ZERO-RANGE HAMILTONIANS FOR THREE QUANTUM PARTICLES

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ABSTRACT. Characterisation of the confined states of quantum systems made of many particles interacting via short range forces was the main goal for theoretical physicists investigating the structure of nuclei in the early years of Quantum Mechanics. A rigorous formulation of the problem was given at the beginning of the sixties by the russian school of mathematical physics. The analysis of the threebody problem already revealed intriguing pathologies opening at the same time promising prospects for the future. We summarize history and recent attempts of this line of research

1. INTRODUCTION

The three quantum particle problem is a line of research that Robert A. Minlos has been following for most of his scientific carrier. Together with Berezin and Faddeev he framed the problem of zerorange interactions in Quantum Mechanics inside the theory of self-adjoint extensions of symmetric operators. He was able to formulate in a rigorous way the unboudedness problem for three-particle zero-range Hamiltonians and he also suggested possible way out of such a difficulty.

Following his suggestions, resumed later by Albeverio, Hoegh-Krohn and Wu [2], we attempted to work out partial solutions to the problem. It is worth mentioning that nowadays the interest in the problem shifted toward many other research fields and, e.g., it is actively investigated by physicist and applied mathematicians working in low temperature physics of quantum many particle systems (see e.g. [7] and reference therein). We want first to give an outline of the way zero range interactions and the quantum three-body problem appeared in the physical literature.

Heuristically point interactions are quantum interactions supported on points or "thin sets" (e.g. low dimensional hypersurfaces). They are also called zero-range interactions or contact interactions

They are used whenever the range of interparticle interactions is much shorter than other relevant length scales.

They have the advantage of permitting better insight allowing for "explicit computations": for this reason they are used in the mathematical modeling of many natural phenomena.

Let \mathcal{M} be a submanifold of \mathbb{R}^d of dimension s < d. Consider the operator

$$H_{0,0} := -\Delta \upharpoonright C_0^{\infty}(\mathbb{R}^d \setminus \mathcal{M})$$

As a restriction of a self-adjoint operator $H_{0,0}$ is symmetric but non self-adjoint. In fact,

$$D(H_{0,0}^*) = \left\{ \psi \in L^2(\mathbb{R}^d) : |(\psi, -\Delta\phi)| < C \|\phi\| \ \forall \phi \ \in C_0^\infty(\mathbb{R}^d \setminus \mathcal{M}) \right\}$$

includes any function in $D(-\Delta) = H^2(\mathbb{R}^d)$ as well as any function $\psi \in L^2(\mathbb{R}^d)$ such that

$$-\Delta \psi = \xi + T; \ \xi \in L^2(\mathbb{R}^d), \ T \in D'(\mathbb{R}^d) \text{ with } supp \ T \subseteq \mathcal{M}$$

Definition. Any (non-trivial) self-adjoint extension of $H_{0,0}$ (if any) will be denoted as a Hamiltonian with zero-range interaction on \mathcal{M} .

The simplest case is when $\mathcal{M} = \{y_1, \dots, y_N\}$ $y_i \in \mathbb{R}^d$ $\forall i = 1, \dots, N$, i.e., a discrete set of points of \mathbb{R}^d .

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Take $\psi = G^z(\cdot - y_i)$ where $G^z = \mathcal{F}^{-1}(k^2 - z)^{-1}$ for any $z \in \mathbb{C} \setminus \mathbb{R}^+$. It belongs to $L^2(\mathbb{R}^d)$ for d =1,2,3 and

$$(G^{z}(\cdot - y_{i}), -\Delta_{x}\phi) = ([-\Delta_{x} - z]G^{z}(\cdot - y_{i}), \phi) + (zG^{z}(\cdot - y_{i}), \phi) = (zG^{z}(\cdot - y_{i}), \phi)$$

for all $\phi \in C_0^{\infty}(\mathbb{R}^d \setminus \{y_1, \dots, y_N\})$, which means that $G^z \in D(H_{0,0}^*)$ (but it does not belong to $H^2(\mathbb{R}^d)$) and that $G^z(\cdot - y_i)$ is an eigenvector of $H_{0,0}^*$ relative to the eigenvalue z.

The same result holds true for any partial derivative of G^z belonging to $L^2(\mathbb{R}^d)$ (which is true only for the first derivatives of G^z in d = 1).

