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COMMENT

Response to "Comment on 'On the Coulomb potential in one dimension'" by Fischer, Leschke and Müller

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Abstract. The differential operator $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x)$, $\gamma \in \mathbb{R}$, in one dimension is studied using distribution theory. It is proven that there exists a unique self-adjoint operator corresponding to the differential expression understood in the principle-value sense. Point interactions determined by the singular operator $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x) + \alpha\delta(x)$ are studied.

1. Introduction

Fischer, Leschke and Müller claim in their comment [5] that 'in one dimension a self-adjoint Schrödinger operator with a $1/x$ or $1/|x|$ potential cannot be defined without the specification of a boundary condition at the origin' (see also [4]). I agree with their statement that special boundary conditions at the origin are needed to define a self-adjoint operator. These boundary conditions cannot be specified if one considers self-adjoint operator corresponding to the formal expression as one of the possible extensions of the symmetric operator defined on the domain of smooth functions with support separated from the origin. This approach has been proposed in [5]. The main idea of my paper [9] is the following. The formal differential expression $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x)$ defines a map from the Hilbert space to the space of distributions. The corresponding Hilbert space operator can be formed by restriction. It appears that this operator is self-adjoint and coincides with one of the self-adjoint extensions suggested in [5], i.e. the boundary conditions at the origin are determined by the formal differential expression itself if one considers it in the framework of distribution theory. Maybe it is proper to explain this idea more precisely.

Paper [9] was initiated by the discussion between Newton and Moshinsky on the penetrability of the potential $1/x$ in one dimension (see [13–15]), where the Schrödinger operator

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \gamma\frac{1}{x} \tag{1}$$

in $L_2(\mathbb{R})$ has been investigated. Point zero is a singular point for the corresponding differential operator. It was proposed in [9] to study this operator in the framework of distribution theory with the standard set of test functions $D = C_0^\infty(\mathbb{R})$ [8]. Let us denote the corresponding set of distributions by D'. The operator $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x)$ can be defined in the generalized sense with the set of test functions $D_0 = C_0^\infty(\mathbb{R}\backslash\{0\})$, since the set D_0 is invariant under the action of the operator. To determine an operator acting from $L_2(\mathbb{R})$ to D' the potential has to be defined as a distribution in D'. The function $1/x$ does not determine a unique distribution in D'. In [9] the corresponding distribution has been defined in the principle-value sense $1/x \Rightarrow \mathrm{vp}(1/x)$. The potential $1/x$ is an odd function homogeneous of order -1 and considered distribution is the unique regularization of the function $1/x$, which defines an odd distribution homogeneous of the same order, since the difference between any two distributions corresponding to the function $1/x$ is a distribution with support at the origin. Every odd distribution homogeneous of order -1 having support at the origin is equal to zero. Therefore, it was proposed that we study the following operator

$$H^d = \mathrm{vp}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\gamma}{x}\right) \qquad H^d : L_2(\mathbb{R}) \to D' \tag{2}$$

defined in the distributional sense. The potential $1/|x|$ will not be discussed in the current paper, since the function $1/|x|$ does not determine any bounded functional on $C_0^\infty(\mathbb{R})$ and, therefore, cannot be studied in the framework of our approach, as has been already shown in [9].

After paper [9] had been published Professor A Dijksma and B Bodenstorfer drew my attention to the papers by Boyd, Everitt, Gunson and Zettl (see [2, 3, 7]), where a similar differential equation has been studied. The second-order differential operator with the potential $1/x$ has been studied as a perturbation of the second derivative operator. The perturbation $1/x$ is not infinitesimally form-bounded with respect to the operator $-\mathrm{d}^2/\mathrm{d}x^2$ in one dimension. It was shown that the potential $\mathrm{vp}(1/x)$ is form-bounded with the relative bound zero perturbation of the second derivative operator ([7]). Therefore, it is possible to define the operator (2) using the KLMN theorem [16]. The corresponding perturbed operator coincides with the operator H from [9].

Of course, it is possible to consider different point perturbations at the origin of the determined self-adjoint operator [1]. Using von Neumann theory, self-adjoint operators describing penetrable and impenetrable problems can be constructed. The choice of the boundary conditions at the origin has to be determined by the physical problem which has to be described. The question discussed in [9] was of mathematical origin: Which self-adjoint operator H corresponds to the differential operator H^d? This question has been answered in the framework of the theory of distributions. The differential operator H^d is a natural regularization of the operator (1). The functions from the domain of the corresponding self-adjoint operator H possess a remarkable property: the graph of every such function is given by the C^1 curve.

The current paper is organized as follows. In section 2, the second derivative operator on the line is studied in detail. It is shown how to construct point interactions for this operator. In section 3, the operator H corresponding to the formal expression (1) is calculated. It is proven that this operator is self-adjoint. Point interactions for the operator H are studied in section 4. We concentrate our attention on the interactions with support at the singular point.

