2} + \sum_{n=1}^{N} \left(\alpha_n\,\delta(x-x_n) + \beta_n\,\delta'(x-x_n)\right). \tag{48}$$

Then, when applied to $\psi(x) \in \mathcal{D}_\Omega$ gives:

$$\left[-\frac{d^2\psi(x)}{dx^2}\right]$$

$$+\sum_{n=1}^{N}\left(-[\psi']_{x_n}+\alpha_n\,\tilde{\delta}_{x_n}(\psi)+\beta_n\,\tilde{\delta}'_{x_n}(\psi)\right)\delta(x-x_n)$$

$$+\sum_{n=1}^{N}\left(-[\psi]_{x_n}+\beta_n\,\tilde{\delta}_{x_n}(\psi)\right)\delta'(x-x_n)\,. \tag{49}$$

This gives a function in $L^2(\mathbb{R})$ if and only if the coefficients of $\delta(x-x_n)$ and $\delta'(x-x_n)$ vanish identically.

This is equivalent to say that for each $x_n \in \Omega$, one has the following matching condition for the function ψ:

$$\begin{pmatrix} \psi(x_n+) \\ \psi'(x_n+) \end{pmatrix} = \begin{pmatrix} \dfrac{2+\beta_n}{2-\beta_n} & 0 \\ \dfrac{4\alpha_n}{4-\beta_n^2} & \dfrac{2-\beta_n}{2+\beta_n} \end{pmatrix} \begin{pmatrix} \psi(x_n-) \\ \psi'(x_n-) \end{pmatrix} . \tag{50}$$

Note.- For the matrix giving the matching conditions in, say, the origin,

$$\begin{pmatrix} 1 & \beta \\ 0 & 1 \end{pmatrix} , \tag{51}$$

we obtain another self adjoint extension:

$$-\frac{d^2}{dx^2} + \beta\,\delta'(x)\,. \tag{52}$$

Contents

Tempered distributions

A one dimensional Schwartz function is

$$f(x) : \mathbb{R} \longmapsto \mathbb{C}\,, \tag{53}$$

such that

1.- $f(x) \in C^\infty(\mathbb{R})$, and
2.- For all $n, m = 0, 1, 2, \dots$, one has

$$\lim_{|x|\to\infty} x^n \, \frac{d^m}{dx^m} \, f(x) = 0\,. \tag{54}$$

These Schwartz functions form a linear space $\mathcal{S}$, the Schwartz space. In addition,

$$\mathcal{S} \subset L^2(\mathbb{R}) \subset \mathcal{S}^\times\,. \tag{55}$$

Any $T \in \mathcal{S}^\times$ is a tempered distribution.

The order of a distribution.

Regularity Theorem: Let $T \in \mathcal{S}$. Then, $T = g^{(k}(x)$, in the distributional sense, for some polynomially bounded continuous function $g(x) : \mathbb{R} \longmapsto \mathbb{C}$, so that for all $\varphi(x) \in \mathcal{S}$, we have

$$\langle T|\varphi\rangle = \int_{-\infty}^{\infty} (-1)^k g(x)\, \varphi^{(k}(x)\, dx\,. \qquad (56)$$

Singular order: A distribution $T \in \mathcal{S}^\times$ is said to have singular order $r \in \mathbb{Z}$ on a closed finite interval $I \subset \mathbb{R}$ if $T = f^{(r+2}(x)$, where $f(x)$ is a distribution corresponding to a continuous although not differentiable function on I and $f^{(r+2}(x)$ is the $(r+2)$-th distributional derivative of $f(x)$.

Examples,

1.- An infinitely smooth function, $f(x) \in C^\infty(I)$, is said to have order $r = -\infty$.

2.- The Heaviside step function, $H(x)$, has singular order $r = -1$.

3.- The primitive of $H(x)$ has singular order $r = -2$.

4.- The Dirac delta $\delta(x)$ has singular order $r = 0$.

5.- The derivative in the distributional sense $\delta'(x)$ has singular order $r = 1$.

Distributions with $r \leq -2$ are regular, while distributions with $r \geq 0$ are singular.

The Schödinger equation with point potentials

Let us consider the Schrödinger equation,

$$\psi''(x) + k^2\psi(x) = V(x)\,\psi(x)\,, \tag{57}$$

and assume that the potential $V(x)$ is not given by a regular locally integrable function, but instead to other kind of interaction such as a tempered distribution. Let us see how this interaction should be.

Let us consider

$$\psi''(x) + k^2\psi(x) = s[\psi](x)\,. \tag{58}$$

Here, the prime indicates distributional derivative.

In (58), in any interval which does not include the singularities of $V(x)$, the potential is regular and the function $\psi(x)$ continuous. At these points, $V(x)\,\psi(x) \equiv s[\psi](x)$.

To determine the most general kind of interaction $s[\psi](x)$, supported at the origin, we require that

- The following relation between the supports: $\text{supp } s[\psi](x) \subset \text{supp } V(x)$.
- The singular order of the distribution $s[\psi](x)$ cannot exceed the singular order of $V(x)$ in any closed subset of its support.
- The probability current density must be conserved everywhere, in particular across the singular point.

The probability current density is given by

$$j(x) := \frac{\hbar}{2mi}\left[\psi^*(x)\,\frac{\partial\,\psi(x)}{\partial\,x} - \psi(x)\,\frac{\partial\,\psi^*(x)}{\partial\,x}\right]. \tag{59}$$

An important result is the following:

A necessary and sufficient condition for a distribution $T \equiv f(x)$ to have the origin as a support is that it can be written as a finite sum of the form:

$$f(x) = \sum_{m=0}^{r_s} \alpha_m \, \delta^{(m}(x) \,, \qquad \alpha_{r_s} \neq 0 \,. \tag{60}$$

Consequently,

$$s[\psi](x) = \sum_{m=0}^{r_s} \alpha_m[\psi] \, \delta^{(m}(x) \,. \tag{61}$$

Note that m is the singular order of the corresponding term in (61). Also,

$$\alpha_m[\psi] = \alpha_m[\psi(0\pm), \psi'(0\pm)] \tag{62}$$

is a linear functional.

