How to model p-scattering using point interactions and related problems

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October 13, 2008

Classical point interaction in $\mathbb{R}^3$

Formal expression

$$L_\alpha = -\Delta + \alpha\delta \equiv -\Delta + \alpha\delta\langle\delta,\cdot\rangle.$$

Rigorous interpretation (in $L_2(\mathbb{R}^3)$):
The operator L^γ is defined on the functions possessing the following asymptotic expansion

$$U(x) = \frac{u_-}{4\pi|\mathbf{x}|} + u_0 + o(1),\ \mathbf{x} \to 0$$

and the "boundary conditions"

$$u_0 = \gamma u_-,\ \ \gamma \in \mathbb{R} \cup \{\infty\}.$$

The real parameters α and γ are *somehow* connected, but precise relation between them cannot be established without additional assumptions.[1] We know only

$$\alpha = 0 \Leftrightarrow \gamma = \infty.$$

[1] See our book with S. Albeverio, where this connection is established using homogeneity properties of the formal operator L_α.

Alternative definition

The self-adjoint operator L^γ in $L_2(\mathbb{R}^3)$ is defined on the functions possessing the following representation

$$U(x) = U_r(x) + u_- \frac{e^{-\beta|\mathbf{x}|}}{4\pi|\mathbf{x}|}, \;\; \beta > 0,$$

with

$$U_r \in \mathrm{Dom}\,(-\Delta) (= W_2^2(\mathbf{R}^3)), \quad u_- \in \mathbb{C}$$

and the "boundary conditions"

$$U_r(0) = \left(\gamma + \frac{\beta}{4\pi}\right) u_1.$$

The parameter $\tilde{\gamma} = \gamma + \frac{\beta}{4\pi}$ runs over $\mathbb{R} \cup \{\infty\}$ again.
We extend the domain of the original operator $-\Delta$ by adding one-dimensional subspace spanned by $\frac{e^{-\beta|\mathbf{x}|}}{4\pi|\mathbf{x}|} = \frac{1}{-\Delta+\beta^2}\delta$, but as a compensation we need extra boundary condition. As a result the resolvent equation

$$(L^\gamma - \lambda)U = F$$

is again solvable for any $F \in L_2(\mathbb{R}^3)$ and $\Im\lambda > 0$.

Properties of the standard model

- The operator L^γ is self-adjoint.
- The spectrum contains the absolutely continuous branch $[0, \infty)$ (inherited from the Laplacian) and at most one negative eigenvalue $E_0 = -(4\pi\gamma)^2$ provided $\gamma < 0$.
- The eigenfunction corresponding to $E_0 = -\chi^2$ is spherically symmetric

$$\Psi_0 = \frac{e^{-\chi|\mathbf{x}|}}{4\pi|\mathbf{x}|}, \;\; \chi = -4\pi\gamma.$$

- The scattered waves are

$$V(\lambda, \mathbf{k}, \mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + a(k)\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|},$$

where the scattering amplitude is calculated by substituting $\mathbb{V}$ into the boundary conditions

$$a = a(|\mathbf{k}|) = \frac{-1}{ik/4\pi - \gamma}.$$

- The scattering amplitude a does not depend on the direction of the incoming wave $\Rightarrow$ the scattering matrix is non-trivial in the s-channel only.

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Why p-type point interactions are impossible in L_2?

1. All self-adjoint extensions of the operator $-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}$ coincide with the family L^γ.
2. It is expected that the operator is defined on the functions possessing the representation
$$U_r(x) + u_1 g_1,$$
where g_1 has p-symmetry, for example
$$g_1 = \frac{\partial}{\partial x_1}\frac{e^{-\beta_1|\mathbf{x}|}}{4\pi|\mathbf{x}|} = -\frac{\beta_1|\mathbf{x}|+1}{4\pi|\mathbf{x}|^3}x_1 \notin L_2(\mathbb{R}^3).$$
3. It is natural to expect that the boundary conditions take the form
$$\frac{\partial}{\partial x_1}U_r(0) = \tilde{\gamma}u_1,$$
but if U_r just belongs to the domain of $-\Delta$, then the value $\frac{\partial}{\partial x_1}U_r(0)$ is not properly defined!

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Conclusions

In order to define p-type point interactions one has to

- extend the original Hilbert space ($L_2(\mathbb{R}^3)$) by adding elements like g_1,
- use smoother functions in order to make sense of the boundary condition.

