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1D point interactions in nonrelativistic quantum mechanics

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The problem of a nonrelativistic quantum particle moving on a real line with the most general point interaction at a single point can be treated in two equivalent modes: (i) by considering an alternative system without a singular potential but excluding the point, in which case the interaction is exclusively encoded in proper boundary conditions, and (ii) by explicitly considering a singular potential written in terms of the Dirac delta and derivatives $\mathrm{d}/\mathrm{d}x$ positioned properly. How can this be possible? The aim of this seminar is to discuss these two approaches.

1:30 - 2:30 p.m. Friday, 4$^{\text{th}}$ March 2022

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What is a point interaction?

Answer

- By a [point] interaction we mean an idealized localized singular interaction with zero range occurring at a point in a region. However, this kind of interaction can also be described by a free system in the same region with the singular point excluded (a hole or a single defect or an obstacle), in which case the interaction is encoded in boundary conditions rather than in a formal singular Hamiltonian operator.

- [Point = contact = zero-range = delta] interaction

- Point interactions can be considered as a good approximation of highly localized real (two-body) interactions or potentials

- Quantum systems with point interactions have been under an intensive investigation in the recent years, both theoretically, numerically and experimentally

- In this seminar, we will only consider Schrödinger Hamiltonians in one dimension, and the singular interaction will be located at $x = 0$. This is the simplest case but it has a very rich structure

A bit of history

- R. De L. Kronig and W. G. Penney, “Quantum mechanics of electrons in crystal lattices”, Proc. Roy. Soc. (London) 130A, 499–513 (1931)

This paper presented the first relevant model in quantum mechanics based on point interactions. Using this model, Kronig and Penney obtained the band structure of the metals

- H. Bethe and R. Peierls, “Quantum theory of the diplon”, Proc. Roy. Soc. (London) 148A, 146–156 (1935); L. H. Thomas, “The interaction between a neutron and a proton and the structure of H3”, Phys. Rev. 47, 903–909 (1935).

Bethe-Peierls and Thomas used point interactions as theoretical models to solve the neutron–proton scattering in the approximation of very short interaction range

- E. Fermi, “Sul moto dei neutroni nelle sostanze idrogenate”, Ricerca Scientifica 7, 13–52, (1936).

The Bethe-Peierls and Thomas results were developed by Fermi with the introduction of the so-called “delta pseudo-potential” (very common in nuclear physics)

- F. A. Berezin y L. D. Faddeev, “A remark on Schrödinger’s equation with a singular potential”, Soviet Math. Dokl. 2, 372–375 (1961)

The work of Berezin and Faddeev was the first rigorous analysis of a 3D two-particle system with point interaction

- S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden, “Solvable Models in Quantum Mechanics”, (Springer, New York, 1988); M. Carreau, “Four-parameter point-interaction in 1D quantum systems”, J. Math. Gen. 26, 427-432 (1993); P. Kurasov, “Distribution theory for discontinuous test functions and differential operators with generalized coefficients”, J. Math. Anal. Appl. 201, 297-323 (1996); S. Albeverio, L. Dabrowski and P. Kurasov, “Symmetries of Schrödinger Operators with Point Interactions”, Lett. Math. Phys. 45, 33-47 (1998); S. Albeverio and P. Kurasov, “Singular Pertubations of Differential Operators”, (University Press, Cambridge, 2000).

The works of Albeverio, Kurasov, Gesztesy, Dabrowski, Carreau *et al*, in the 1980s and 1990s, produced a significant number of new results. Since then, the topic has remained very active and models using point interactions are today under active theoretical and experimental investigation

Point interactions as boundary conditions (BCs)

- **Hamiltonian operator in $\mathbb{R} - \{0\}$ $(= \mathbb{R} \setminus \{0\})$**

$$\hat{\mathrm{h}} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

- **Self-adjoint on $D(\hat{\mathrm{h}})\,(= D(\hat{\mathrm{h}}^\dagger))$ $[\,D(\hat{\mathrm{h}})$ is the domain of $\hat{\mathrm{h}}\,]$**

$$\Psi \in D(\hat{\mathrm{h}}) \;:\; \left\{ \begin{bmatrix} \Psi(0+) - \mathrm{i}\lambda\Psi'(0+) \\ \Psi(0-) + \mathrm{i}\lambda\Psi'(0-) \end{bmatrix} = \hat{U} \begin{bmatrix} \Psi(0+) + \mathrm{i}\lambda\Psi'(0+) \\ \Psi(0-) - \mathrm{i}\lambda\Psi'(0-) \end{bmatrix} \right\} \text{[1]}$$