This result is rather straightforward:

The maximum singular order for the interaction $s[\psi](x)$ compatible with $\psi(x)$ being square integrable is $r_s = 1$. Then,

$$s[\psi](x) = \alpha_0[\psi]\,\delta(x) + \alpha_1[\psi]\,\delta'(x)\,. \tag{63}$$

The coefficients $\alpha_0[\psi]$ and $\alpha_1[\psi]$ should be determined in accordance with the previous requirements. Let us go back to equation (58) with (63), which gives:

$$\psi''(x) + k^2\psi(x) = \alpha_0[\psi]\,\delta(x) + \alpha_1[\psi]\,\delta'(x)\,, \tag{64}$$

and take the first primitive. This gives:

$$\psi'(x) + k^2\,\psi^{(-1)}(x) = \alpha_0[\psi]\,H(x) + \alpha_1[\psi]\,\delta(x) + c_1\,, \tag{65}$$

which, taking into account the continuity of $\psi^{(-1)}(x)$ at the origin, gives

$$\psi'(0+) - \psi'(0-) = \alpha_0[\psi]\,. \tag{66}$$

Now, taken the primitive of (65) and using the same idea, we have that

$$\psi(0+) - \psi(0-) = \alpha_1[\psi]\,. \tag{67}$$

Let us write

$$\Phi(x) := \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix}. \tag{68}$$

Using the current conservation at the origin, i.e., $j(0+) = j(0-)$, and after some procedures, it results that (66)-(67) can be written in the following form:

$$\Phi(0+) = \Lambda\,\Phi(0-)\,, \quad \Lambda = e^{i\varphi}\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad ad - cd = 1\,. \tag{69}$$

The final result is

$$s[\psi](x) = \left[c\, e^{i\varphi}\, \psi(0-) + \left(d\, e^{i\varphi} - 1\right) \psi'(0-)\right] \delta(x)$$

$$+ \left[\left(a\, e^{i\varphi} - 1\right) \psi(0-) + b\, e^{i\varphi}\, \psi'(0-)\right] \delta'(x)\,. \tag{70}$$

There is another possibility, which is

$$\psi'(0\pm) = h_\pm\, \psi(0\pm)\,, \qquad h_\pm \in \mathbb{R} \cup \{\infty\}\,, \tag{71}$$

which gives

$$s[\psi](x) = [h_+\, \psi(0+) - h_- \psi(0-)]\; \delta(x) + [\psi(0+) - \psi(0-)]\; \delta'(x)$$

$$= [\psi'(0+) - \psi'(0-)]\; \delta(x) + \left[h_+^{-1}\, \psi'(0+) - h_-^{-1} \psi'(0-)\right]\; \delta'(x)\,. \tag{72}$$

M. Calçada, J.T. Lunardi, L.A. Manzoni, W. Monteiro, Distributional approach to point interactions in one-dimensional quantum mechanics, Frontiers in Physics, **2**, 23 (2014).

One dimensional Dirac equation

Let us consider the Dirac equation:

$$\left(i\alpha_x \frac{d}{dx} - \beta\, m + E\right)\psi(x) = V(x)\,\psi(x)\,, \tag{73}$$

with

$$\alpha_x := \sigma_3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \beta := \sigma_1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{74}$$

and

$$\psi(x) = (u(x), v(x))^T\,. \tag{75}$$

The Dirac equation with an arbitrary potential supported at the origin should have the form:

$$\left(i\alpha_x \frac{d}{dx} - \beta\, m + E\right)\psi(x) = S[\psi](x)\,. \tag{76}$$

Under the same requirements than in the Schrödinger case, we must have that

$$S[\psi](x) = \sum_{n=1}^{r_s} \Omega_n[\psi]\,\delta^{(n}(x)\,, \tag{77}$$

with

$$\Omega_n[\psi] = (\varphi_n^0[\psi], \varphi_n^1[\psi])^T\,. \tag{78}$$

Here, the equation has a first order derivative only, so that

$$S[\psi](x) = \Omega_0[\psi]\,\delta(x)\,, \qquad \Omega_0[\psi] = \begin{pmatrix} \varphi^0[\psi] \\ \\ \varphi^1[\psi] \end{pmatrix}\,. \tag{79}$$

If we use relation (79) into the Dirac equation (76), we obtain by following a similar procedure as in the Schrödiger case (note that the primitive of $\psi(x)$ is continuous at the origin),

$$\psi(0+) - \psi(0-) = -i\alpha_x\,\Omega_0[\psi]\,. \tag{80}$$

Then, using (79) into (76), we obtain two equations, one for each component of $\psi(x) = (u(x), v(x))^T$, which are

$$v(x) = \frac{1}{E+m}\left[\varphi^1[\psi]\,\delta(x) - iu'(x)\right], \tag{81}$$

and

$$u''(x) + k_r^2\, u(x) = (E+m)\, \varphi^0[\psi]\, \delta(x) - i\varphi^1[\psi]\, \delta'(x)\,, \tag{82}$$

with

$$k_r := \sqrt{E^2 - m^2}\,. \tag{83}$$

Let us recall the Schrödinger equation (58)

$$\psi''(x) + k^2\, \psi(x) = \alpha_0\, \delta(x) + \alpha_1\, \delta'(x)\,, \tag{84}$$

and compare it with (83). It results that $\alpha_0 = (E+m)\,\varphi^0[\psi]$ and $\alpha_1 = -i\varphi^1[\psi]$. Consequently, all results of the previous section are valido for the $u(x)$ component of the spinor.

For the $v(x)$ component and taking into account (81), we obtain the following relations at the origin:

$$v(0\pm) = -\frac{i}{E+m}\, u'(0\pm)\,. \tag{85}$$

In the Schrödinger case, we have used the probability current conservation in order to establish the boundary conditions at the origin. Here, we should do the same for $u(x)$. Here,

$$j^1(x) = \psi^\dagger(x)\,\alpha_x\,\psi(x) = u^*(x)\,v(x) + u(x)\,v^*(x)\,. \qquad (86)$$

Then, using (85) one concludes that

$$j^1(0\pm) = \frac{1}{i(E+m)}\;\left[u^*(\pm)\,u'(0\pm) - {u'}^*(0\pm)\,u(0\pm)\right] \qquad (87)$$

The conservation of (87) ate the origin provide the boundary conditions ate the origin. In the ordinary case, we have that

$$\psi(0+) = \Lambda_r\,\psi(0-)\,, \qquad (88)$$

with

$$\Lambda_r = e^{i\varphi_r}\begin{pmatrix} a_r & ib_r \\ -ic_r & d_r \end{pmatrix}\,, \qquad a_r\,d_r - b_r\,c_r = 1\,. \qquad (89)$$

Nonetheless, there exists some other possible boundary conditions:

$$v(0\pm) = ih_r^{\pm}\, u(0\pm)\,, \qquad h_r^{\pm} \in \mathbb{R} \cup \{\infty\}\,. \tag{90}$$

Observe that if $h_r^{\pm} = 0$, then $v(0\pm) = 0$ and if $h_r^{\pm} = \infty$, then, $u(0\pm) = 0$. These are called the separated solutions.