It is possible to classify the entire family of self-adjoint extensions of $H_{0,0}$ for d=1,2 and 3. It turns out that in each dimension the family of self-adjoint extensions shows peculiar properties. We will be interested in particular in the following operators that can be proved (see [1]) to be a subset of the family of self-adjoint extensions of $H_{0,0}$ in $L^2(\mathbb{R}^3)$.

For any $\underline{\alpha} = \{\alpha_1, \ldots, \alpha_n\}$ with $\alpha_i \in \mathbb{R}$, $i = 1, \ldots, n$ and $\underline{y} = \{y_1, \ldots, y_n\}$, $y_i \in \mathbb{R}^3$, $i = 1, \ldots, n$ the operator $H_{\underline{\alpha}, \underline{y}}$ defined by

$$D(H_{\underline{\alpha},\underline{y}}) = \left\{ u \in L^2(\mathbb{R}^3) \mid u = \phi_{\lambda} + \sum_{k=1}^n q_k G_{\lambda}(\cdot - y_k) \\ \phi_{\lambda} \in H^2(\mathbb{R}^3), \quad \phi_{\lambda}(y_j) = \sum_{k=1}^n [\Gamma_{\underline{\alpha},\underline{y}}(\lambda)]_{jk} q_k, \ j = 1, ..., n \right\}$$
(1)

$$(H_{\underline{\alpha},\underline{y}} + \lambda)u = (-\Delta + \lambda)\phi_{\lambda} \tag{2}$$

where $G_{\lambda} \equiv G^{z}|_{z=-\lambda}$ and

$$[\Gamma_{\underline{\alpha},\underline{y}}(\lambda)]_{jk} = \left(\alpha_j + \frac{\sqrt{\lambda}}{4\pi}\right)\delta_{jk} - G_{\lambda}(y_j - y_k)(1 - \delta_{jk})$$
(3)

vanishing at $y_1, ..., y_n$ one has q = 0 and then, from (2), $H_{\alpha,y}u = -\Delta u$.

At each point y_j the elements of the domain satisfy a boundary condition expressed by the last equality in (1). If we define $r_j = |x - y_j|$ it is easy to see that the boundary condition can be equivalently written as

$$\lim_{r_j \to 0} \left[\frac{\partial(r_j u)}{\partial r_j} - 4\pi \alpha_j(r_j u) \right] = 0, \quad j = 1, ..., n$$
(4)

This explains the term "local" given to this class of extensions.

The spectral structure of local point interaction Hamiltonians is not at all trivial and it is easily investigated. In fact, $-\lambda$ is a negative eigenvalues of the Hamiltonian $H_{\underline{\alpha},\underline{y}}$ if and only if det $\Gamma_{\underline{\alpha},\underline{y}}(\lambda) =$ 0 and the generalised eigenfunctions are non-trivial and explicitly known. Details can be found in [1]. Here, we want only to point out that if two scatterer positions come close one to the other the off-diagonal terms of the matrix (3) become very large with respect to any value of the strength parameters $\underline{\alpha}$. It is easy to check that in the limit of zero distance the ground state eigenvalue of the Hamiltonian is approaching $-\infty$ (for details when n=2, see [1]).

Let us now consider the much more difficult case of many particles. The Hamiltonians for a system of N particles interacting via zero-range forces will be defined as any self-adjoint extension of

$$-\sum_{i=1}^N \Delta_{x_i} \upharpoonright C_0^\infty(\mathbb{R}^{dN} \setminus \bigcup_{i < j} \sigma_{ij})$$

$$\sigma_{ij} = \{x = (x_1, ..., x_N) \in \mathbb{R}^{dN} | x_i = x_j\}$$

acting on state vectors with symmetry properties which will depend on the type of particles under investigation.

In the following, we will consider the case of three identical bosons with masses 1/2, in the center of mass reference frame.