- $\Psi(0\pm) = \lim_{\epsilon\to 0}\Psi(0\pm\epsilon)$, $\Psi'(0\pm) = \lim_{\epsilon\to 0}\Psi'(0\pm\epsilon)$
- $\lambda \in \mathbb{R}$ is a parameter (inserted for dimensional reasons)
- **$\hat{U}$ is a unitary matrix $\Rightarrow$ four real parameters**

$$\hat{U} = \exp(\mathrm{i}\phi)\begin{bmatrix} m_0 - \mathrm{i}\,m_3 & -m_2 - \mathrm{i}\,m_1 \\ m_2 - \mathrm{i}\,m_1 & m_0 + \mathrm{i}\,m_3 \end{bmatrix}$$

- $\phi \in [0, \pi]$
- $m_A \in \mathbb{R}$ $(A = 0, 1, 2, 3)$, $(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$

[1] For example, use von Neumann's theory of self-adjoint extensions

The most general family of BCs can be written in distinct ways

$$\Psi \in D(\hat{\mathrm{h}}) \ : \ \left\{ \begin{bmatrix} \lambda\Psi'(0+) - \lambda\Psi'(0-) \\ \Psi(0+) - \Psi(0-) \end{bmatrix} = \hat{S} \begin{bmatrix} \Psi(0+) + \Psi(0-) \\ \lambda\Psi'(0+) + \lambda\Psi'(0-) \end{bmatrix} \right\}$$

$$\hat{S} = \frac{1}{m_1 + \sin(\phi)} \begin{bmatrix} -m_0 + \cos(\phi) & -m_3 - \mathrm{i}\, m_2 \\ m_3 - \mathrm{i}\, m_2 & -m_0 - \cos(\phi) \end{bmatrix}$$

$S_{11} \in \mathbb{R}$, $S_{22} \in \mathbb{R}$, $S_{21} = -S_{12}^*$

Each example of BC encodes a different kind of wall at $x = 0$

(a) The Dirac delta interaction

$$\begin{bmatrix} \Psi(0+) \\ \lambda\Psi'(0+) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -2\frac{m_0}{m_1} & 1 \end{bmatrix} \begin{bmatrix} \Psi(0-) \\ \lambda\Psi'(0-) \end{bmatrix}$$

$[\, m_0 = -\cos(\phi),\ m_1 = \sin(\phi),\ m_2 = m_3 = 0 \,]$

(b) The first derivative of the Dirac delta interaction

$$\begin{bmatrix} \Psi(0+) \\ \lambda\Psi'(0+) \end{bmatrix} = \begin{bmatrix} \frac{1+m_3}{m_1} & 0 \\ 0 & \frac{1-m_3}{m_1} \end{bmatrix} \begin{bmatrix} \Psi(0-) \\ \lambda\Psi'(0-) \end{bmatrix}$$

$[\, m_0 = m_2 = 0 \Rightarrow ((1 - m_3)/m_1) = m_1/(1 + m_3),\ \phi = \pi/2 \,]$

(c) The quasi-periodic interaction

$$\begin{bmatrix} \Psi(0+) \\ \lambda\Psi'(0+) \end{bmatrix} = \begin{bmatrix} m_1 - \mathrm{i}m_2 & 0 \\ 0 & m_1 - \mathrm{i}m_2 \end{bmatrix} \begin{bmatrix} \Psi(0-) \\ \lambda\Psi'(0-) \end{bmatrix}$$

$\left[\, m_0 = m_3 = 0 \Rightarrow (m_1)^2 + (m_2)^2 = 1,\ \phi = \pi/2 \,\right]$

(d) The so-called "delta-prime" interaction

$$\begin{bmatrix} \Psi(0+) \\ \lambda\Psi'(0+) \end{bmatrix} = \begin{bmatrix} 1 & -2\frac{m_0}{m_1} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \Psi(0-) \\ \lambda\Psi'(0-) \end{bmatrix}$$

$\left[\, m_0 = \cos(\phi),\ m_1 = \sin(\phi),\ m_2 = m_3 = 0 \,\right]$

(e) The Dirichlet BC

$$\Psi(0+) = \Psi(0-) = 0$$

$\left[\, m_0 = +1,\ m_2 = m_3 = 0 \Rightarrow m_1 = 0,\ \phi = \pi \,\right]$

(f) The Neumann BC

$$\Psi'(0+) = \Psi'(0-) = 0$$

$\left[\, m_0 = +1,\ m_2 = m_3 = 0 \Rightarrow m_1 = 0,\ \phi = 0 \,\right]$

Point interactions as singular potentials

(Heuristic) Hamiltonian operator in $\mathbb{R}$

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \hat{V}(x)$$

A plausible general singular potential operator

$$\hat{V}(x) = a\langle\delta,\cdot\rangle\delta(x) + b\langle\delta',\cdot\rangle\delta(x) + c\langle\delta,\cdot\rangle\delta'(x) + d\langle\delta',\cdot\rangle\delta'(x)$$

