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On the Coulomb potential in one dimension

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Abstract. A mathematically rigorous definition of the one-dimensional Schrödinger operator $-\mathrm{d}^2/\mathrm{d}x^2 - \gamma/x$ is given. It is proven that the domain of the operator is defined by the boundary conditions connecting the values of the function on the left and right half-axes. The investigated operator is compared with the Schrödinger operator containing the Coulomb potential $-\gamma/|x|$.

1. Introduction

The one-dimensional Schrödinger operator with a Coulomb potential has been discussed in the literature. This operator attracts the attention of mathematicians because it contains the simplest potential with a non-integrable singularity. This potential which depends on the absolute value of the coordinate $-\gamma/|x|$ is important in physical applications and is one of the natural generalizations of the Coulomb potential for the one-dimensional case [3]. See [2] for an excellent review on the present status of the problem. Recently another class of Schrödinger operators with potentials having a first-order singularity was analysed by Moshinsky [4]. These operators have potentials with a different sign of the singularity on the left- and right-hand sides of the singular point. The simplest representative of this family is the potential $-\gamma/x$ with the singularity at the origin. Such operators appear in the problems of nuclear physics (see [4] for references). The Schrödinger operator

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

can be defined in the principal value sense on the entire line. Boundary conditions connecting the boundary values of the function from the domain of the operator on the left- and right-hand sides of the origin were given in [4] but no motivation (physical or mathematical) has been given. Strong scientific discussion shows that there is a certain misunderstanding around this point [5, 6]. A mathematically rigorous definition of the self-adjoint Schrödinger operator with this potential can be given using the distribution theory. It is shown that this operator is 'penetrable' in contrast to the even Coulomb Hamiltonian.

A similar analysis can be applied to the Schrödinger operator with the Coulomb potential

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

It is shown that the corresponding operator is symmetric but not self-adjoint (see the appendix). The Friedrichs extension of the symmetric operator leads to the operator defined on the functions satisfying the Dirichlet boundary conditions at the origin. One can speak about the 'non-penetrability' of the one-dimensional Coulomb potential.

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2. Potential with an odd singularity

Consider the Schrödinger operator with the odd potential (1). This operator can be defined in the principal value sense as proposed in [4]. The corresponding operator H is defined by the generalized differential expression (1) on the domain

$$\mathrm{Dom}(H) = \left\{ \psi \in L_2(\mathbb{R}) : \mathrm{PV}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi - \frac{\gamma}{x}\psi \right) \in L_2(\mathbb{R}) \right\}. \tag{3}$$

This domain is contained in the domain of the operator H_0^*, where H_0 is the restriction of the operator H on the set of $C_0^\infty(\mathbb{R}\backslash\{0\})$ functions.

Each function from the domain of the adjoint operator H_0^* has the following asymptotics at the origin [2, 4]:

$$\psi(x) = \psi(\pm 0) + o(1) \qquad x \to \pm 0 \tag{4}$$

$$\psi'(x) = -\gamma\psi(x)\ln(|\gamma x|) + b_\pm(\psi) + o(1) \qquad x \to \pm 0. \tag{5}$$

Each function from the domain of the adjoint operator is bounded in the neighbourhood of the origin. The derivative has a logarithmic singularity at the origin if the function is not equal to zero there. The following lemma will be important later.

Lemma 1. Let $\psi \in \mathrm{Dom}(H_0^*)$, $\psi(\pm 0) = 0$, then $\psi(x) = \mathrm{O}(x)$, $\psi'(x) = \mathrm{O}(1)$ when $x \to \pm 0$.

Proof. We are going to prove this lemma for positive values of x. The negative case can be treated similarly. For any positive a there exists $\epsilon > 0$ such that $x \in (0, \epsilon) \Rightarrow |\psi(x)| < a$. Then the following estimates are valid for all $x \in (0, \epsilon)$

$$|\psi'(x)| \leqslant |\gamma a \ln(|\gamma x|)| + \mathrm{O}(1).$$

It follows that

$$|\psi(x)| \leqslant \left| \gamma a \int_0^x \ln(|\gamma x|)\,\mathrm{d}x \right| + \mathrm{O}(x) = \mathrm{O}(x\ln|x|).$$

The last estimate can be substituted into the representation for the derivative

$$|\psi'(x)| \leqslant \mathrm{O}(x\ln^2|x|) + \mathrm{O}(1) = \mathrm{O}(1).$$

It follows that

$$\psi(x) =_{x\to+0} \mathrm{O}(x). \qquad \square$$

Deficiency indices of the symmetric operator H_0 are equal to $(2, 2)$. All self-adjoint extensions of the operator H_0 can be constructed with the help of the von Neumann theory. All these extensions are parametrized by the boundary conditions at the origin.