2. The operator $-\mathrm{d}^2/\mathrm{d}x^2$ and point interactions

To clarify our approach, let us consider first the operator of the second derivative in $L_2(\mathbb{R})$. The differential operator $L^d = -\mathrm{d}^2/\mathrm{d}x^2$ is defined on the whole Hilbert space in the weak sense. However, the range of the linear operator L^d does not belong to the Hilbert space.

In order to consider this operator in the framework of the theory of self-adjoint operators one has to restrict this operator to the following domain:

$$\mathrm{Dom}(L) = \{\psi \in L_2(\mathbb{R}) : L^d\psi \in L_2(\mathbb{R})\}. \tag{3}$$

The operator L^d restricted to this domain will be denoted by L. One can easily show that the domain $\mathrm{Dom}(L)$ coincides with the Sobolev space $W_2^2(\mathbb{R})$. One can also prove that the operator L is self-adjoint on the described domain. Therefore, the operator L is the unique self-adjoint operator corresponding to the second derivative differential operator L^d. The point zero is not a singular point for the differential operator L^d but let us study this point in more detail. The functions from the domain of the operator L and their first derivatives are continuous at the origin as elements from $W_2^2(\mathbb{R})$. The latter statement can be written in the form of boundary conditions at the origin:

$$\psi(-0) = \psi(+0) \qquad \psi'(-0) = \psi'(+0). \tag{4}$$

It is true that 'self-adjointness is the only property of a Hamiltonian required by the axioms of quantum mechanics' ([5]). However, a symmetric differential expression can determine a unique self-adjoint operator as we have already seen. Let us consider point interactions ([1]) of the described self-adjoint operator. The same differential expression $-\mathrm{d}^2/\mathrm{d}x^2$ defines self-adjoint operators L_J and $L_{\boldsymbol{h}}$ on the domains of functions in $W_2^2(\mathbb{R}\backslash\{0\})$ satisfying respectively the following boundary conditions at the origin of one of the types,

$$\begin{aligned} &\begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = J \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix} \qquad J = \mathrm{e}^{\mathrm{i}\varphi} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \\ &\varphi \in [-\pi/2, \pi/2] \qquad a, b, c, d \in \mathbb{R} \qquad ad - bc = 1 \end{aligned} \tag{5}$$

or

$$h_0^+\psi'(+0) = h_1^+\psi(+0) \qquad h_0^-\psi'(+0) = h_1^-\psi(+0) \qquad \boldsymbol{h}^\pm = (h_0^\pm, h_1^\pm) \in \boldsymbol{P}^1 \tag{6}$$

where $\boldsymbol{P}^1$ denotes the projective space (see [10–12]). Each of these operators can be obtained as a self-adjoint extension of the operator L_0 which is equal to the restriction of L to the set of functions satisfying the boundary conditions

$$\psi(0) = 0 \qquad \psi'(0) = 0.$$

However, these operators in general do not coincide with the restriction of the differential operator L^d to the corresponding domain. For any $\psi \in \mathrm{Dom}(L_J)$ and $\varphi \in \mathrm{Dom}(L_{\boldsymbol{h}})$ the differences between the ranges of the operators $L_J\psi - L^d\psi$ and $L_{\boldsymbol{h}}\varphi - L^d\varphi$ are given by certain distributions with support at the origin. Every such distribution is equal to a linear combination of the delta function and its derivatives. The operator L is the unique operator which coincides on its domain $\mathrm{Dom}(L)$ with the differential operator L^d. Therefore, the operator L is the correct self-adjoint operator corresponding to the differential expression $-\mathrm{d}^2/\mathrm{d}x^2$ on the real line. Different self-adjoint operators L_J and $L_{\boldsymbol{h}}$ can be considered as point perturbations of the operator L. It has been shown in [10] that each of these operators corresponds to a certain singular differential operator, which can be obtained as a combination of the following three operators:

- the Schrödinger operator with the generalized potential

$$L_{X_1X_2} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + X_1\delta + X_2\delta^{(1)} \tag{7}$$

- the regularized Schrödinger operator with the singular gauge field

$$L_{X_3} = \left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} + X_3\delta\right)^2 - (X_3\delta)^2 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathrm{i}X_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta - \delta^{(1)}\right) \tag{8}$$

- the Schrödinger operator with the singular density

$$L_{X_4} = -\frac{\mathrm{d}}{\mathrm{d}x}(1 + X_4\delta)\frac{\mathrm{d}}{\mathrm{d}x}. \tag{9}$$

The total family of singular differential operators is described by four real parameters X_1, X_2, X_3, X_4. To obtain the whole family of self-adjoint perturbations of the operator L at the origin it is necessary to consider even infinite values of the parameters ([10]). Similar analysis can be carried out for the operator $\mathrm{d}^n/\mathrm{d}x^n$ in $L_2(\mathbb{R})$ [11].