- a, b, c, and d are complex numbers
- $\langle F, \Psi\rangle$ (with $F = \delta$ or $\delta' \equiv \mathrm{d}\delta/\mathrm{d}x$) denotes the action $F[\Psi]$ of the distribution F on the test function Ψ
- $\langle\delta, \Psi\rangle = \int_{\mathbb{R}} \mathrm{d}x\, \delta(x)\Psi(x) = \int_{\mathbb{R}} \mathrm{d}x\, \delta(x)\Psi(0) = \Psi(0)$
- $\langle\delta', \Psi\rangle = \int_{\mathbb{R}} \mathrm{d}x\, \delta'(x)\Psi(x) = \int_{\mathbb{R}} \mathrm{d}x\, \delta'(x)\Psi(0) - \int_{\mathbb{R}} \mathrm{d}x\, \delta(x)\Psi'(0) = -\Psi'(0)$

Formally self-adjoint, i.e., $\hat{\mathrm{H}} = \hat{\mathrm{H}}^\dagger \Rightarrow a \in \mathbb{R}$, $d \in \mathbb{R}$, $c = b^*$

- $\hat{\mathrm{P}}$-symmetric, i.e., $\hat{\mathrm{P}}^{-1}\hat{\mathrm{H}}\,\hat{\mathrm{P}} = \hat{\mathrm{H}}^\dagger \Rightarrow a \in \mathbb{R}$, $d \in \mathbb{R}$, $c = -b^*$

General singular potential operator (four real parameters)

$$\hat{V}(x) = g_1\langle\delta,\cdot\rangle\delta(x) + (g_2 - \mathrm{i}g_3)\langle\delta',\cdot\rangle\delta(x) + (g_2 + \mathrm{i}g_3)\langle\delta,\cdot\rangle\delta'(x) + g_4\langle\delta',\cdot\rangle\delta'(x)$$

- $g_B \in \mathbb{R}$, $B = 1,2,3,4$

$\hat{V}(x)$ can be written in various ways

$$\hat{V}(x) = g_1\delta(x) - (g_2 - \mathrm{i}g_3)\delta(x)\frac{\mathrm{d}}{\mathrm{d}x} + (g_2 + \mathrm{i}g_3)\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)$$

- i.e.,

$$\hat{V}(x)\Box = g_1\delta(x)\Box - (g_2 - \mathrm{i}g_3)\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\Box + (g_2 + \mathrm{i}g_3)\frac{\mathrm{d}}{\mathrm{d}x}\left(\,\delta(x)\Box\,\right) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\Box\right)$$

Also

$$\hat{V}(x) = g_1\delta(x) + g_2\delta'(x) + \mathrm{i}g_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x)\right) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)$$

Just to clarify

$$\hat{\mathrm{H}}_{g_1} \equiv -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \hat{V}_{g_1}(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g_1\delta(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g_1\langle\delta,\cdot\rangle\delta(x) \quad (\hbar^2 = 2m = 1)$$

- $\hat{\mathrm{H}}_{g_1}$ should be defined only on a subset of $\mathcal{L}^2(\mathbb{R})$, its domain $D(\hat{\mathrm{H}}_{g_1})$. Why? Answer: Because $\Psi \in \mathcal{L}^2(\mathbb{R})$ ($\Rightarrow \|\Psi\|^2 \equiv \langle\Psi,\Psi\rangle < \infty$), but also $\hat{\mathrm{H}}_{g_1}\Psi \in \mathcal{L}^2(\mathbb{R})$. However, $\hat{\mathrm{H}}_{g_1}\Psi \notin \mathcal{L}^2(\mathbb{R})$. In effect,

$$\| \hat{V}_{g_1}\Psi \|^2 \equiv \langle \hat{V}_{g_1}\Psi, \hat{V}_{g_1}\Psi\rangle = \int_{\mathbb{R}} \mathrm{d}x \mid \hat{V}_{g_1}\Psi \mid^2 = g_1^2 \int_{\mathbb{R}} \mathrm{d}x \, |\langle\delta,\Psi\rangle\delta(x)|^2$$

$$= g_1^2 \, |\Psi(0)|^2 \int_{\mathbb{R}} \mathrm{d}x \, \delta(x)\delta(x) = g_1^2 \, |\Psi(0)|^2 \, \delta(0) = +\infty \qquad (\text{unless } \Psi(0) = 0)$$

- Thus, $\hat{\mathrm{H}}_{g_1}$ is not a proper operator on $\mathcal{L}^2(\mathbb{R})$

- If there is a self-adjoint operator corresponding to $\hat{\mathrm{H}}_{g_1}$, it could coincide with $\hat{\mathrm{h}}$ (unperturbed operator) but restricted to act on the set of functions that only satisfy the condition $\Psi(0) = 0$. Well, this operator is not self-adjoint (although it can be extended to be self-adjoint).