Theorem 1. Operator H is the self-adjoint operator $-\mathrm{d}^2/\mathrm{d}x^2 - \gamma/x$ defined on the domain of functions from $\mathrm{Dom}(H_0^*)$, satisfying the following boundary conditions at the origin:

$$\begin{cases} \psi(-0) = \psi(+0) \\ b_-(\psi) = b_+(\psi). \end{cases} \tag{6}$$

Proof. Calculation of the expression $\text{PV}(-(\mathrm{d}^2/\mathrm{d}x^2)\psi - (\gamma/x\psi))$ in the principal value sense gives the following result for any test function $\varphi \in C_0^\infty(\mathbb{R})$

$$
\begin{aligned}
\text{PV}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi - \frac{\gamma}{x}\psi\right)(\varphi) &= \text{PV}\int_{-\infty}^{+\infty}\left(-\psi\varphi'' - \frac{\gamma}{x}\psi\varphi\right)\mathrm{d}x \\
&= \lim_{\epsilon\to+0}\left\{\int_{-\infty}^{-\epsilon}\left(-\psi\varphi'' - \frac{\gamma}{x}\psi\varphi\right)\mathrm{d}x + \int_{\epsilon}^{+\infty}\left(-\psi\varphi'' - \frac{\gamma}{x}\psi\varphi\right)\mathrm{d}x\right\} \\
&= \lim_{\epsilon\to+0}\left(\int_{-\infty}^{-\epsilon}\left(-\psi''\varphi - \frac{\gamma}{x}\psi\varphi\right)\mathrm{d}x + \int_{\epsilon}^{+\infty}\left(-\psi''\varphi - \frac{\gamma}{x}\psi\varphi\right)\mathrm{d}x\right. \\
&\quad \left. +[\psi(\epsilon)\varphi'(\epsilon) - \psi(-\epsilon)\varphi'(-\epsilon)] + \{-\psi'(\epsilon)\varphi(\epsilon) + \psi'(-\epsilon)\varphi(-\epsilon)\}\right).
\end{aligned}
$$

The integrals in the last expression converge to a finite limit when $\epsilon \to +0$ because ψ is from the domain of the adjoint operator H_0^*. The expression in the square brackets has a limit due to the asymptotics (4) and continuity of the function φ at the origin. The expression in the curly brackets converges to a finite limit only if the functions $\psi(x)$ are continuous at the origin: $\psi(+0) = \psi(-0)$. Applying lemma 1 to the function $\psi(x) - \psi(-x)$ vanishing at the origin we obtain the following limit:

$$
\begin{aligned}
\lim_{\epsilon\to+0}(\psi'(\epsilon) - \psi'(-\epsilon)) &= \lim_{\epsilon\to+0}(2\gamma(-\psi(\epsilon) + \psi(-\epsilon))\ln(|\gamma\epsilon|) + b_+(\psi) - b_-(\psi) \\
&= b_+(\psi) - b_-(\psi).
\end{aligned}
$$

Thus the distribution $\text{PV}(-(\mathrm{d}^2/\mathrm{d}x^2)\psi - (\gamma/x)\psi)$ has the following singularity at the origin

$$
(b_+(\psi) - b_-(\psi))\delta.
$$

It follows that $\text{PV}(-(\mathrm{d}^2/dx^2)\psi - (\gamma/x)\psi)$ is contained in $L_2(\mathbb{R})$ if and only if conditions (6) are satisfied. These conditions together with the differential expression (1) define a self-adjoint operator. This is a unique self-adjoint operator corresponding to the odd Coulomb potential. The theorem is proven. □

This operator was investigated in [4] without discussing the definition. The scattering matrix and eigenvalues were calculated.

3. Conclusions

We have shown that Schrödinger operators with the potentials $-\gamma/x$ and $-\gamma/|x|$ possess different properties. The operator with the even potential cannot be defined correctly in the framework of the theory of self-adjoint operators (see the appendix)—the corresponding operator is only symmetric, but not self-adjoint. The self-adjoint operator can be defined by the Friedrichs extension, but it can be presented by the orthogonal sum of the operators defined on the positive and negative half-axes. One can speak about the 'non-penetrability' of the even Coulomb potential. In contrast, the Schrödinger operator with the odd potential is perfectly defined in the framework of the theory of self-adjoint operators. The boundary conditions corresponding to this operator glue together the values of the functions on the positive and negative half-lines. The one-dimensional potential $-\gamma/x$ is 'penetrable'. Using the extension theory for symmetric operators other 'penetrable' and 'non-penetrable' Schrödinger operators with these potentials can be constructed but all these self-adjoint perturbations should be considered to be Hamiltonians with point interactions [1]. This family of self-adjoint perturbations for the even potential was analysed in [2]. A similar analysis can be carried out for the odd potential.