Then for the first situation, we have that

$$S[\psi](x) = i\alpha_x\,(\Lambda_r - 1)\,\psi(0-)\,\delta(x)\,. \tag{91}$$

For the second,

$$S[\psi](x) = i\alpha_x \left[\begin{pmatrix} 1 & 0 \\ ih_r^{+} & 0 \end{pmatrix} \psi(0+) - \begin{pmatrix} 1 & 0 \\ ih_r^{-} & 0 \end{pmatrix} \psi(0-) \right] \delta(x)\,. \tag{92}$$

In order to analyze the non-relativistic limit, its is interesting to write the equation on $u(x)$ in terms of the above parameters. For the first case, we have:

$$u''(x) + k_r\, u(x) = \left[(E+m)c_r\, e^{i\varphi_r}\, u(0-) + \left(d_r\, e^{i\varphi_r} - 1\right) u'(0-)\right] \delta(x)$$

$$+ \left[\left(a_r\, e^{i\varphi_r} - 1\right) u(0-) + \frac{b_r}{E+m}\, e^{i\varphi_r}\, u'(0-)\right] \delta'(x)\,. \quad (93)$$

For the second case,

$$u''(x) + k_r\, u(x) = (E+m)\left[-h_r^+\, u(0+) + h_r^-\, u(0-)\right]\, \delta(x)$$

$$+[u(0+) - u(0-)]\, \delta'(x)\,. \qquad (94)$$

The non-relativistic limit is reached with $E \to m$, $k_r \to k$.

For instance, the relativistic interaction with a non-relativistic limit corres ponding to an interaction of type $\gamma\,\delta(x)$ is given by the values of the parameters $\varphi_r = b_r = 0$, $a_r = d_r = 1$, $c_r = \gamma$.

For $\varphi_r = c_r = 0$, $a_r = d_r = 1$ and $b_r = -\gamma$, one would have as non-relativistic limit $-\gamma/(4m^2)\,\delta'(x)$.

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A semirelativistic model

Let us consider the one dimensional Salpeter Hamiltonian:

$$H_0 = \sqrt{P^2 + m^2}\,, \qquad P = -i\frac{d}{dx}\,. \tag{95}$$

On the domain,

$$\mathcal{D} = \{\varphi(x) \in C_0^\infty(\mathbb{R})\,,\ \ \varphi(0) = 0\}\,. \tag{96}$$

This operator is symmetric with deficiency indices $n_\pm = 1$. Then, one may expect that its self adjoint extensions have the form

$$H = \sqrt{P^2 + m^2} - \lambda\,\delta(x)\,, \qquad \lambda \in \mathbb{R}\,. \tag{97}$$

Similarly, using the domain

$$\mathcal{D} = \{\varphi(x) \in C_0^\infty(\mathbb{R})\,, \;\; \varphi(a_1) = \cdots = \varphi(a_n) = 0\}\,, \tag{98}$$

one expect that its self adjoint extensions are of the form:

$$H = \sqrt{P^2 + m^2} - \sum_{i=1}^{n} \lambda_i\, \delta(x - a_i)$$

$$= H_0 - \sum_{i=1}^{n} \lambda_i\, \delta(x - a_i)\,, \quad \lambda_i \in \mathbb{R}\,, \;\; i = 1, 2, \ldots, n\,. \tag{99}$$

Let us analyze the possibility of a definition of this formal Hamiltonian as a self adjoint extension of the Salpeter Hamiltonian.

For convenience, we use here a notation a la Dirac, so that

$$\psi(x) \equiv \langle x|\psi\rangle \,. \tag{100}$$

Then, for $a \in \mathbb{R}$,

$$\delta(x-a) \equiv |a\rangle\langle a| \,, \tag{101}$$

since,

$$\langle x|a\rangle\langle a|\psi\rangle = \delta(x-a)\,\psi(a) = \delta(x-a)\,\psi(x) \,. \tag{102}$$

The Schrödinger equation is now:

$$\langle x| \left(H_0 - \sum_{i=1}^{n} \lambda_i \, |a_i\rangle\langle a_i| \right) |\psi\rangle = \langle x|E\psi\rangle = E\psi(x) \,. \tag{103}$$

The heat kernel and regularization of the Hamiltonian

The Heat kernel for H_0 is a solution of the following equation:

$$H_0\, K_t(x,y) = -\frac{\partial\, K_t(x,y)}{\partial\, t}\,. \tag{104}$$

Now for the regularization of the Hamiltonian, we propose,

$$H_\epsilon := H_0 - \sum_{i=1}^{n} \lambda_i(\epsilon)\, |a_i^\epsilon\rangle\langle a_i^\epsilon|\,, \tag{105}$$

with

$$K_{\epsilon/2}(x,y) = \langle x|a_i^\epsilon\rangle\,, \tag{106}$$

$\epsilon > 0$ being a short time cut off. This definition is motivated by the fact that

$$\lim_{\epsilon\to 0^+} \langle x|a_i^\epsilon\rangle = \langle x|a_i\rangle = \delta(x-a_i)\,. \tag{107}$$

Resolvent

To find the resolvent $R_\epsilon = (H_\epsilon - E)^{-1}$, we assume that $E \notin \sigma(H_0)$ and write

$$\left(H_0 - \sum_{i=1}^{n} \lambda_i(\epsilon) \, |a_i^\epsilon\rangle\langle a_i^\epsilon| - E \right) |\psi\rangle = |\rho\rangle \,. \tag{108}$$

Let

$$|f_i^\epsilon\rangle := \sqrt{\lambda_i(\epsilon)} \, |a_i^\epsilon\rangle \Longrightarrow \langle x | f_i^\epsilon \rangle = \sqrt{\lambda_i(\epsilon)} \, K_{\epsilon/2}(x, a_i) \,, \tag{109}$$

and apply $(H_0 - E)^{-1}$ to (108), so as to get

$$|\psi\rangle = \sum_{j=1}^{n} (H_0 - E)^{-1} \, |f_j^\epsilon\rangle\langle f_j^\epsilon | \psi\rangle + (H_0 - E)^{-1} \, |\rho\rangle \,. \tag{110}$$

We apply $\langle f_i^\epsilon|$ to (110) and obtain

$$\sum_{j=1}^{n} T_{ij}(\epsilon, E)\,\langle f_j^\epsilon|\psi\rangle = \langle f_i^\epsilon|H_0 - E)^{-1}\,|\rho\rangle\,, \tag{111}$$

where,

$$T_{ij}(\epsilon, E) := \left\{ \begin{array}{ll} 1 - \langle f_i^\epsilon|(H_0 - E)^{-1}|f_i^\epsilon\rangle & \text{if} \quad i = j\,, \\ \\ -\langle f_i^\epsilon|(H_0 - E)^{-1}|f_j^\epsilon\rangle & \text{if} \quad i \neq j\,. \end{array} \right. \tag{112}$$