The first problem can be resolved by just adding to the origianl Hilbert space a finite dimensional space.

The second problem can be resolved by considering the Sobolev space $W_2^1(\mathbb{R}^3)$ instead of $L_2(\mathbb{R}^3)$. The space $W_2^1(\mathbb{R}^3)$ is the space of all functions $f(\mathbf{x}), \mathbf{x} \in \mathbb{R}^3$ with the finite norm

$$\| f \|_{W_2^1} = \| \sqrt{-\Delta + 1} f \|_{L_2} .$$

It is a Hilbert space and from the mathematical point of view there is no preference in using the space L_2 instead of W_2^1.

The domain of the Laplace operator coincides with the set of functions such that

$$\| (\sqrt{-\Delta + 1})^3 f \| < \infty.$$

Important fact (Sobolev embedding theorem)

Every function f of three variables, such that $\| (\sqrt{-\Delta+1})^3 f \| < \infty$ has continuous first derivatives, i.e. $\frac{\partial}{\partial x_j} f(0)$ are perfectly defined.

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The model space

Our aim is to get a model for p-type spherically symmetric point interaction. One may think about giving definition for the following formal operator

$$-\Delta + \sum_{i=1}^{3} \alpha \partial_{x_i} \delta \langle \partial_{x_i} \delta, \cdot \rangle.$$

Introduce the notation $g_j(\lambda) = \frac{\partial}{\partial x_j} \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|} = \frac{ik|\mathbf{x}| - 1}{4\pi|\mathbf{x}|^3} e^{ik|\mathbf{x}|} x_j$. The new Hilbert space can be chosen equal to

$$\mathbb{H} = W_2^1(\mathbb{R}^3) \dot{+} \mathcal{L}\{g_1(-\beta_1^2), g_2(-\beta_1^2), g_3(-\beta_1^2)\} \ni \mathbb{U} = U + \sum_{i=1}^{3} u_1^i g_i(-\beta_1^2)$$

with the norm $\| \mathbb{U} \|_{\mathbb{H}}^2 = \| U \|_{W_2^1}^2 + \gamma \| \mathbf{u}_1 \|^2$. Real positive numbers β_1 and γ are free parameters of the model. Every function from this space possesses the representation

$$\mathbb{U} = U - \frac{\beta_1|\mathbf{x}| + 1}{4\pi|\mathbf{x}|^3} e^{-\beta_1|\mathbf{x}|} \mathbf{x} \cdot \mathbf{u}_1$$

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The differential operator in $\mathbb{H}$

The model operator $\mathbb{A}$ should be defined so that it acts as Laplacian outside the origin, namely

$$\mathbb{A}\mathbb{U} = -(\mathbb{U}_{x_1x_1} + \mathbb{U}_{x_2x_2} + \mathbb{U}_{x_3x_3}), \quad \mathbf{x} \neq 0.$$

Consider another free parameter $\beta \neq \beta_1$ and introduce

$$G_i = \frac{1}{\beta_1^2 - \beta^2}(g_i(-\beta^2) - g_i(-\beta_1^2)).$$

The Laplacian acts on such function as follows

$$\begin{array}{rcl} -\Delta G_i & = & -\Delta \left(\frac{1}{\beta_1^2 - \beta^2}(g_i(-\beta^2) - g_i(-\beta_1^2)) \right) \\ & = & \frac{1}{\beta_1^2 - \beta^2}\left(-\beta^2 g_i(-\beta^2) + \beta_1^2 g_i(-\beta_1^2)\right) \\ & = & -\beta^2 G_i + g_i(-\beta_1^2). \end{array}$$

The functions G_i and g_i form a sort of cascade and the operator $-\Delta + \beta^2$ is a cascade operator

$$(-\Delta + \beta^2)G_i = g_i, \;\; (-\Delta + \beta_1^2)g_i = \partial_{x_i}\delta.$$