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Appendix. Potential with an even singularity

The Schrödinger operator H^c with the Coulomb potential is defined by the differential expression (2) on the domain:

$$\mathrm{Dom}(H^c) = \left\{ \psi \in L_2(\mathbb{R}) : -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi - \frac{\gamma}{|x|}\psi \in L_2(\mathbb{R}) \right\}. \tag{7}$$

Let us consider the symmetric operator H_0^c and restriction of the operator H^c on the set of functions $C_0^\infty(\mathbb{R}\backslash\{0\})$. Then the operator H^c coincides with one of the restrictions of the adjoint operator H_0^{c*}. The symmetric operator H_0^c has deficiency indices $(2, 2)$. Self-adjoint extensions of this operator have been studied recently in [2]. It was shown that every function ψ from the domain of the adjoint operator H_0^{c*} has the following representation in the neighbourhood of the origin:

$$\psi(x) = \psi(\pm 0) + o(1) \qquad x \to \pm 0 \tag{8}$$

$$\psi'(x) = \mp\gamma\psi(x)\ln(|\gamma x|) + b_\pm(\psi) + o(1) \qquad x \to \pm 0. \tag{9}$$

Theorem A1. Operator $H^c = -\mathrm{d}^2/\mathrm{d}x^2 - \gamma/|x|$ is a symmetric, but not self-adjoint operator in the Hilbert space $L_2(\mathbb{R})$.

Proof. Calculations similar to those used during the proof of theorem 1 can be carried out:

$$\begin{aligned}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi - \frac{\gamma}{|x|}\psi\right)(\varphi) &= \int_{-\infty}^{+\infty}\left(-\psi\varphi'' - \frac{\gamma}{|x|}\psi\varphi\right)\mathrm{d}x \\ &= \lim_{\epsilon_+,\epsilon_-\to+0}\left(\int_{-\infty}^{-\epsilon_-}\left(-\psi\varphi'' - \frac{\gamma}{|x|}\psi\varphi\right)\mathrm{d}x + \int_{\epsilon_+}^{+\infty}\left(-\psi\varphi'' - \frac{\gamma}{|x|}\psi\varphi\right)\mathrm{d}x\right) \\ &= \lim_{\epsilon_+,\epsilon_-\to+0}\left(\int_{-\infty}^{-\epsilon_-}\left(-\psi''\varphi - \frac{\gamma}{|x|}\psi\varphi\right)\mathrm{d}x + \int_{\epsilon_+}^{+\infty}\left(-\psi''\varphi - \frac{\gamma}{|x|}\psi\varphi\right)\mathrm{d}x\right. \\ &\quad \left. +[\psi(\epsilon_+)\varphi'(\epsilon_+) - \psi(-\epsilon_-)\varphi'(-\epsilon_-)] + \{-\psi'(\epsilon_+)\varphi(\epsilon_+) + \psi'(-\epsilon_-)\varphi(-\epsilon_-)\}\right).\end{aligned} \tag{10}$$

The expression in the curly brackets has a finite limit if and only if the derivatives of ψ has finite limits on both sides of the origin. It follows that functions ψ from the domain $\mathrm{Dom}(H^c)$ satisfy the Dirichlet conditions at the origin:

$$\psi(-0) = \psi(+0) = 0. \tag{11}$$

It follows from lemma 1 that the derivative of ψ has finite limits from the right- and left-hand sides of the origin. For every $\psi \in \mathrm{Dom}(H_0^{c*})$, $\psi(0) = 0$ the distribution $-(\mathrm{d}^2/\mathrm{d}x^2)\psi - (\gamma/|x|)\psi$ belongs to $L_2(\mathbb{R})$ if and only if the derivative of ψ is continuous at the origin

$$\psi'(-0) = \psi'(+0). \tag{12}$$

Boundary conditions (11), (12) define a symmetric, but non-self-adjoint restriction of the operator H_0^{c*}. Each function from the domain of the adjoint operator H_0^{c*} is an element of the Sobolev space $W_2^2(\mathbb{R}\backslash[-\epsilon, \epsilon])$ for any positive ϵ. Thus integrating by parts one can prove that operator H^c is symmetric on the domain, defined by the boundary conditions (11), (12). The theorem is proven. □

We would like to make two comments. One can try to define the considered operator in the principal value sense, but such calculations do not define a self-adjoint operator such as used for the operator with an odd potential. The limit (10) is finite only if $\psi(-0) = -\psi(0)$, but distribution $-(\mathrm{d}^2/\mathrm{d}x^2)\psi - (\gamma/|x|)\psi$ is from $L_2(\mathbb{R})$ only if the function and its derivative are continuous at the origin. These conditions coincide with the conditions (11), (12) and the corresponding operator is not self-adjoint.

It is natural to define a self-adjoint operator, corresponding to the linear operator (2), by the Friedrichs extension of the symmetric operator H^c. This self-adjoint extension is defined by the Dirichlet boundary conditions at the origin. This operator has been studied rigorously in [3]. The same operator was obtained in [2] with the help of the functional-integral approach.

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