Next, solve equation (111) in the variables $\langle f_j^\epsilon|\psi\rangle$ and use this result in (110). One obtains:

$$R_\epsilon(E) = (H_\epsilon - E)^{-1} = (H_0 - E)^{-1} + (H_0 - E)^{-1}$$

$$\times \left(\sum_{i,j=1}^{n} |f_i^\epsilon\rangle [T^{-1}(\epsilon, E)]_{ij} \langle f_j^\epsilon| \right) (H_0 - E)^{-1}\,. \tag{113}$$

We may write the above resolvent in terms of the original variables as

$$R_\epsilon(E) = (H_\epsilon - E)^{-1} = (H_0 - E)^{-1} + (H_0 - E)^{-1} \times \left(\sum_{i,j=1}^{n} |a_i^\epsilon\rangle [\Phi^{-1}(\epsilon, E)]_{ij} \langle a_j^\epsilon| \right) (H_0 - E)^{-1} \,, \tag{114}$$

with

$$\Phi_{ij}(\epsilon, E) := \begin{cases} \lambda_i^{-1}(\epsilon) - \langle a_i^\epsilon|(H_0 - E)^{-1}|a_i^\epsilon\rangle & \text{if} \quad i = j \,, \\ -\langle a_i^\epsilon|(H_0 - E)^{-1}|a_j^\epsilon\rangle & \text{if} \quad i \neq j \,. \end{cases} \tag{115}$$

We can express the resolvent of the free Hamiltonian in terms of the heat kernel associated with H_0 as

$$(H_0 - E)^{-1} = \int_0^\infty dt\, e^{-t(H_0 - E)}\,, \tag{116}$$

which have sense if Real $E < m$, ($H_0 = \sqrt{P^2 + m^2}$) and $t \geq 0$. In terms of the Green function, one may write

$$\langle x|(H_0 - E)^{-1}|y\rangle = \int_0^\infty dt\, K_t(x,y)\, e^{tE}\,. \tag{117}$$

Then, using the properties of the heat Kernel, one has

$$\langle a_i^\epsilon|(H_0 - E)^{-1}|a_j^\epsilon\rangle = \int_0^\infty dt\, K_{t+\epsilon}(a_i, a_j)\, e^{tE}\,. \tag{118}$$

The explicit expression of the Heat kernel has been obtained (Lieb and Loss) and is ($x, y \in \mathbb{R}$ and $t \geq 0$)

$$K_t(x,y) = \frac{mt}{\pi\sqrt{(x-y)^2+t^2}}\, K_1\left(m\sqrt{(x-y)^2+t^2}\right)\,, \qquad (119)$$

where $K_1(-)$ is the modified Bessel function of the first kind.

If we take the limit as $\epsilon \longmapsto 0^+$, under the above conditions, we have

$$\lim_{\epsilon\to 0^+} \langle a_i^\epsilon|(H_0-E)^{-1}|a_j^\epsilon\rangle = \int_0^\infty dt\, K_t(a_i,a_j)\, e^{tE}\,. \qquad (120)$$

This integral converges if $i \neq j$ and diverges if $i = j$.

For $i \neq j$, we have obtained a proper limit

$$\Phi_{i,j}(E) = -\int_0^\infty dt\, K_t(a_i,a_j)\, e^{tE}\,. \qquad (121)$$

For $i = j$, we need to use a regularization process. Recall that

$$\Phi_{i,i}(\epsilon, E) = \frac{1}{\lambda_i(\epsilon)} - \int_0^\infty dt\, K_{t+\epsilon}(a_i, a_i)\, e^{tE}\,. \tag{122}$$

Here, the usual procedure is to compensate the divergence on the limit $\epsilon \to 0^+$ in the integral with a divergence on the other term. Then,

$$\frac{1}{\lambda_i(\epsilon)} = \frac{1}{\lambda_i(M_i)} + \int_0^\infty dt\, K_{t+\epsilon}(a_i, a_i)\, e^{tM_i}\,, \tag{123}$$

where M_i is a renormalization scale. Then, in the limit as $\epsilon \to 0^+$,

$$\Phi_{i,i}(E) = \frac{1}{\lambda_i(M_i)} + \int_0^\infty dt\, K_{t+\epsilon}(a_i, a_i)\,(e^{tM_i} - e^{tE})\,. \tag{124}$$

However, the physical meaning of M_i is not clear.

The good news are that the renormalization scale may be eliminated. In fact, bound states are the poles of the resolvent, so that the bound state energy at the center i, E_B^i, is a solution of $\Phi_{i,i}(E_B^i) = 0$ with $E < m$. Then, one may replace (124) by

$$\Phi_{i,i}(E) = \int_0^\infty dt\, K_{t+\epsilon}(a_i, a_i)\, (e^{tE_B^i} - e^{tE})\,. \tag{125}$$

Then, the $\lim_{\epsilon\to 0^+} R_\epsilon(E)$ is given by

$$R(E) = (H-E)^{-1} = (H_0 - E)^{-1} + (H_0 - E)^{-1}$$

$$\times \left(\sum_{i,j} |a_i\rangle [\Phi^{-1}(E)]_{i,j} \langle a_j| \right) (H_0 - E)^{-1}\,. \tag{126}$$

One can prove that this is the resolvent of a self adjoint operator H, identified with (99) .

Using this model, we have analyzed among other issues

- Bound state spectrum, which are real solutions of $\det[\Phi(E)] = 0$.
- Scattering wave functions. Transmission and reflection coefficients.
- Bound states and scattering coefficients in the massless case,

F. Erman, M. Gadella, H. Uncu, One-dimensional semi-relativistic Hamiltonian with multiple Dirac delta potentials, Phys. Rev. D, **95**, 045004 (2017).

E. H. Lieb and M. Loss, *Analysis*, AMS, Providence, RI, 2001.

Contents

N deltas

Now, let us consider the following Schrödinger equation:

$$-\frac{\hbar}{2m}\,\frac{d^2\psi(x)}{dx^2}-\sum_{i=1}^{N}\lambda_i\,\delta(x-a_i)\,\psi(x)=E\,\psi(x)\,, \tag{127}$$

where a_i, $\lambda_i>0$, $i=1,2,\dots,N$ are real numbers. This is the Schrödinger equation of a Hamiltonian of the type $H=H_0+V$, where $H_0=P^2/(2m)$ corresponds to the free particle and

$$V=-\sum_{i=1}^{N}\lambda_i\,|a_i\rangle\langle a_i|\,. \tag{128}$$

Writing $|f_i\rangle:=\sqrt{\lambda_i}\,|a_i\rangle$, one has

$$\langle x|\frac{P^2}{2m}|\psi\rangle-\sum_{i=1}^{N}\langle x|f_i\rangle\langle f_i|\psi\rangle=E\,\langle x|\psi\rangle\,. \tag{129}$$