- The one-parameter (self-adjoint) extension matches with $-\mathrm{d}^2/\mathrm{d}x^2$ and its domain is essentially $W_2^2(\mathbb{R}\setminus\{0\})$ –the Sobolev space of continuous functions with continuous bounded first derivative, except for a finite jump at $x = 0$ – and the boundary condition $\Psi(0+) = \Psi(0-) \equiv \Psi(0)$ and $\Psi'(0+) - \Psi'(0-) = g_1\Psi(0)$

- The latter operator could be considered a natural definition for $\hat{\mathrm{H}}_{g_1}$ in the framework of the theory of self-adjoint operators

Still clarifying

$$\hat{\mathrm{H}}_{g_4} \equiv -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \hat{V}_{g_4}(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - g_4 \frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g_4 \langle \delta', \cdot \rangle \delta'(x) \qquad (\hbar^2 = 2m = 1)$$

- $\hat{V}_{g_4}(x)$ coincides with $\hat{V}_{g_1}(x)$ with the replacement $\delta \to \delta'$, but $\hat{V}_{g_4}(x)$ is not the first derivative of $\hat{V}_{g_1}(x)$
- Again, we start with $\Psi \in \mathcal{L}^2(\mathbb{R})$ ($\Rightarrow \|\Psi\|^2 \equiv \langle \Psi, \Psi \rangle < \infty$), but $\hat{\mathrm{H}}_{g_4}\Psi \notin \mathcal{L}^2(\mathbb{R})$. In effect (just formal manipulations!),

$$\| \hat{V}_{g_4}\Psi \|^2 \equiv \langle \hat{V}_{g_4}\Psi, \hat{V}_{g_4}\Psi \rangle = \int_{\mathbb{R}} \mathrm{d}x \; | \hat{V}_{g_4}\Psi |^2 = g_4^2 \int_{\mathbb{R}} \mathrm{d}x \; |\langle \delta', \Psi \rangle \delta'(x)|^2$$

$$= g_4^2 \, |\Psi'(0)|^2 \int_{\mathbb{R}} \mathrm{d}x \; |\delta'(x)|^2 = g_4^2 \, |\Psi'(0)|^2 \int_{\mathbb{R}} \mathrm{d}x \, \delta'(x)\delta'(x)$$

$$= g_4^2 \, |\Psi'(0)|^2 \, (-\delta''(0)) = +\infty \qquad (\text{unless } \Psi'(0) = 0)$$

- Thus, $\hat{\mathrm{H}}_{g_4}$ is not a proper operator on $\mathcal{L}^2(\mathbb{R})$
- In any case, the (self-adjoint) operator $-\mathrm{d}^2/\mathrm{d}x^2$ (no singular potential!) with the boundary condition $\Psi(0+) - \Psi(0-) = -\alpha g_4 \Psi'(0)$ and $\Psi'(0+) = \Psi'(0-) \equiv \Psi'(0)$ could be considered a natural definition for $\hat{\mathrm{H}}_{g_4}$ in the framework of the theory of self-adjoint operators

Plausible choice for discontinuous test functions at $x = 0$

$$\langle \delta, \Psi \rangle = \Psi(0) \equiv \frac{\Psi(0+) + \Psi(0-)}{2}$$

$$\langle \delta', \Psi \rangle = -\Psi'(0) \equiv -\frac{\Psi'(0+) + \Psi'(0-)}{2}$$

- i.e., $\hat{\mathrm{H}}$ (in a generalized sense) is determined by resorting to a theory of distributions where the test functions $\Psi(x)$ and $\Psi'(x)$ are discontinuous at the origin
- There are situations in which the latter choices do not hold, for example, if $\Psi(x)$ is defined by a differential equation in which $\delta(x)$ is involved, the relation $\langle \delta, \Psi \rangle = \Psi(0) = (\Psi(0+) + \Psi(0-))/2$ does not hold

Connecting singular potentials with boundary conditions

$$\hat{\mathrm{H}}\Psi(x) = -\alpha^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x) + \hat{V}(x)\Psi(x) = E\Psi(x)$$

$$\hat{V}(x)\Psi(x) = g_1\Psi(0)\delta(x) - (g_2 - \mathrm{i}g_3)\Psi'(0)\delta(x) + (g_2 + \mathrm{i}g_3)\Psi(0)\delta'(x) - g_4\Psi'(0)\delta'(x)$$

- $\alpha \equiv 2m/\hbar^2$

By integrating the Schrödinger equation I

$$\lambda\Psi'(0+) - \lambda\Psi'(0-) = \frac{1}{2}\lambda\alpha g_1 \left(\Psi(0+) + \Psi(0-)\right) - \frac{1}{2}\alpha(g_2 - \mathrm{i}g_3)\left(\lambda\Psi'(0+) + \lambda\Psi'(0-)\right)$$

- Hint: integrate $\hat{\mathrm{H}}\Psi = E\Psi$ from $-\epsilon$ to $+\epsilon$ and take the limit $\epsilon \to 0$