3. One-dimensional Coulomb Hamiltonian

The differential operator H^d with an internal singularity at the origin has already been discussed in [9]. In the introduction we have defined this operator acting as follows: $L_2(\mathbb{R}) \to D'$. The linear operator acting in the Hilbert space is defined on the domain

$$\mathrm{Dom}(H) = \{\psi \in L_2(\mathbb{R}) : H^d\psi \in L_2(\mathbb{R})\}. \tag{10}$$

The latter definition is similar to the definition of the domain of the operator L given by (3). Following the approach described above, the operator H acting in the Hilbert space is the restriction of the differential operator H^d to the domain $\mathrm{Dom}(H)$. To determine the operator H it is necessary to describe its domain more precisely.

Lemma 1. If $\psi \in \mathrm{Dom}(H)$ then the following inclusion holds,

$$\psi \in W_2^2(\mathbb{R}\backslash[-\epsilon, \epsilon]) \tag{11}$$

for every positive $\epsilon > 0$.

Proof. Let $\psi \in \mathrm{Dom}(H)$ and let φ be an arbitrary test function from $C_0^\infty(\mathbb{R}\backslash\{0\})$. The support of the function φ is separated from the origin. Therefore, the potential $1/x$ is continuous and bounded on the support of φ. It follows that $\psi \in W_2^2(\mathbb{R}\backslash[-\epsilon, \epsilon])$, since the function φ can be chosen arbitrary. The lemma is proven. □

Lemma 1 implies that every function from the domain of the operator H and its first derivative are continuous outside the origin.

Lemma 2. Let $\psi \in L_2(\mathbb{R}_\pm)$ and assume that

$$\psi'' + \frac{\gamma}{x}\psi = g \in L_2(\mathbb{R}_+).$$

Then the limits $\psi(\pm 0)$ exist and the following asymptotic representations hold:

$$\psi(x) = \psi(\pm 0) + O(\sqrt{|x|}) \qquad x \to \pm 0 \tag{12}$$

$$\psi'(x) = -\gamma\psi(\pm 0)\ln|x| + b_\pm + o(1) \qquad x \to \pm 0. \tag{13}$$

Proof. The assumption implies that $\psi = \psi_1 + \psi_2$, where $\psi_1'' = g \in L_2(\mathbb{R}_+)$, $\psi_1(\pm 0) = 0$ and $\psi_2'' = -(\gamma/x)\psi$. It is clear that ψ_1 and ψ_2 are in $C^1(\mathbb{R}_\pm)$ and that $\psi_1'(x)$ has a limit as $x \to \pm 0$. We present here the proof for the positive half-axis $x > 0$ only. The proof for the negative half-axis is similar. To study the asymptotic behaviour of $\psi_2(x)$ we write

$$\psi_2'(x) = \psi_2'(1) + \gamma\int_x^1 \frac{1}{y}\psi(y)\,\mathrm{d}y$$

$$\psi_2(x) = \psi_2(1) - (1-x)\psi_2'(1) - \gamma \int_x^1 \frac{y-x}{y}\psi(y)\,\mathrm{d}y. \tag{14}$$

Since ψ is integrable over (0,1) and $0 < (y-x)/y < 1$, the Lebesque dominated convergence theorem implies that the last term tends to

$$-\gamma \int_0^1 \psi(y)\,\mathrm{d}y$$

as $x \to +0$. Then the $\lim_{x\to+0}\psi_2(x)$ exists. Using the fact that $\psi \in L_2(\mathbb{R}_+)$ we can improve this argument and prove (12) as follows:

$$|\psi_2(x) - \psi_2(+0)| \leqslant x|\psi_2'(1)| + |\gamma| \int_0^x |\psi(y)|\,\mathrm{d}y + x|\gamma| \int_x^1 \frac{1}{y}|\psi(y)|\,\mathrm{d}y.$$

Since ψ is bounded, the last term is less than $Cx|\ln x| \leqslant C_1\sqrt{x}$, and by the Schwarz inequality

$$\int_0^x |\psi(y)|\,\mathrm{d}y \leqslant \left\{ \int_0^x 1\,\mathrm{d}y \int_0^x |\psi(y)|^2\,\mathrm{d}y \right\}^{1/2} \leqslant C\sqrt{x}.$$

This proves (12). Plugging the representation (12) into (14) gives (13). □

The following lemma is similar to theorem 1 from [9].