Expressed in terms of the Jacobi coordinates

$$\mathbf{x} = \mathbf{x}_2 - \mathbf{x}_3, \qquad \mathbf{y} = \frac{1}{2}(\mathbf{x}_2 + \mathbf{x}_3) - \mathbf{x}_1 \tag{5}$$

the space of square integrable functions completely symmetric in the exchange of particle coordinates is

$$L_s^2(\mathbb{R}^6) = \left\{ \psi \in L^2(\mathbb{R}^6) \text{ s.t. } \psi(\mathbf{x}, \mathbf{y}) = \psi(-\mathbf{x}, \mathbf{y}) = \psi\left(\frac{1}{2}\mathbf{x} + \mathbf{y}, \frac{3}{4}\mathbf{x} - \frac{1}{2}\mathbf{y}\right) \right\}$$
(6)

Zero-range interactions among particles will be confined on the three-dimensional hyperplanes

$$\Sigma = \{ \mathbf{x} = 0 \} \cup \{ \mathbf{y} - \mathbf{x}/2 = 0 \} \cup \{ \mathbf{y} + \mathbf{x}/2 = 0 \}.$$
(7)

As we pointed out already, this means that we are looking for Hamiltonians in $L^2_s(\mathbb{R}^6)$ which are non trivial s.a. extension of the operator

$$\tilde{H}_0 = -\Delta_{\mathbf{x}} - \frac{3}{4} \Delta_{\mathbf{y}}, \quad D(\tilde{H}_0) = \left\{ \psi \in L^2_s(\mathbb{R}^6) \text{ s.t. } \psi \in H^2(\mathbb{R}^6), \ \psi \big|_{\Sigma} = 0 \right\}.$$
(8)

The defect spaces of \tilde{H}_0 are now of infinite dimensions. This makes the examination of classes of self-adjoint extensions much more difficult and their physical interpretation more complicate.

Ter-Martirosian and Skorniakov [16], on the basis of the analogy with the point interaction potentials, proposed to define an operator H_{α} acting as the free Hamiltonian outside the hyperplanes and satisfying a boundary condition close to the hyperplanes. Specifically, they impose for the functions in the domain of the Hamiltonian the boundary condition

$$\psi(\mathbf{x}, \mathbf{y}) = \frac{\xi(\mathbf{y})}{|\mathbf{x}|} + \alpha \,\xi(\mathbf{y}) + o(1) \,, \quad \text{for } |\mathbf{x}| \to 0 \quad \text{and } \mathbf{y} \neq 0 \tag{9}$$

where ξ is a function depending on ψ . The same behaviour must hold close to the other coincidence hyperplanes for symmetry reasons.

Being the singular part in (9) the behaviour of the potential of a charge ξ distributed on the hyperplane, the operators H_{α} and the boundary condition were expressed in terms of charge distribution potentials, i.e. imposing that functions in the domain of H_{α} were the sum of a regular and a singular part in the following way

$$\psi = w^{\lambda} + \mathcal{G}^{\lambda} \xi, \qquad w^{\lambda} \in H^2(\mathbb{R}^6)$$
(10)

where $\lambda > 0$ and

$$\widehat{\mathcal{G}^{\lambda}\xi}(\mathbf{k},\mathbf{p}) = \sqrt{\frac{2}{\pi}} \, \frac{\hat{\xi}(\mathbf{p}) + \hat{\xi}(\mathbf{k} - \frac{1}{2}\mathbf{p}) + \hat{\xi}(-\mathbf{k} - \frac{1}{2}\mathbf{p})}{|\mathbf{k}|^2 + \frac{3}{4}|\mathbf{p}|^2 + \lambda} \,. \tag{11}$$

is the $(\lambda -)$ potential of a charge density ξ identically distributed on each coincidence plane. The behaviour of the function $\mathcal{G}^{\lambda}\xi(\mathbf{x},\mathbf{y})$ close to the planes is easily computed

$$\mathcal{G}^{\lambda}\xi(\mathbf{x},\mathbf{y}) = \frac{\xi(\mathbf{y})}{|\mathbf{x}|} - \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \, e^{i\mathbf{p}\cdot\mathbf{y}} \left(T^{\lambda}\hat{\xi}\right)(\mathbf{p}) + o(1) \tag{12}$$

where

$$\left(T^{\lambda}\hat{\xi}\right)(\mathbf{p}) := \sqrt{\frac{3}{4}|\mathbf{p}|^{2} + \lambda} \,\,\hat{\xi}(\mathbf{p}) - \frac{1}{\pi^{2}} \int d\mathbf{p}' \,\frac{\hat{\xi}(\mathbf{p}')}{|\mathbf{p}|^{2} + |\mathbf{p}'|^{2} + \mathbf{p} \cdot \mathbf{p}' + \lambda} \,. \tag{13}$$

In this way the boundary condition (9) can be rephrased as an integral equation for the "charges" ξ (for details see [5] and references therein).