The identity in the momentum space may be represented as

$$I = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,|p\rangle\langle p|\,, \tag{130}$$

where $P|p\rangle = p\,|p\rangle$, for all $p \in \mathbb{R}$. Let us carry this identity to each of the terms of (129):

$$\langle x|\frac{P^2}{2m}|\psi\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,\langle x|\frac{P^2}{2m}|p\rangle\langle p|\psi\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,\frac{p^2}{2m}\,\langle x|p\rangle\,\tilde{\psi}(p)$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,\frac{p^2}{2m}\,e^{\frac{i}{\hbar}\,px}\,\tilde{\psi}(p)\,. \tag{131}$$

Analogously,

$$E\,\langle x|\psi\rangle = E\,\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,e^{\frac{i}{\hbar}\,px}\,\tilde{\psi}(p)\,. \tag{132}$$

$$\langle x|f_i\rangle\langle f_i|\psi\rangle = \lambda_i \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\,\langle x|p\rangle\langle p|a_i\rangle\langle a_i|\psi\rangle$$

$$= \sqrt{\lambda_i}\,\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{\frac{i}{\hbar}\,px}\, e^{-\frac{i}{\hbar}\,pa_i}\,\sqrt{\lambda_i}\,\tilde{\psi}(a_i)\,. \tag{133}$$

This integral does not converges in the ordinary sense, but in the distributional sense. Then writing $\phi(a_i) := \sqrt{\lambda_i}\,\psi(a_i)$, the original equation takes the form:

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}\,px}\,\tilde{\psi}(p)\left(\frac{p^2}{2m}-E\right) = \sum_{i=1}^{N}\sqrt{\lambda_i}\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}\,p(x-a_i)}\,\phi(a_i)\,. \tag{134}$$

This implies,

$$\tilde{\psi}(p) = \sum_{i=1}^{N} \sqrt{\lambda_i}\, \frac{e^{-\frac{i}{\hbar}\, p a_i}}{\dfrac{p^2}{2m} - E}\, \phi(a_i)\,. \tag{135}$$

Since,

$$\psi(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}\, p x}\, \tilde{\psi}(p)\,, \tag{136}$$

we have that

$$\psi(a_i) = \sum_{i=1}^{N} \sqrt{\lambda_i}\, \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \frac{e^{\frac{i}{\hbar}\, p(a_i - a_j)}}{\dfrac{p^2}{2m} - E}\, \phi(a_i)\,. \tag{137}$$

Multiplying by $\sqrt{\lambda_i}$, one finds (i fixed)

$$\left[1-\lambda_i\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\frac{1}{\dfrac{p^2}{2m}-E}\right]\phi(a_i)$$

$$-\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\sum_{j=1,j\neq i}^{N}\sqrt{\lambda_i\lambda_j}\left[\frac{e^{\frac{i}{\hbar}\,p(a_i-a_j)}}{\dfrac{p^2}{2m}-E}\right]\phi(a_j)=0\,. \tag{138}$$

This can be written as

$$\sum_{j=1}^{N}\Phi_{i,j}(E)\,\phi(a_j)=0\,, \tag{139}$$

with

$$\Phi_{i,j}(E) = \begin{cases} 1 - \lambda_i \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \dfrac{1}{\dfrac{p^2}{2m} - E} & \text{if} \quad i = j\,, \\ \sqrt{\lambda_i \lambda_j} \left[\dfrac{e^{\frac{i}{\hbar}\, p(a_i - a_j)}}{\dfrac{p^2}{2m} - E} \right] & \text{if} \quad i \neq j\,. \end{cases} \tag{140}$$

Assume that $E < 0$, so that $E = -|E|$, so that the integrals in (140) may be calculated by the residue method. This gives:

$$\Phi_{i,j}(E) = \begin{cases} 1 - \frac{m\lambda_i}{\hbar\sqrt{2m|E|}} & \text{if} \quad i = j\,, \\ -\frac{m\sqrt{\lambda_i\lambda_j}}{\hbar\sqrt{2m|E|}}\, \exp\left\{ -\sqrt{2m|E|}\, |a_i - a_j|/\hbar \right\} & \text{if} \quad i \neq j\,. \end{cases} \tag{141}$$

Bound states are solutions of $\det \Phi(E) = 0$. In this model, bound states always exist. Let us calculate the wave function of a bound state with negative energy $E_B = -|E_B|$. First of all from (139) ,

$$\sum_{j=1}^{N} \Phi_{i,j}(-|E_B|)\, \phi_B(a_j) = 0\,, \qquad i = 1, 2, \ldots, N\,, \tag{142}$$

then ($\phi_B(x) = \sqrt{\lambda_i}\psi(x)$),

$$\tilde{\psi}_B(p) = \sum_{i=1}^{N} \sqrt{\lambda_i}\, \frac{e^{-\frac{i}{\hbar}\, p a_i}}{\frac{p^2}{2m} + |E_B|}\, \phi_B(a_i)\,. \tag{143}$$

In the coordinate representation, we have after the inverse Fourier transform,

$$\psi_B(x) = \sum_{i=1}^{N} \lambda_i\, \phi_B(a_i)\, \sqrt{m/2}\, \frac{e^{-\frac{\sqrt{2m|E_B|}}{\hbar}\, |x - a_i|}}{\hbar\sqrt{E_B}}\,. \tag{144}$$

For $E \geq 0$, no square integrable wave functions exists and, therefore, all bound states must be negative.
Two particular cases:

- A single center localized at $x = 0$ with coupling constant $\lambda > 0$.

$$\Phi(E) = 1 - \frac{m\lambda}{\hbar\sqrt{2m|E|}}\,, E_B = -\frac{m\lambda^2}{2\hbar^2}\,, \psi_B(x) = \frac{\sqrt{m\lambda}}{\hbar}\, e^{-\frac{m\lambda}{\hbar^2}\,|x|}\,. \tag{145}$$

- Two centers at $a_1 = 0$, $a_2 = a$ and $\lambda_1 = \lambda_2 = \lambda$. Then, if $\kappa := \frac{\sqrt{2m|E|}}{\hbar}$,

$$\det \Phi(E) = 0 \Longrightarrow e^{-a\kappa_\pm} = \pm\left(\frac{\hbar^2\kappa_\pm}{m\lambda} - 1\right) \tag{146}$$

The solutions in terms of the energy are:

$$E_\pm = -\left(\frac{\lambda}{2} + \frac{1}{a}\,W\left[\pm\frac{a\lambda}{2}\,e^{-\frac{a\lambda}{2}}\right]\right)^2 , \tag{147}$$

where $W(-)$ is the Lambert function, solution of the equation,

$$y\,e^y = z \Longrightarrow y = W(z)\,. \tag{148}$$

F. Erman, M. Gadella, S. Tunalı, H. Uncu, A singular one-dimensional bound state problem and its degeneracies, Eur. Phys. J. Plus, **132**, 352 (2017).