By integrating the Schrödinger equation II

$$\Psi(0+) - \Psi(0-) = \frac{1}{2}\alpha(g_2 + \mathrm{i}g_3)\left(\Psi(0+) + \Psi(0-)\right) - \frac{1}{2}\frac{\alpha g_4}{\lambda}\left(\lambda\Psi'(0+) + \lambda\Psi'(0-)\right)$$

- Hint: integrate $\hat{\mathrm{H}}\Psi = E\Psi$ first from $x = -L$ $(L > 0)$ to x, then once more from $-\epsilon$ to $+\epsilon$ and take the limit $\epsilon \to 0$ again

General boundary condition (four real parameters)

$$\begin{bmatrix} \lambda\Psi'(0+) - \lambda\Psi'(0-) \\ \Psi(0+) - \Psi(0-) \end{bmatrix} = \hat{M} \begin{bmatrix} \Psi(0+) + \Psi(0-) \\ \lambda\Psi'(0+) + \lambda\Psi'(0-) \end{bmatrix}$$

$$\hat{M} = \frac{1}{2}\alpha \begin{bmatrix} \lambda g_1 & -(g_2 - \mathrm{i}g_3) \\ g_2 + \mathrm{i}g_3 & -\frac{g_4}{\lambda} \end{bmatrix}$$

- $M_{11} \in \mathbb{R}$, $M_{22} \in \mathbb{R}$, $M_{21} = -M_{12}^*$

The connection

$$\frac{1}{2}\alpha\lambda g_1 = \frac{-m_0 + \cos(\phi)}{m_1 + \sin(\phi)}$$

$$\frac{1}{2}\alpha g_2 = \frac{m_3}{m_1 + \sin(\phi)}$$

$$\frac{1}{2}\alpha g_3 = \frac{-m_2}{m_1 + \sin(\phi)}$$

$$\frac{1}{2}\alpha\frac{g_4}{\lambda} = \frac{m_0 + \cos(\phi)}{m_1 + \sin(\phi)}$$

- Compare the general BC obtained by integrating the Schrödinger equation with the most general family of BCs for $\hat{\mathrm{h}}$

- Every formal or heuristic (formally) self-adjoint operator $\hat{\mathrm{H}}$ with a singular potential $\hat{V}(x)$, coincides with a certain self-adjoint operator $\hat{\mathrm{h}}$

- In other words, any local potential that depends on the Dirac delta and derivatives $\mathrm{d}/\mathrm{d}x$ positioned conveniently, can be associated with a boundary condition, and viceversa

Examples

(a) The Dirac delta interaction

$$\hat{V}(x) = g_1 \delta(x) \qquad [\, = g_1 \langle \delta, \cdot \rangle \delta(x) \,]$$

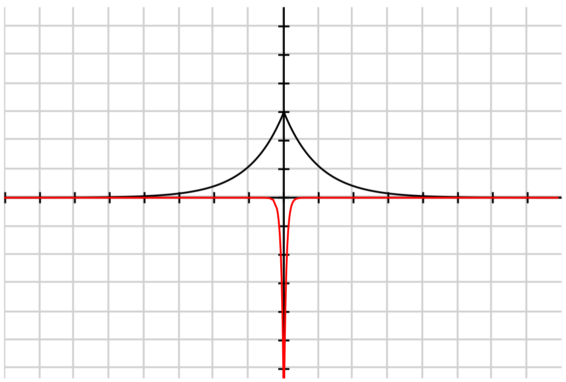
$$[\, m_0 = -\cos(\phi),\ m_1 = \sin(\phi),\ m_2 = m_3 = 0 \,] \Rightarrow [\, g_1 = 2\cot(\phi)/\alpha\lambda,\ g_2 = g_3 = g_4 = 0 \,]$$

- $[\, \phi = \pi/2 \Rightarrow g_1 = 0 \Rightarrow \hat{V}(x) = 0 \,]$
- $[\, \phi \to \pi- \Rightarrow g_1 \to -\infty \Rightarrow$ **(e)** $]$
- **One single (even-parity) bound state**

$$\Psi(x) = \sqrt{-\frac{1}{2}\alpha g_1}\, \exp\left(\frac{1}{2}\alpha g_1 \,|\, x \,|\right), \qquad E = -\frac{1}{4}\alpha (g_1)^2, \qquad g_1 < 0$$

$$\Psi(0+) = \Psi(0-) \equiv \Psi(0)$$

$$\Psi'(0+) - \Psi'(0-) = \alpha g_1 \Psi(0)$$



(b) The first derivative of the Dirac delta interaction

$$\hat{V}(x) = g_2\,\delta'(x) \qquad [\, = g_2\langle\delta', \cdot\,\rangle\delta(x) + g_2\langle\delta, \cdot\,\rangle\delta'(x)\ ]$$

$[\,m_0 = m_2 = 0 \Rightarrow ((1-m_3)/m_1) = m_1/(1+m_3),\ \phi = \pi/2\,] \Rightarrow [\,g_2 = 2m_3/\alpha(1+m_1),$
$g_1 = g_3 = g_4 = 0\,]$