Lemma 3. If $\psi \in \mathrm{Dom}(H)$ then the boundary values $\psi(\pm)$, $b_\pm(\psi)$ determined by (12) and (13) satisfy the following boundary conditions:

$$\psi(-0) = \psi(+0) \qquad b_-(\psi) = b_+(\psi). \tag{15}$$

Proof. This coincides with the proof of theorem 1 from [9]. □

The graph of each function from the domain $\mathrm{Dom}(H)$ is continuous at the origin. Moreover, the corresponding curve is C^1. If $\psi(0) \neq 0$ then the tangent line to the graph at the origin is vertical.

The three lemmas imply the following theorem.

Theorem 1. The operator H is the self-adjoint operator $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x)$ defined on the domain of functions from $W_2^2(\mathbb{R}\backslash[-\epsilon, \epsilon])$ for every positive $\epsilon > 0$ possessing the representation (12) and (13) and satisfying the boundary conditions (15).

Proof. To finish the proof of the theorem one needs to show that every function from the described domain is mapped by the operator H^d to an element from the Hilbert space. This follows from the proof of theorem 1 from [9]. This operator is self-adjoint, since it is closed, symmetric and has zero deficiency indices. The theorem is proven. □

Thus, we have shown that there exists a unique self-adjoint operator corresponding to the differential operator H^d. The domain of this operator is determined by the boundary conditions connecting the boundary values of the functions on the left- and right-hand sides of the origin. Therefore, it is natural to speak about the penetrability of the potential $1/x$. Different boundary conditions at the origin determine operators which can be considered as self-adjoint point perturbations of the original operator H. Let us illustrate the latter statement by considering singular differential operator with the delta interaction at the origin.

4. Point interactions for Coulomb Hamiltonian

We are going to study in this section the following singular differential operator:

$$H_\alpha = \mathrm{vp}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\gamma}{x}\right) + \alpha\delta(x). \tag{16}$$

The delta function $\delta(x)$ has support at the singular point of the differential operator. Point perturbations with support outside the origin can be considered following the main lines of section 2, since the potential $1/x$ is a bounded function at every point $x, x \neq 0$. The perturbation $\alpha\delta(x)$ is a form-bounded perturbation with the relative bound zero of the operator H. Lemmas 1 and 2 are valid even for the functions from the domain of the operator H_α. In fact the operator H_α is equal to a certain self-adjoint extension of the operator H_0, which is the restriction of the operator H on the set of $C_0^\infty(\mathbb{R}\backslash\{0\})$ functions. The operator H_0 has deficiency indices $(2, 2)$ and its self-adjoint extensions can be described by a certain unitary 2×2 matrix using von Neumann theory.

Theorem 2. The operator H_α is the self-adjoint operator $-(\mathrm{d}^2/\mathrm{d}x^2) - (\gamma/x)$ defined on the domain of functions from $W_2^2(\mathbb{R}\backslash[-\epsilon, \epsilon])$ for every positive $\epsilon > 0$ possessing the representation (12) and (13) and satisfying the boundary conditions

$$\psi(-0) = \psi(+0) = \frac{1}{\alpha}(b_+(\psi) - b_-(\psi)). \tag{17}$$

Proof. The proof of the theorem is similar to the proof of lemma 3 and theorem 1. The distribution $\mathrm{vp}(-(\mathrm{d}^2\psi/\mathrm{d}x^2) - (\gamma/x)\psi)$ is equal to the sum of a delta function and a square integrable function if and only if the function ψ is continuous at the origin $\psi(-0) = \psi(+0)$. The singular part of the latter distribution at the origin is equal to $-\alpha\psi(0)\delta(x)$ if and only if the following condition is satisfied:

$$-b_+(\psi) + b_-(\psi) = -\alpha\psi(0).$$

Hence we have proven that every function from the domain of the operator H_α satisfies the boundary conditions (17).

The self-adjointness of the operator H_α follows from the fact that the boundary conditions (17) describe a self-adjoint extension of the operator H_0 and the operators H_α and H_0^* coincide on this domain. The theorem is proven. □

One can consider the operator H_α even for the infinite value of the parameter α. The operator H_∞ is defined by the Dirichlet boundary conditions at the origin

$$\psi(+0) = \psi(-0) = 0.$$

This operator can be decomposed into the orthogonal sum of two self-adjoint operators defined on the positive and negative half-axes. The physical problem described by this self-adjoint operator has an impenetrable singularity at the origin. However, the nature of the impenetrability is not related to the singularity of the potential $1/x$ at the origin. It is due to the special boundary conditions. Fischer, Leschke and Müller are right in saying that 'penetrable' and 'impenetrable' quantum systems can be described by choosing different boundary conditions at the origin. Certain physical problems can force us to use 'impenetrable' boundary conditions, but the boundary conditions corresponding to the differential operator H^d has been determined in a unique way.

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