Scattering properties and resonances have been studied in: F. Erman, M. Gadella, H. Uncu, On scattering from the one-dimensional multiple Dirac delta potentials, Eur. J. Physics, **39**, 035403 (2018).

Contents

Position of the problem.

The one-dimensional stationary Dirac equation for a particle of mass m and energy E scattered by a double barrier of singular interactions can be written as a distributional differential equation of the form

$$(i\gamma^1\,\partial_1 - m\mathbb{I} + \gamma^0 E)\psi(x) = D[\psi](x)\,, \tag{149}$$

with $\gamma^0 = \sigma_3$ and $\gamma^1 = i\sigma_2$.

For a potential $V(x) = \gamma^0\mathcal{I}(x)$ that has singularities in a finite set of points σ, the interaction distribution $D[\psi](x)$ is required to satisfy the following conditions:

- The distribution $D[\psi](x)$, defined on the entire real line, must coincide with $\mathcal{I}(x)\psi(x)$ on $\mathbb{R}/\{0\}$.

- The components of the Dirac spinor $\psi(x)$ must correspond to regular distributions in the entire real line (i.e. they must be slow growth functions and locally integrable in the Lebesgue sense). Thus, the order r_ψ of the spinor components is bounded from above by $r_\psi \leq -1$.
- The distribution $D[\psi](x)$ must be such that the current density is conserved across all singular points in the set σ.

To fix ideas, assume that $\sigma \equiv \{0\}$. Using the two first conditions above, one concludes that

$$D[\psi](x) = \Omega[\psi]\delta(x)\,, \tag{150}$$

where $\Omega[\psi]$ is a 2 x 1 complex matrix, independent of the coordinate x.

Then taking the primitive of (150), one finds:

$$i\gamma^1\psi(x) + (\gamma^0 E - m\mathbb{I})\psi^{(-1)}(x) = \Omega[\psi]\,\theta(x) + c\,. \tag{151}$$

This implies that:

$$i\gamma^1[\psi(0+) - \psi(0-)] = \Omega[\psi]\,. \tag{152}$$

The current conservation across the origin (for the moment our only singular point) should be conserved. The one dimensional current conservation is

$$j^1(x) = \psi^\dagger(x)\gamma^0\gamma^1\psi(x)\,. \tag{153}$$

Its conservation across the origin implies that

$$\psi^\dagger(0+)\sigma_1\psi(0+) = \psi^\dagger(0-)\sigma_1\psi(0-)\,. \tag{154}$$

After (153) and (154) and some non-trivial manipulations, one finds that

$$\Omega[\psi] = (B\mathbb{I} + A_0\gamma^0 + A_1\gamma^1 + iW\gamma^5)\,\frac{\psi(0+)+\psi(0-)}{2}\,, \qquad (155)$$

with $\gamma^5 = \gamma^0\gamma^1 = \sigma_1$.

The parameters in (155) are the strengths of scalar B, vector, A_μ, $\mu = 0, 1$, and pseudoescalar, W, physical interactions.

After some manipulations, one finds that the above considerations yield to the existence of matching conditions ate the origin of the type

$$\psi(0+) = \Lambda\,\psi(0-)\,, \;\; \Lambda = e^{i\varphi}\begin{pmatrix} a & ib \\ -ic & d \end{pmatrix}\,, \;\; ad - bc = 1\,,\; \varphi \in [0,\pi)\,. \qquad (156)$$

C.A. Bonin, J.T. Lunardi, L.A. Manzoni, The physical interpretation of point interactions in one-dimensional relativistic quantum mechanics, J. Phys. A: Math. Theor., **57**, 095204 (2024).

Analogously, let us assume that one has point interactions supported at the points $\pm\ell/2$. In such a case, ($\mu = 0, 1$)

$$D[\psi](x) = (B^{(1)}\,\mathbb{I} + A^{(1)}_{\mu}\gamma^{\mu} + iW^{(1)}\gamma^{5})\,\delta\left(x + \frac{\ell}{2}\right)\,\frac{\psi(\ell/2+) + \psi(\ell/2-)}{2}$$

$$+(B^{(2)}\,\mathbb{I} + A^{(2)}_{\mu}\gamma^{\mu} + iW^{(2)}\gamma^{5})\,\delta\left(x - \frac{\ell}{2}\right)\,\frac{\psi(-\ell/2+) + \psi(-\ell/2-)}{2}\,. \quad (157)$$

At the points $x = \pm\ell/2$, the singularities may also be described by some matching conditions given by 2×2 matrices depending of four real independent parameters. These parameters depend on those written in (157).

General eigenstates

The Dirac particle moves freely outside the singular points, those supporting the deltas. The solution of the wave equation can be written as

$$\psi(x) = \begin{cases} \psi_1(x) & \text{if} \quad x < -\ell/2\,, \\ \psi_2(x) & \text{if} \quad -\ell/2 < x < \ell/2\,, \\ \psi_3(x) & \text{if} \quad \ell/2 < x\,, \end{cases} \tag{158}$$

where ($j = 1, 2, 3$)

$$\psi_j(x) = F_j\, e^{ikx}\, u_E(k) + G_j\, e^{-ikx}\, u_E(-k) \equiv \mathbb{P}(k, x) \begin{pmatrix} F_j \\ G_j \end{pmatrix}\,, \tag{159}$$

with

$$k := \sqrt{E^2 - m^2}\,, \qquad u_E(k) = (1, k/(E+m))^T\,. \tag{160}$$

In (159),

$$\mathbb{P}(k,x) = \begin{pmatrix} e^{ikx} & e^{-ikx} \\ \frac{k}{E+m}\, e^{ikx} & -\frac{k}{E+m}\, e^{-ikx} \end{pmatrix} . \tag{161}$$

Transfer matrix

$$\begin{pmatrix} F_3 \\ G_3 \end{pmatrix} = \mathbb{M}(\Lambda_1, \Lambda_2, k, x_1, x_2) \begin{pmatrix} F_1 \\ G_1 \end{pmatrix} , \tag{162}$$

with

$$\mathbb{M}(\Lambda_1, \Lambda_2, k, x_1, x_2) = [\mathbb{P}^{-1}(k, x_2)\Lambda_2\, \mathbb{P}(k, x_2)][\mathbb{P}^{-1}(k, x_1)\Lambda_1\, \mathbb{P}(k, x_1)] . \tag{163}$$