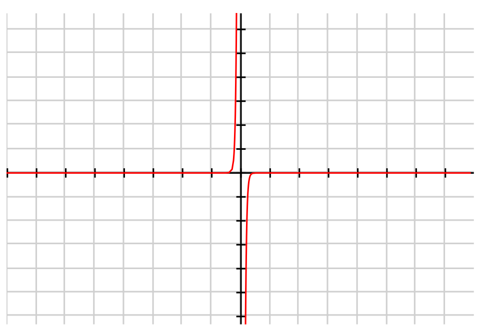
- $[\,m_3 = 0 \Rightarrow (m_1)^2 = 1$, **and choosing** $m_1 = 1 \Rightarrow g_2 = 0 \Rightarrow \hat{V}(x) = 0\,]$

- $[\,m_1 = 0 \Rightarrow (m_3)^2 = 1 \Rightarrow g_2 = 2m_3/\alpha\,]$
  [**(A) Mixed BC** $m_3 = 1 \Rightarrow g_2 = 2/\alpha \Rightarrow \Psi(0-) = \Psi'(0+) = 0\,]$
  [**(B) Mixed BC** $m_3 = -1 \Rightarrow g_2 = -2/\alpha \Rightarrow \Psi'(0-) = \Psi(0+) = 0\,]$

- **The trivial bound state (i.e. the discrete spectrum is empty)**

$$\Psi(x) = 0, \qquad E = 0$$

$$\Psi(0+) - \Psi(0-) = \frac{\alpha g_2}{2}\,(\Psi(0+) + \Psi(0-))$$
$$\Psi'(0+) - \Psi'(0-) = -\frac{\alpha g_2}{2}\,(\Psi'(0+) + \Psi'(0-))$$



(c) The quasi-periodic (or quasi-free) potential

$$\hat{V}(x) = \mathrm{i}g_3 \left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x) \right) \qquad [\, = -\mathrm{i}g_3\langle\delta', \cdot\,\rangle\delta(x) + \mathrm{i}g_3\langle\delta, \cdot\,\rangle\delta'(x)\,]$$

$[\,m_0 = m_3 = 0 \Rightarrow (m_1)^2 + (m_2)^2 = 1,\ \phi = \pi/2\,] \Rightarrow [\,g_3 = -2m_2/\alpha(1+m_1),$ $g_1 = g_2 = g_4 = 0\,]$

- $[\,m_1 = 1,\ m_2 = 0 \Rightarrow \hat{V}(x) = 0 \Rightarrow \Psi(0+) = \Psi(0-),\ \Psi'(0+) = \Psi'(0-)\,]$

- $[\,m_1 \to -1,\ m_2 \to 0 \Rightarrow g_3 \to -\infty,$

$$\Rightarrow \hat{V}(x) = \lim_{g_3 \to -\infty} \mathrm{i}g_3 \left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x) \right) \Leftrightarrow \left\{ \begin{array}{l} \Psi(0+) = -\Psi(0-) \\ \Psi'(0+) = -\Psi'(0-) \end{array} \right. \;]$$

- $\hat{\mathrm{H}}$ is equivalent to a Schrödinger operator with a singular gauge field at $x = 0$ (just formal manipulations!)

$$\hat{\mathrm{H}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathrm{i}g_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x) \right) = \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - g_3\,\delta(x) \right)^2 - g_3^2(\delta(x))^2$$

- The trivial bound state (i.e. the discrete spectrum is empty)

$$\Psi(x) = 0, \qquad E = 0$$

(d) The so-called “delta-prime” interaction potential

$$\hat{V}(x) = -g_4 \frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) \qquad [= +g_4 \langle \delta', \cdot \rangle \delta'(x)]$$

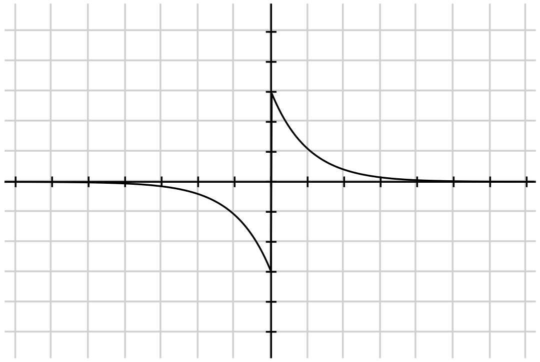
$$[\, m_0 = \cos(\phi),\ m_1 = \sin(\phi),\ m_2 = m_3 = 0\,] \Rightarrow [\, g_4 = 2\lambda \cot(\phi)/\alpha,\ g_1 = g_2 = g_3 = 0\,]$$

- $[\, \phi = \pi/2 \Rightarrow g_4 = 0 \Rightarrow \hat{V}(x) = 0\,]$
- $[\, \phi \to 0+ \Rightarrow g_4 \to +\infty \Rightarrow$ **(f)** $]$

