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Perturbation theory for point interactions in three dimensions

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Abstract. The formal manipulation with δ-potentials modelling contact interactions is compared with the recent mathematical theory of this phenomenon.

1. Introduction

Contact interactions are widely used as an approximation of short-range potentials especially in those cases in which the explicit form of the potentials is unknown (cf Albeverio *et al* 1984a and references therein). This contact interaction is often modelled by a heuristic Hamiltonian

$$\tilde{H}_\lambda = -\Delta + V(x) + \lambda\delta(x) \tag{1}$$

on a Hilbert space $L^2(R^3)$, λ being a coupling constant and δ the Dirac measure at the origin. In one dimension, Hamiltonians with δ-potentials can be defined rigorously (Reed and Simon 1975, Ex. 3 to Th. 10.17) and they are the most applied potentials of solid state physics (Kronig and Penney 1931, Erdős and Herndon 1982, Englisch 1983). Though it has been known for a long time (Berezin and Fadeev 1961) that in more than one dimension the singularities of the δ-potential become so strong that it is not possible to define the heuristic Hamiltonian $\tilde{H}_\lambda$ for non-zero λ as a self-adjoint operator on $L^2(R^3)$, δ-potentials are widely used in physics, especially in nuclear physics, molecular physics and solid state physics, for the description of short-range effects and one gets reasonable results (Thomas 1935, Fermi 1936, Das and Behrson 1959, Schwartz 1959, Zeldovič 1960, Schaefer and Yaris 1967, Blinder 1978). For example the first order of the perturbation theory applied to

$$\tilde{H}_\lambda = H_0 + \lambda\delta(x) \qquad H_0 = -\Delta + V(x),$$

predicts an energy shift

$$E - E^{(0)} \approx \lambda |f^{(0)}(0)|^2.$$

where $f^{(0)}$ is the eigenfunction of H_0 corresponding to $E^{(0)}$. Since the eigenfunctions of the usual Hamiltonians H_0 are bounded (Reed and Simon 1978, Th. 13.38) the energy shift is also bounded.

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On the other hand there is a second possibility to describe contact interactions which is correct from the mathematical point of view (Berezin and Fadeev 1961, Alberverio *et al* 1979). Let us first define the restricted operator H_0^r

$$H_0^r = H_0 \upharpoonright C_0^\infty(\mathbf{R}^3 \backslash \{0\}).$$

($C_0^\infty(\Omega)$ denotes the set of infinitely differentiable functions with compact support contained in Ω.) H_0^r is a symmetric operator with deficiency indices (1, 1) (Behnke and Focke 1978). Therefore a one-parameter family H_α of its self-adjoint extensions exists (Reed and Simon 1975, Th. 10.2). These operators H_α are used as Hamiltonians describing a particle moving under the influence of the potential $V(x)$ and an additional contact interaction at 0. It is also possible to obtain these Hamiltonians H_α as a perturbation of the operator H_0 by sequences of potentials with shrinking supports (Albeverio and Høegh-Krohn 1981, Šeba 1985).

The aim of this paper is to compare the formal δ-potential description of contact interactions with the rigorous one. Thus this article can be understood as a continuation of Englisch (1984). In § 2 we describe all self-adjoint extensions of H_0^r. In § 3 we show that the formal δ-potential approach yields in the first order of the perturbation theory the same eigenvalues as the rigorous approach does. The same holds for the scattering amplitudes as is shown in § 4.

Thus the reasonable results obtained by the formal application of perturbation theory to formal Hamiltonians can be explained.

2. Hamiltonians with point interactions

Following Albeverio and Høegh-Krohn (1981) we describe Hamiltonians with point interactions by self-adjoint extensions of H_0^r, where

$$H_0^r = -\Delta + V(x), \qquad D(H_0^r) = C_0^\infty(\mathbf{R}^3 \backslash \{0\}).$$

In order to avoid inessential technicalities we confine ourselves to the potentials satisfying

$$V(x) \in L^2(\mathbf{R}^3) + L^\infty(\mathbf{R}^3),$$

i.e. $V = V_2 + V_\infty$ with $\int |V_2(x)|^2 \, d^3x < \infty$ and $\sup_x |V_\infty(x)| < \infty$. (Cf Albeverio *et al* (1983) and Zorbas (1980) for the special case $V(x) = 1/|x|$ and Gesztesy and Pittner (1984) for short-range potentials V.) The conditions concerning V guarantee that

$$H_0 = -\Delta + V(x)$$

is a self-adjoint operator with domain

$$D(H_0) = D(-\Delta) = \{f \in L^2(\mathbf{R}^3) : \Delta f \in L^2(\mathbf{R}^3) \text{ in the sense of distributions}\}$$

(Reed and Simon 1975, § 10.2). It is known from the mathematical literature (Behnke and Focke 1978) that H_0^r has deficiency indices (1, 1). Consequently there is a one-parameter family H_α of its self-adjoint extensions. We interpret these operators H_α as Hamiltonians describing a particle under the additional influence of a zero-range interaction at 0. Obviously H_0 is one of the self-adjoint extensions of H_0^r.