Scattering states

For scattering solutions with the particle incident from the left and no incident wave from the right, one may set $F_1 = 1$, $G_1 = r(k)$, $G_3 = 0$ and $F_3 = t(k)$, where $r(k)$ and $t(k)$ are the reflection and transmission amplitudes, respectively.

$$\begin{pmatrix} F_3 \\ G_3 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} F_1 \\ G_1 \end{pmatrix} . \tag{164}$$

Then,

$$F_3 = M_{11} + M_{12} G_1 \,, \qquad 0 = M_{21} + M_{22} G_1 \,, \tag{165}$$

so that

$$r(k) = -\frac{M_{21}}{M_{22}} \,, \qquad t(k) = \frac{\det \mathbb{M}}{M_{22}} \,. \tag{166}$$

The matrix $\mathbb{M}$ is often called the transmission matrix. The elements of the scattering matrix, S, are defined as

$$\begin{pmatrix} G_1 \\ F_3 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} F_1 \\ G_3 \end{pmatrix} . \tag{167}$$

Thus,

$$S = \frac{1}{M_{22}} \begin{pmatrix} -M_{21} & 1 \\ \det \mathbb{M} & T_{12} \end{pmatrix} . \tag{168}$$

Purely outgoing boundary conditions imply that $F_1 = G_3 = 0$, so that

$$\boxed{M_{22} = 0} . \tag{169}$$

Bound states and resonances

Bound states are square integrable solutions of the equation. Recall the purely outgoing boundary conditions $F_1 = 0 = G_3$:

$$\psi_3(x) = F_3\, e^{ikx}\,, \quad x > \ell/2\,, \quad \psi_1(x) = G_1\, e^{-ikx}\,, \quad x < -\ell/2\,. \tag{170}$$

This gives a bound state if $k = i\kappa$ with $\kappa > 0$. The value of κ can be obtained from

$$M_{22}(i\kappa) = 0\,. \tag{171}$$

Bound states exists if and only if, we have solutions on κ from (171). For some particular cases, we have shown the existence of bound states.

Resonances are also solutions of purely outgoing boundary conditions $F_1 = 0 = G_3$. They are given for complex values of k solutions of $M_{22}(k) = 0$. These values do not provide square integrable wave functions. These solutions appear into pairs

$$k_\pm = \sqrt{(E_R \pm i\Gamma/2)^2 - m^2}\,, \qquad \Gamma > 0\,. \tag{172}$$

Critical and Supercritical states

Critical states are bounded solutions of the equation with $E = m$, i.e., solutions of

$$[i\gamma^1 \partial_1 - m(\mathbb{I} - \gamma^0)]\psi(x) = D[\psi](x)\,. \tag{173}$$

Solutions are of the form ($j = 1, 2, 3$):

$$\psi_j(x) = F_j \begin{pmatrix} 2imx \\ 1 \end{pmatrix} + G_j \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbb{P}_{crit} \begin{pmatrix} F_j \\ G_j \end{pmatrix}, \tag{174}$$

with

$$\mathbb{P}_{crit} = \begin{pmatrix} 2imx & 1 \\ 1 & 0 \end{pmatrix}. \tag{175}$$

The requirement for boundedness implies that $F_1 = F_2 = 0$, so that

$$\begin{pmatrix} 0 \\ G_3 \end{pmatrix} = \mathbb{M}^{crit}(\Lambda_1, \Lambda_2, x_1, x_2) \begin{pmatrix} 0 \\ G_1 \end{pmatrix}, \tag{176}$$

which implies:

$$\begin{pmatrix} M_{12}^{crit} & 1 \\ M_{22}^{crit} & -1 \end{pmatrix} = \begin{pmatrix} G_1 \\ G_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{177}$$

This system has non trivial solutions if

$$M_{12}^{crit} = 0\,, \tag{178}$$

which is not a transcendental equation on k.

For instance, if $A_0^{(0)} = A_0^{(1)} = B$ and $A_1^{(0)} = -A_1^{(1)} = W^{(0)} = -W^{(1)} = 0$ (even arrangement), there are critical states if

$$B = 0\,, \qquad \text{or} \qquad B = \frac{1}{2m\ell}\,. \tag{179}$$

Supercritical states are bounded solutions of the equation with $E = -m$, i.e., solutions of

$$[i\gamma^1\,\partial_1 - m(\mathbb{I} + \gamma^0)]\psi(x) = D[\psi](x)\,. \tag{180}$$

The discussion in supercritical states is similar to that of critical states.

C.A. Bonin, M. Gadella, J.T. Lunardi, L.A. Manzoni, Bound states and resonance analysis of one-dimensional relativistic parity-symmetric two-point interactions, Front. Phys., **14**, 1776432 (2026).

Contents

The Birman-Schwinger operator

This is a method to obtain eigenvalues for the Schrödinger equation under some conditions.

Assume we have the following eigenvalue problem

$$(H_0 - E)\psi = V\psi\,, \tag{181}$$

with $V \geq 0$ and $E < 0$. Then, the square root $V^{1/2}$ is well defined. If $0 \notin \sigma(V)$, also is $V^{-1/2}$.

Let us write (181) as

$$(H_0 - E)\,V^{-1/2}V^{1/2}\,\psi = V^{1/2}V^{1/2}\,\psi\,, \tag{182}$$

Write,

$$\chi := V^{1/2}\,\psi\,. \tag{183}$$

Then, (182) becomes,

$$\chi = V^{1/2}(H_0 - E)^{-1}\, V^{1/2}\,\chi = B_{BS}(E)\chi\,. \tag{184}$$

Then,

$$B_{BS}(E) := V^{1/2}(H_0 - E)^{-1}\, V^{1/2}\,, \tag{185}$$

is the Birman-Schwinger operator for H_0 and V.

Then, the eigenvalues $E < 0$ of the Schrödinger equation are the values of E for which the operator $B_{BS}(E)$ has eigenvalue one.

Another operator. Let us write the Schrödinger equation as ($H_0 \geq 0$, $E < 0$)

$$(H_0 - E)^{1/2}\psi = (H_0 - E)^{-1/2}\, V\, (H_0 - E)^{-1/2}(H_0 - E)^{1/2}\,\psi\,. \quad (186)$$

Then, if

$$\chi := (H_0 - E)^{1/2}\psi\,, \quad (187)$$

one writes (186) as

$$\chi = (H_0 - E)^{-1/2}\, V\, (H_0 - E)^{-1/2}\,\chi\,. \quad (188)$$

The operator

$$R(E) := (H_0 - E)^{-1/2}\, V\, (H_0 - E)^{-1/2} \tag{189}$$

has the following properties:

- The eigenvalues of the Schrödinger equation are those values of E for which $R(E)$ has the eigenvalue one.
- The operator $R(E)$ and the Birman-Schwinger operator $B_{BS}(E)$ are isospectral.