One single (odd-parity) bound state

$$\Psi(x) = \sqrt{\frac{2}{\alpha g_4}}\, \mathrm{sgn}(x) \exp\left(-\frac{2}{\alpha g_4}\,|\,x\,|\right), \qquad E = -\frac{4}{\alpha^3 (g_4)^2}, \qquad g_4 > 0$$

$$\Psi(0+) - \Psi(0-) = -\alpha g_4 \Psi'(0)$$
$$\Psi'(0+) = \Psi'(0-) \equiv \Psi'(0)$$



(e) The Dirichlet potential

$$\hat{V}(x) = \lim_{g_1 \to -\infty} g_1 \delta(x)$$

$[m_0 = +1,\ m_2 = m_3 = 0\ (\Rightarrow m_1 = 0),\ \phi = \pi] \Rightarrow [g_1 = -4/\alpha\lambda m_1 \to -\infty,$ $g_2 = g_3 = g_4 = 0]$

- This potential is (heuristically) the square of the Dirac delta

$$\hat{V}(x) = -\delta(0)\delta(x) = -\delta(x)\delta(x) = -(\delta(x))^2$$

- The bound state could be calculated from the example (a)

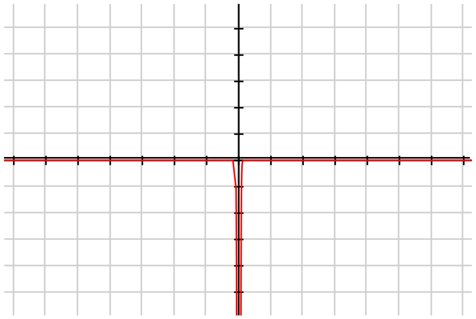
$$\Psi(x) = \lim_{g_1 \to -\infty} \sqrt{-\frac{1}{2}\alpha g_1}\, \exp\left(\frac{1}{2}\alpha g_1 \,|\, x \,|\right) \equiv \lim_{g_1 \to -\infty} \Psi_{g_1}(x) \ \Rightarrow\ (\Psi(x))^2 = \delta(x)$$

- $\Psi(x)$ looks like a highly localized state with $E = \lim_{g_1 \to -\infty} -\frac{1}{4}\alpha(g_1)^2 = -\infty$
- But, the distribution (or linear functional) associated with the state $\Psi(x)$, $\Psi[\Phi]$, is precisely zero ($\Phi \in \mathcal{L}^2(\mathbb{R})$ is the test function)

$$F[\Phi] = \Psi[\Phi] = \langle \Psi, \Phi \rangle = \lim_{g_1 \to -\infty} \int_{-\infty}^{+\infty} \mathrm{d}x\, \Psi_{g_1}(x)\Phi(x) = \lim_{g_1 \to -\infty} 2\sqrt{-\frac{2}{\alpha g_1}}\,\Phi(0) = 0$$

- The eigenfunction is really trivial, i.e., $\Psi(x) = 0$ everywhere, and it satisfies the Dirichlet BC, i.e., $\Psi(0+) = \Psi(0-) \equiv \Psi(0) = 0$

- We have an impenetrable barrier at $x = 0$



(f) The Neumann potential

$$\hat{V}(x) = \lim_{g_4 \to \infty} -g_4 \frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)$$

$[\, m_0 = +1,\ m_2 = m_3 = 0\ (\Rightarrow m_1 = 0),\ \phi = 0\,] \Rightarrow [\, g_4 = 4\lambda/\alpha m_1 \to +\infty,\ g_1 = g_2 = g_3 = 0\,]$

- This potential is the "delta-prime" interaction potential with infinite strength
- Thus, the bound state could be calculated from the example (d)

$$\Psi(x) = \lim_{g_4 \to \infty} \sqrt{\frac{2}{\alpha g_4}}\, \mathrm{sgn}(x) \exp\left(-\frac{2}{\alpha g_4}\,|\,x\,|\right) = 0$$

$$E = \lim_{g_4 \to \infty} -\frac{4}{\alpha^3 (g_4)^2} = 0$$

- The eigenfunction is trivial, and it satisfies the Neumann BC, i.e., $\Psi'(0+) = \Psi'(0-) \equiv \Psi'(0) = 0$

- We have an impenetrable barrier at $x = 0$

Other results

- For every function $\Psi \in D(\hat{\mathrm{h}})$, the probability current density

$$j(x) = \frac{\hbar}{\mathrm{m}} \mathrm{Im}\left(\Psi^*(x)\Psi'(x)\right)$$

satisfies

$$j(0+) = j(0-) \qquad \left[= -\frac{\hbar}{\mathrm{m}}\frac{1}{\lambda}\left(\frac{1}{m_0 + \cos(\phi)}\right) \mathrm{Re}\left((m_2 + \mathrm{i}\, m_1)\Psi^*(0+)\Psi(0-)\right) \right]$$