Knowing H_0 we can apply the results by Zorbas (1980) who represents all the remaining extensions H_α by means of H_0 in the following way:

$$H_\alpha = -\Delta + V(x),$$
$$D(H_\alpha) = \{f \in L^2(R^3) : f(x) = g(x) + c(G(x, 0, i) - e^{i\alpha} G(x, 0, -i)),$$
$$g(x) \in D(\overline{H_0^r}),\ c \in C\} \quad \alpha \in [0, 2\pi),$$

where $G(x, y, z)$ is the Green function of H_0,

$$[(H_0 - z)^{-1} f](x) = \int G(x, y, z) f(y)\, d^3y,$$

and $\overline{H_0^r}$ is the closure of H_0^r (Reed and Simon 1972, § 8.1). The Green function $G_\alpha(x, y, z)$ of H_α is given by

$$G_\alpha(x, y, z) = G(x, y, z) + \mu(z, \alpha) G(x, 0, z) G(y, O, z) \tag{2}$$

with

$$\mu(z, \alpha) = (1 - e^{i\alpha}) \Big((i - z) \int G(y, 0, z) G(y, 0, i)\, d^3y$$
$$- e^{i\alpha} (i + z) \int G(y, 0, z) G(y, 0, -i)\, d^3y \Big)^{-1}. \tag{3}$$

This relation implies that $H_{\alpha=0} = H_0$.

Now we want to compare the eigenvalues of the Hamiltonian H_α with the formal eigenvalues obtained by applying the perturbation theory to the formal Hamiltonian $\tilde{H}_\lambda$ from (1).

3. Perturbation of eigenvalues by point interactions

We note once more that $\tilde{H}_\lambda$ as defined in (1) represents only a formal Hamiltonian since it cannot be defined as a self-adjoint operator on $L^2(R^3)$ for non-zero λ. Moreover the term $\lambda\delta(x)$ is not bounded with respect to H_0 in any sense such that the conditions for the applicability of perturbation theory (Reed and Simon 1978, Th. 12.8) are not fulfilled.

Nevertheless, applying the perturbation theory to the formal Hamiltonian (1) and assuming that there is no degeneracy of the eigenvalues of H_0, one gets for the nth eigenvalue $E_n(\lambda)$ of $\tilde{H}_\lambda$

$$E_n(\lambda) = E_n^{(0)} + \lambda |f_n^{(0)}(0)|^2 + O(\lambda^2) \tag{4}$$

where $E_n^{(0)}$ and $f_n^{(0)}(x)$ are the nth eigenvalue and the nth eigenvector of H_0, respectively:

$$H_0 f_n^{(0)}(x) = E_n^{(0)} f_n^{(0)}(x).$$

The term $|f_n^{(0)}(0)|^2$ is bounded since eigenfunctions of the operator H_0 are bounded in R^3 (Reed and Simon 1978, Th. 13.38). In spite of its very formal derivation, relation (4) is often used in physics and yields reasonable results. The following theorem reveals the cause for this.

Theorem. Let $E_n^{(\alpha)}$ be the nth eigenvalue of H_α. Then for every n and small α it holds that

$$E_n^{(\alpha)} = E_n^{(0)} + \alpha |f_n^{(0)}(0)|^2 \Big(2 \int |G(x, 0, i)|^2\, d^3x \Big)^{-1} + O(\alpha^2).$$

Proof. Let $e_n(\alpha)$ be an eigenvalue of $(H_\alpha + \mathrm{i})^{-1}$:

$$[(H_\alpha + \mathrm{i})^{-1} f_n^{(\alpha)}](x) = e_n(\alpha) f_n^{(\alpha)}(x).$$

Obviously it holds that

$$E_n^{(\alpha)} = (1 - \mathrm{i} e_n(\alpha))/e_n(\alpha). \tag{5}$$

Using relations (2) and (3), choosing $z = -\mathrm{i}$ and developing $\mu(-\mathrm{i}, \alpha)$ up to first order we get

$$(H_\alpha + \mathrm{i})^{-1} = (H_0 + \mathrm{i})^{-1} - \alpha G(x, 0, -\mathrm{i}) \times \langle \overline{G(x, 0, -\mathrm{i})}, \cdot \rangle \left(2 \int |G(x, 0, \mathrm{i})|^2 \, \mathrm{d}^3 x \right)^{-1} + O(\alpha^2). \tag{6}$$