One dimensional Coulomb

Let us consider the operator $-d^2/dx^2$ on $L^2(\mathbb{R}^+)$ with the following domain:

$$\mathcal{D} := \{f(x) \in W_2^2(\mathbb{R}^+)\,, \quad f(0) = 0\}\,. \tag{190}$$

This operator is self adjoint and represented as

$$\left(-\frac{d^2}{dx^2}\right)_{D^+} \quad . \tag{191}$$

Its Green function (kernel of the resolvent operator) is given by ($E < 0$, $x, y \geq 0$)

$$\left[\left(-\frac{d^2}{dx^2}\right)_{D^+} + |E|\right]^{-1}(x,y) = \frac{e^{-|E|^{1/2}|x-y|} - e^{-|E|^{1/2}(x+y)}}{2|E|^{1/2}} \,. \tag{192}$$

Then, let us consider the following Hamiltonian with domain $\mathcal{D}$ ($x > 0$, $\lambda > 0$):

$$H_{D^+} := \left(-\frac{d^2}{dx^2}\right)_{D^+} - \frac{\lambda}{x} \,. \tag{193}$$

This is self adjoint on $\mathcal{D}$.

The Kernel for the $B_{BS}(E)$ operator for (193) is

$$K_{BS}^{+}(x,y;|E|) = \frac{\lambda}{x^{1/2}}\left[\left(-\frac{d^2}{dx^2}\right)_{D^+} + |E|\right]^{-1}(x,y)\,\frac{1}{y^{1/2}}$$

$$= \frac{\lambda}{x^{1/2}}\,\frac{e^{-|E|^{1/2}|x-y|} - e^{-|E|^{1/2}(x+y)}}{2|E|^{1/2}}\,\frac{1}{y^{1/2}}\,. \tag{194}$$

Now a relevant question. Is $B_{BS}(E)$ trace class. If this were the case, the energy values E solutions of the Schrödinger equation, would be the zeros of the Fredholm determinant:

$$\det[I - \lambda\, B_{BS}(E)] = 0\,. \tag{195}$$

The Fredholm determinant is defined as

$$\det[I - \lambda\, B_{BS}(E)] = 1 + \sum_{m=1}^{\infty} \frac{(-\lambda)^m}{m!}\, \Phi_m(E)\,, \tag{196}$$

with

$$\Phi_m(E) = \int \det \begin{pmatrix} K_{BS}^{+}(t_1, t_1) & \dots & K_{BS}^{+}(t_1, t_m) \\ \cdot & \dots & \cdot \\ K_{BS}^{+}(t_m, t_1) & \dots & K_{BS}^{+}(t_m, t_m) \end{pmatrix} dt_1\, dt_2\, \dots\, dt_m\,. \tag{197}$$

In our case,

$$\int \left|K_{BS}^{+}(x,y;|E|)\right| \,dx\,dy = \infty\,, \tag{198}$$

so that $K_{BS}(E)$ is not trace class.

It is nevertheless Hilbert-Schmidt, with Hilbert-Schmidt norm given by:

$$||B_{BS}(E)||^2 = \int \left|K_{BS}^{+}(x,y;|E|)\right|^2 \,dx\,dy = \frac{\pi^2}{24\,|E|^{1/2}}\,. \tag{199}$$

S. Fassari, M. Gadella, J.T. Lunardi, L.M. Nieto, F. Rinaldi. The One-Dimensional Coulomb Hamiltonian: Properties of Its Birman-Schwinger Operator, Mathematical Methods in the Applied Sciences, **48**, 11813-11822 (2025).

Nevertheless, in the present case, we can obtain exactly the eigenvalues of H_{D^+}.

For any $\phi(x) \in L^2(\mathbb{R}^+)$, we have that

$$\langle \phi | B_{BS}(E) \phi \rangle = \frac{1}{|E|^{1/2}} \langle U_{|E|}\, \phi | B_{BS}(1)\, U_{|E|}\, \phi \rangle\,, \tag{200}$$

with

$$U_{|E|}\, \phi(x) = \frac{1}{|E|^{1/4}}\, \phi\left(\frac{x}{|E|^{1/2}} \right)\,, \tag{201}$$

so that

$$B_{BS}(E) = \frac{1}{|E|^{1/2}}\, U_{|E|}^{-1}\, B_{BS}(1)\, U_{|E|} \tag{202}$$

Hence,

$$\sigma\left(B_{BS}(E)\right) = \frac{1}{|E|^{1/2}}\,\sigma\left(B_{BS}(1)\right)\,. \tag{203}$$

Then if $E < 0$, $E \in \sigma_{disc}(H_{D^+})$ if and only if $1 \in \sigma(B_{BS}(1))$.

Equivalently, if

$$|E|^{1/2} \in \sigma\left(B_{BS}(1)\right)\,, \quad \text{or} \quad |E| \in \left(B_{BS}^2(1)\right) \tag{204}$$

This means that solving the Schrödinger equation

$$[H_{D^+}\,\psi](x) = \left[\left(-\frac{d^2}{dx^2}\right)_{D^+}\right](x) - \frac{\psi(x)}{x} = -\lambda^2\psi(x)\,, \tag{205}$$

is equivalent to solve

$$\int_0^\infty K^+_{BS}(x,y;|E|)\,\phi(y)\,dy = \lambda\,\phi(x)\,, \qquad \lambda > 0\,. \tag{206}$$

Setting $\phi(x) = \sqrt{x}\,e^{-x}\,p(x)$ and after some algebra, (206) becomes

$$\int_0^x [e^{2y}-1]e^{-2y}\,p(y)\,dy + [e^{2x}-1]\int_x^\infty e^{-2y}\,p(y)\,dy = 2\lambda\,x\,p(x)\,. \tag{207}$$

After differentiating twice, we obtain

$$x\,p''(x) + 2(1-x)p'(x) + 2\left(\frac{1}{2\lambda} - 1\right)p(x) = 0\,. \tag{208}$$

This is the Laguerre differential equation, so that

$$\frac{1}{2\lambda} - 1 = n\,, \quad n = 0, 1, 2, \dots\,. \tag{209}$$

Then, the eigenvalues of $B_{BS}(1)$ are

$$\lambda_n = \frac{1}{2(n+1)}\,, \qquad n = 0, 1, 2, \dots\,, \tag{210}$$

so that the eigenvalues of H_{D^+} are

$$\lambda_n^2 = \frac{1}{4(n+1)^2}\,, \qquad n = 0, 1, 2, \dots\,. \tag{211}$$

S. Fassari, M. Gadella, F. Rinaldi, Novel properties of the Birman-Schwinger operator of the one-dimensional Coulomb Hamiltonian. Analysis and Mathematical Physics, , , (2026).