As noticed by Danilov [9], the operators constructed in this way are not self-adjoint and admit a continuum set of eigenvalues tending to minus infinity.

2. Minlos and Faddeev seminal papers (1962)

In two fundamental papers [13], [14] on the subject Minlos and Faddeev succeeded in translating rigorously the attempts of Ter-Martirosian and Skornyakov in terms of Birman's theory of self-adjoint extensions of positive symmetric operators. They proved that the boundary condition (9) about the behaviour of functions in the domain of the Hamiltonians close to the coincidence planes was not enough to guarantee their self-adjointness.

The final result can be summarised in the following characterisation, written in momentum space, of a two-parameter family of self-adjoint Hamiltonians

$$D(H_{\alpha,\beta}) = \left\{ \psi \in L^2_s(\mathbb{R}^6) \mid \psi = w^{\lambda} + \mathcal{G}^{\lambda}\xi, \ w^{\lambda} \in H^2(\mathbb{R}^6), \ \hat{\xi} \in D(T^{\lambda}_{\beta}), \\ \alpha \,\hat{\xi}(\mathbf{p}) + \left(T^{\lambda}\hat{\xi}\right)(\mathbf{p}) = \left. (w^{\lambda} \right|_{\mathbf{x}=0})^{\wedge}(\mathbf{p}) \right\},$$
(14)

$$(H_{\alpha,\beta} + \lambda)\psi = (H_0 + \lambda)w^{\lambda}, \qquad (15)$$

where

$$H_0 = -\Delta_{\mathbf{x}} - \frac{3}{4}\Delta_{\mathbf{y}}, \qquad D(H_0) = H^2(\mathbb{R}^6).$$
(16)

with

$$D(T_{\beta}^{\lambda}) = \left\{ \hat{\xi} \in L^{2}(\mathbb{R}^{3}) \mid \hat{\xi} = \hat{\xi}_{1} + \hat{\xi}_{2}, \quad \hat{\xi}_{1} \in D(T^{\lambda}), \\ \text{and} \quad \hat{\xi}_{2}(\mathbf{k}) = \frac{c}{|\mathbf{k}|^{2} + 1} \left(\beta \sin\left(s_{0} \log|\mathbf{k}|\right) + \cos\left(s_{0} \log|\mathbf{k}|\right) \right) \right\}$$
(17)

where c is an arbitrary constant, s_0 is the positive solution of the equation

$$1 - \frac{8}{\sqrt{3}} \frac{\sinh \frac{\pi s}{6}}{s \cosh \frac{\pi s}{2}} = 0.$$
 (18)

Apart from technical complications due to the self-adjointness requirement, one should notice the similarity between (14 - 15) and (1). Each function in the domain of the Hamiltonians is the sum of a regular part and the potential of some charge density distributed on the coincidence planes, the Hamiltonians operate as the free Hamiltonian acting on the regular part and the boundary condition can be expressed as an equation on the charges.

The Hamiltonians defined in the way described above were finally self-adjoint, but Minlos and Faddeev realised that their spectral structure made those Hamiltonians unphysical models for a threebody quantum system. In fact, the authors found that their point spectrum contains an infinite sequence of negative eigenvalues unbounded from below (see [10] for an alternative proof). The authors also suggest a possible way out of this unboudedness pathology. In short, their hint amounts to substitute the constant α in (14) with the operator A defined, in Fourier space, by

$$(A\hat{\xi})(\mathbf{p}) = \alpha\hat{\xi}(\mathbf{p}) + (K\hat{\xi})(\mathbf{p})$$
(19)

with $\alpha \in \mathbb{R}$ and K the convolution operator with kernel K(p) behaving for large $|\mathbf{p}|$ as

$$K(\mathbf{p}) \sim \frac{\gamma}{|\mathbf{p}|^2}, \quad \text{for} \quad |\mathbf{p}| \to \infty$$