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Definition of the operator

The operator $\mathbb{A}_\theta$, $\theta \in [0, \pi)$ is defined on the functions possessing the representation

$$\begin{array}{rcl} \mathbb{U} & = & U_r + \sum_{i=1}^{3} u^i G_i(-\beta^2) + \sum_{i=1}^{3} u_1^i g_i(-\beta_1^2), \\ & & U_r \in W_2^3(\mathbb{R}^3), \mathbf{u}, \mathbf{u}_1 \in \mathbb{C}^3, \end{array}$$

and the boundary conditions

$$\sin\theta \left(\nabla U_r(0) + \gamma \mathbf{u}_1 \right) = \cos\theta \, \mathbf{u},$$

by the formula

$$\mathbb{A}_\theta \left(U_r + \sum_{i=1}^{3} u^i G_i(-\beta^2) + \sum_{i=1}^{3} u_1^i g_i(-\beta_1^2) \right)$$

$$= -\Delta U_r - \beta^2 \sum_{i=1}^{3} u^i G_i(-\beta^2) + \sum_{i=1}^{3} g_i(-\beta_1^2) \left(\mathbf{x} \cdot \mathbf{u} - \beta_1^2 \mathbf{x} \cdot \mathbf{u}_1 \right).$$

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$$= -\Delta U_r - \beta^2 \sum_{i=1}^{3} u^i G_i(-\beta^2) + \sum_{i=1}^{3} g_i(-\beta_1^2) \left(\mathbf{x} \cdot \mathbf{u} - \beta_1^2 \mathbf{x} \cdot \mathbf{u}_1 \right).$$

Properties of the operator

- The operator $\mathbb{A}_\theta$ is self-adjoint in the Hilbert space $\mathbb{H} = W_2^1(\mathbb{R}^3) \oplus \mathbb{C}^3$.
- The operator $\mathbb{A}_\theta$ commutes with the rotations around the origin and reflections in planes passing through the origin.
- Spectral properties of the operator are encoded in the following rational function

$$Q(\lambda) = \frac{1}{12\pi}\left\{ik + \frac{\beta_1^2}{ik-\beta_1} + \beta + \frac{\beta_1^2}{\beta+\beta_1}\right\} + \frac{\gamma}{-\beta_1^2 - k^2}.$$

- The resolvent of the operator on $W_2^1 \subset \mathbb{H}$ is given by

$$(\mathbb{A}_\theta - \lambda)^{-1}U = \frac{1}{-\Delta-\lambda}U$$
$$-\frac{1}{(k^2+\beta_1^2)(Q(\lambda)+\cot\theta)}\left(\int_{\mathbb{R}^3}\frac{(ik|\mathbf{y}|-1)e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|^3}\mathbf{y}^t U(\mathbf{y})d^3\mathbf{y}\right)\frac{(ik|\mathbf{x}|-1)e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|^3}\mathbf{x}.$$

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Spectral properties

The model operator may have several bound states. Each one has mutiplicity 3. The corresponding eigenfunctions are

$$\mathbb{V}_{\lambda_0} = -\frac{\chi|\mathbf{x}|+1}{4\pi|\mathbf{x}|^3} e^{-\chi|\mathbf{x}|}\mathbf{x}\cdot\mathbf{a}, \quad \lambda_0 = -\chi^2,$$

where $\chi > 0$ is a solution to the equation

$$Q(-\chi^2) + \cot\theta = 0.$$

To prove this fact one writes the function $\mathbb{V}$ as a linear combination

$$\mathbb{V} = \sum_{i=1}^{3} g_i a_i + \sum_{i=1}^{3} G_i b_i + V,$$

where $V \in W_2^3(\mathbb{R}^3)$. Substituting into the boundary conditions one gets the dispersion equation.

Scattering properties

- Absolutely continuous spectrum covers the branch $[0, \infty)$ inherited from the Laplacian.
- Continuous spectrum (generalized) eigenfunctions are

$$\mathbb{V}(\lambda, \mathbf{k}/k, \mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{i}{(k^2+\beta_1^2)(Q(k^2)+\cot\theta)} \frac{ik|\mathbf{x}|-1}{4\pi|\mathbf{x}|^3} e^{ik|\mathbf{x}|}\mathbf{x}\cdot\mathbf{k} \ \lambda > 0,$$

- The scattering amplitude depends on the angle between incoming and outgoing waves.
  The scattering matrix is non-trivial in the p-channel!
- New type of eigenfunction expansions can be obtained by integrating the jump of the resolvent of $\mathbb{A}_\theta$ on the real axis.

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Perspectives

- Developed model can be used to describe scattering processes for atoms where *p*-electrons play an essential role;
- One may combine *s*- and *p* -type point interactions;
- The model can be generalized to include higher singularities: *d*, *f*, ... -orbitals;
- Model all atoms from Mendeleev's table!
- The model can be used to calculate electron levels in simple molecules like H_2O;
- Few-body problems;
- ...

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