The ordinary perturbation theory applied to (6) yields for small α

$$e_n(\alpha) = e_n(0) + \alpha e_n^{(1)} + O(\alpha^2) \tag{7}$$

with

$$e_n^{(1)} = -\left(\int G(x, 0, -\mathrm{i}) f_n^{(0)}(x) \, \mathrm{d}^3 x \right)^2 \left(2 \int |G(x, 0, \mathrm{i})|^2 \, \mathrm{d}^3 x \right)^{-1}.$$

Due to

$$G(x, 0, -\mathrm{i}) f_n^{(0)}(x) \, \mathrm{d}^3 x = [(H_0 + \mathrm{i})^{-1} f_n^{(0)}](0) = e_n(0) f_n^{(0)}(0)$$

it follows that

$$e_n^{(1)} = -e_n(0)^2 (f_n^{(0)}(0))^2 \left(2 \int |G(x, 0, \mathrm{i})|^2 \, \mathrm{d}^3 x \right)^{-1}. \tag{8}$$

Inserting (7) and (8) into (5) we complete the proof.

This theorem rigorously provides the eigenvalues of the true point-interaction Hamiltonian H_α in the first order of perturbation theory. We see that for every n they coincide with the formal expression (4) if we put the coupling constant

$$\lambda = \alpha \left(2 \int_{R^3} |G(x, 0, \mathrm{i})|^2 \, \mathrm{d}^3 x \right)^{-1}.$$

The second order of the perturbation theory for $\tilde{H}_\lambda$ diverges as was already remarked in several papers (cf for example Velenik *et al* (1970)), but every order for H_α is converging.

4. Perturbation of scattering amplitudes by point interactions

Here we only treat the perturbation of the free Hamiltonian $H_0 = -\Delta$ by a point interaction. The investigation of the free Hamiltonian was not possible in § 3 since the Laplacian has no eigenvalues.

Formally applying the Born approximation, i.e. the perturbation theory for scattering, to the formal Hamiltonian

$$\tilde{H}_\lambda = -\Delta + \lambda \delta(x) \tag{9}$$

we get in the first order the on-shell scattering amplitude

$$f_\lambda(k, k') = -\lambda/(4\pi). \tag{10}$$

But the second order is divergent since

$$\frac{\int\int e^{-ikx}\, e^{i|k||x-y|}\, e^{ik'y}}{(4\pi|x-y|)}\, \delta(x)\delta(y)\, d^3x\, d^3y = \infty. \tag{11}$$

In spite of its purely formal character the first-order Born approximation (10) is also used in physics (Dawydow 1967, § 115) and it again leads to reasonable results.

For the correct Hamiltonian H_α Albeverio *et al* (1984b) explicitly calculated the on-shell scattering amplitude

$$f^{(\alpha)}(k, k') = \{2\pi[\sin(\alpha/2+\pi/4)/\cos(\alpha/2+\pi/2) - i|k|/(4\pi)]\}^{-1}.$$

The Taylor expansion of $f^{(\alpha)}(k, k')$ yields for small α

$$f^{(\alpha)} \approx -\alpha/(2\sqrt{2}\pi)$$

which agrees for all k and k' with the formal expression (10) if we put the coupling constant $\lambda = \sqrt{2}\alpha$. But in contrast to (11) the true scattering amplitude exhibits no divergences in the second order.

5. Conclusions

The δ-distribution in three dimensions has sometimes been considered (Harrison 1966, Dawydow 1967, § 115, Bartram *et al* 1968, Weber and Dick 1969) as a pseudopotential, i.e. as a potential producing nearly the same eigenvalues or scattering amplitudes as the true short-range potential. On the other hand it has been known for a long time that the δ-potential in three dimensions leads to unphysical features like non-self-adjoint operators. Nevertheless it was successfully used in many calculations which may be explained now by the fact that the δ-distribution is a pseudopotential in a new sense: in the first order the formal application of the perturbation theory to $H_0 + \lambda\delta$ results in the same values as the correct perturbation theory applied to a rigorously defined Hamiltonian with point interaction does.

For a recent attempt to define pseudopotentials in five dimensions, cf Grossmann and Wu (1984). Their paper is based on an alternative approach to define point interactions in three dimensions, cf e.g. Breit (1947), Breit and Zilsel (1947), Huang and Yang (1957), Huang *et al* (1957), Lee *et al* (1957), Wu (1959) and Blatt and Weisskopf (1959, § II.3).

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