- This condition is equivalent to the hermiticity of the (self-adjoint) operator $\hat{\mathrm{h}}$

- If $m_1 = m_2 = 0$, then $j(0+) = j(0-) = 0$. In this case, $x = 0$ is an impenetrable barrier (otherwise it is penetrable)

There are situations in which the following choice (my plausible choice)

$$\langle \delta, \Psi \rangle = \Psi(0) \equiv \frac{\Psi(0+) + \Psi(0-)}{2}$$

does not hold (also for $\langle \delta', \Psi \rangle = -\Psi'(0) = -\left(\Psi(0+) + \Psi(0-)\right)/2$)

Example 1: The 1D Dirac equation with $\hat{V}(x) = g\delta(x)$

$$\hat{\mathrm{H}}\Psi(x) = -\mathrm{i}\hat{\sigma}_z \frac{\mathrm{d}}{\mathrm{d}x}\Psi(x) + \mathrm{m}c^2\hat{\sigma}_x\Psi(x) + \hat{V}(x)\Psi(x) = E\Psi(x)\,,\ \Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

Note that

$$-\mathrm{i}\hat{\sigma}_z \frac{\mathrm{d}}{\mathrm{d}x}\Psi(x) + g\delta(x)\Psi(x) \approx 0$$

This leads us to the correct boundary condition without using the plausible choice

$$\psi_1(0+) = \exp(-\mathrm{i}g)\psi_1(0-)\,,\ \psi_2(0+) = \exp(+\mathrm{i}g)\psi_2(0-)$$

Integrating the Dirac equation and using the plausible choice, one obtains an incorrect boundary condition

$$\psi_1(0+) = \exp(-\mathrm{i}\theta)\psi_1(0-)\,,\ \psi_2(0+) = \exp(+\mathrm{i}\theta)\psi_2(0-)\,,\ \frac{\theta}{2} = \tan^{-1}\left(\frac{g}{2}\right)$$

Example 2: The mean value of the force operator corresponding to the step potential $\phi(x) = V_0\,\Theta(x)$ in the 1D KFG theory

$$\langle \hat{f} \rangle_{\mathrm{KFG}} = \int_{\mathbb{R}} \mathrm{d}x\, \hat{f}\, \varrho_{\mathrm{KFG}}(x,t) = -\int_{\mathbb{R}} \mathrm{d}x\, \frac{\mathrm{d}}{\mathrm{d}x}\phi(x)\varrho_{\mathrm{KFG}}(x,t) = -V_0 \int_{\mathbb{R}} \mathrm{d}x\, \delta(x)\varrho_{\mathrm{KFG}}(x,t)$$

But the probability density $\varrho_{\mathrm{KFG}}(x,t)$ is not continuous at $x = 0$

$$\varrho_{\mathrm{KFG}} = \frac{\mathrm{i}\hbar}{2\mathrm{m}c^2}\left(\Psi^*\dot{\Psi} - \Psi\dot{\Psi}^*\right) - \frac{\phi}{\mathrm{m}c^2}\Psi^*\Psi$$

Integrating the 1D KFG equation without using the plausible choice, one obtains the correct result

$$\langle \hat{f} \rangle_{\mathrm{KFG}} = -V_0 \frac{1}{2}\left[\, \varrho_{\mathrm{KFG}}(0+,t) - \varrho_{\mathrm{KFG}}(0-,t)\,\right]$$

Therefore

$$\int_{\mathbb{R}} \mathrm{d}x\, \delta(x)\varrho_{\mathrm{KFG}}(x,t) = \frac{1}{2}\left[\, \varrho_{\mathrm{KFG}}(0+,t) - \varrho_{\mathrm{KFG}}(0-,t)\,\right]$$

$$\neq \frac{1}{2}\left[\, \varrho_{\mathrm{KFG}}(0+,t) + \varrho_{\mathrm{KFG}}(0-,t)\,\right]$$

The integral of the Dirac delta with a discontinuous function is not always equal to the average of the discontinuity of the function that accompanies the Dirac delta in the integral

Some concluding remarks

- Any point interaction at $x = 0$ characterized by a BC, can also be characterized by an operator with a singular interaction at $x = 0$. For example, the Dirichlet BC, the Neumann BC, and the antiperiodic BC, three very common BCs, each have their own associated singular potential

- The most general family of BCs we have presented here represents the whole family of BCs that a 1D Schrödinger wave function could satisfy at a point

- The case treated here can be easily generalized to the case of finite or infinite number of point interactions

- Point interactions can also be constructed by renormalizing the strengths of the delta functions present in certain combinations of these functions, and making the distances between them disappear

- Even though nature seems to prefer self-adjoint operators, non-self-adjoint point interactions have also been studied in the framework of nonrelativistic quantum mechanics (for example, PT-symmetric point interactions). It is now that non-self-adjoint relativistic point interactions begin to be studied

Thanks!

Grazie!

¡Gracias!