3. On the negative eigenvalues

In a private communication happened years ago between one of us and L.D. Faddeev, he appeared absolutely confident that zero-range Hamiltonians bounded from below for the three-body quantum system would exist. He renewed the suggestion that he and Minlos gave in their '62 papers, mentioning that, with regret, they did not get involved any longer in the problem. On the other hand, Minlos, in the rest of his scientific career, went back occasionally to zero-range Hamiltonians for many-particle quantum systems approaching the interesting case of $N, N \ge 2$, identical fermions interacting, via zero-range forces, with a different particle, giving important contributions to the stability problem (see, e.g., [11], [12]; for more recent developments see [15] and references therein). Recently, we showed that, at least in the case $\alpha = 0$ the strategy works very well. For details of the proof see [10].

Considering the Ter-Martirosian, Skorniakov boundary condition (9) for $\alpha = 0$ and adding the term suggested by Minlos and Faddeev, we have that $-\lambda$, $\lambda > 0$ is a negative eigenvalue of the Hamiltonian if

$$\frac{\delta}{2\pi^2} \int d\mathbf{p}' \, \frac{\hat{\xi}(\mathbf{p}')}{|\mathbf{p} - \mathbf{p}'|^2} + \sqrt{\frac{3}{4}} |\mathbf{p}|^2 + \lambda \, \hat{\xi}(\mathbf{p}) - \frac{1}{\pi^2} \int d\mathbf{p}' \, \frac{\hat{\xi}(\mathbf{p}')}{|\mathbf{p}|^2 + |\mathbf{p}'|^2 + \mathbf{p} \cdot \mathbf{p}' + \lambda} = 0 \,. \tag{20}$$

where δ is a real parameter.

In the rotationally invariant case $\hat{\xi} = \hat{\xi}(|\mathbf{p}|)$, integrating out the angular variables one gets

$$\frac{\delta}{\pi} \int_0^\infty dp' \, p'\hat{\xi}(p') \log \frac{p+p'}{|p-p'|} + \sqrt{\frac{3}{4}p^2 + \lambda} \, p\,\hat{\xi}(p) \\ -\frac{2}{\pi} \int_0^\infty dp' \, p'\hat{\xi}(p') \, \log \frac{p^2 + p'^2 + pp' + \lambda}{p^2 + p'^2 - pp' + \lambda} = 0\,.$$
(21)

The following statement holds true

Proposition 3.1. Let

$$\delta_0 = \frac{\sqrt{3}}{\pi} \left(\frac{4\pi}{3\sqrt{3}} - 1 \right). \tag{22}$$

Then for $\delta > \delta_0$ the equation (21) has only the trivial solution.

The main technical tool used in the proof is the following change of variable (see [8])

$$p = \frac{2\sqrt{\lambda}}{\sqrt{3}} \sinh x, \qquad x = \log\left(\frac{\sqrt{3}p}{2\sqrt{\lambda}} + \sqrt{\frac{3p^2}{4\lambda} + 1}\right)$$
(23)

which allows to diagonalize equation (21) for the new function

$$\theta(x) = \begin{cases} \lambda \sinh x \cosh x \,\hat{\xi} \left(\frac{2\sqrt{\lambda}}{\sqrt{3}} \sinh x \right) & \text{for } x \ge 0\\ -\theta(-x) & \text{for } x < 0 \end{cases}$$
(24)

giving the following equation for the Fourier transform of the function θ

$$\left(1+2 \ \frac{\delta \sinh \frac{\pi}{2}s - 4 \sinh \frac{\pi}{6}s}{\sqrt{3} s \cosh \frac{\pi}{2}s}\right)\hat{\theta}(s) = 0.$$

$$(25)$$

It is then easy to conclude the proof showing that

$$\left(1+2 \ \frac{\delta \sinh \frac{\pi}{2}s - 4 \sinh \frac{\pi}{6}s}{\sqrt{3} s \cosh \frac{\pi}{2}s}\right) > 0 \quad \text{for} \quad \delta > \delta_0.$$

Other recent attempts to obtain zero-range three-body Hamiltonians bounded from below can be found in [3] and [4].

Dedication. The authors want to dedicate this contribution to the memory of Robert A. Minlos, a leading mind of mathematical physics and a wonderful human being.

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