

Self-adjoint extensions of Coulomb systems in 1,2 and 3 dimensions

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Abstract

We study the nonrelativistic quantum Coulomb hamiltonian (i.e., inverse of distance potential) in \mathbb{R}^n , $n = 1, 2, 3$. We characterize their self-adjoint extensions and, in the unidimensional case, present a discussion of controversies in the literature, particularly the question of the permeability of the origin. Potentials given by fundamental solutions of Laplace equation are also briefly considered.

1 Introduction

In principle the unidimensional (1D) hydrogen atom is a simplification of the three-dimensional (3D) model which has been invoked in theoretical and numerical studies [1, 2, 3]; note that Cole and Cohen [4] and Wong et al. [5] have reported some experimental evidence for the 1D hydrogen atom. In a particular situation the 1D eigenvalues coincide with the well-known eigenvalues of the 3D hydrogen model, as discussed ahead.

Apparently the 1D hydrogen atom was first considered in 1928 by Vrkljan [6]. However, it was a work of Loudon [7] published in 1959, whose potential model is

$$V_C(x) = -\frac{\kappa}{|x|}, \quad \kappa > 0,$$

that increased attention to the subject which has become interesting and quite controversial. We refer to V_C as *the Coulomb potential*.

Loudon stated that the 1D hydrogen atom was twofold degenerate, having even and odd eigenfunctions for each eigenvalue, except for the (even) ground state having infinite binding energy. Typically 1D systems have no degenerate eigenvalues, and Loudon justified the double degeneracy as a consequence of the singular atomic potential. Andrews [8] questioned the existence of a ground state with infinite binding energy. Ten years later Haines and Roberts [9] revised Loudon's work and obtained that their even wave

functions, with continuous eigenvalues, were complementary to odd functions, but such results were criticized by Andrews [10], who did not accept the continuous eigenvalues. Gomes and Zimerman [11] argued that the even states with finite energy should be excluded. Spector and Lee [12] presented a relativistic treatment that removed the problem of infinite binding energy of the ground state. Several other works [13, 14, 15, 16, 17, 18, 19, 20, 21] (see also references therein) have discussed this apparently simple problem.

In this work we advocate that the roots of such controversies is a lack of sufficient mathematical care in some papers: in 1D the Coulomb singularity is so severe that it is not a trivial problem to assign boundary conditions at the origin. The main question is how to properly define the self-adjoint realization(s) of

$$\dot{H} = -\frac{\hbar^2}{2m}\Delta + V_C(x), \quad \text{dom } \dot{H} = C_0^\infty(\mathbb{R} \setminus \{0\}).$$

The domain choice is because functions ψ in $C_0^\infty(\mathbb{R} \setminus \{0\})$ are kept far enough from the origin (i.e., zero does not belong to their support), and so $\dot{H}\psi$ is well defined. \dot{H} is hermitian but not self-adjoint, and it turns out that it has deficiency index $n_+ = 2 = n_-$ and so an infinite family of self-adjoint extensions (see Section 4). Although such extensions appear in [18], details of how they were obtained are missing; in Section 4 we find such extensions by another approach, that is, we use a (modified) boundary form as discussed in [22]. These extensions are the candidates for the energy operator of the 1D hydrogen atom.

With these extensions at hand, we discuss the question of permeability of the origin, that is, whether in 1D the Coulomb singularity acts as barrier that allows the electron to pass through it or not. This is one of the important questions considered in the literature. It is found that the permeability depends on the self-adjoint extension and we present explicit examples of both behaviors.

In Sections 2 and 3 we present the self-adjoint extensions of \dot{H} in 3 and 2 dimensions, respectively. It is well-known that in 3D the operator H , with the same action as \dot{H} but domain $C_0^\infty(\mathbb{R}^3)$, is essentially self-adjoint, that is, it has just one self-adjoint extension, whose domain is the Sobolev space $\mathcal{H}^2(\mathbb{R}^3)$ (this is known as Kato-Rellich Theorem; see ahead). However, if the origin is removed and the initial domain $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$ is considered, then also in 3D there are infinitely many self-adjoint extensions. Note that in both 1D and 2D the origin must be removed in order to get well-defined initial operators \dot{H} .

It is sometimes assumed that the right potential describing the coulombian interaction is given by the fundamental solutions of Laplace equation, that is,

$$V_1(x) = \kappa|x|, \quad V_2(x) = \kappa \ln |x|, \quad V_3(x) = -\frac{\kappa}{|x|},$$

in 1D, 2D and 3D, respectively. For example, in the statistical mechanics of the Coulomb gas in 2D the potential V_2 is often considered, instead of V_3 , and the so-called Kosterlitz-Thouless transition is obtained. So in Section 5 we consider the Schrödinger operator with such potentials and argue that they are always essentially self-adjoint (in suitable domains), independently of dimension. Finally, the conclusions are reported in Section 6.

A notational detail: the dot in \dot{H} means that the origin has been removed from the domain of the initial hermitian operator; e.g., in 1D $\text{dom } \dot{H}$ is $C_0^\infty(\mathbb{R} \setminus \{0\})$ and so on.

2 Self-adjoint extensions: 3D

The initial hermitian operator modelling the nonrelativistic quantum 3D hydrogen atom is (write $r = |x|, \theta, \varphi$ for the spherical coordinates)

$$H = -\frac{\hbar^2}{2m}\Delta + V_C(x), \quad \text{dom } H = C_0^\infty(\mathbb{R}^3) \subset L^2(\mathbb{R}^3),$$

which is well defined since for $\psi \in \text{dom } H$

$$\|V_C\psi\|^2 = \kappa^2 \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2} dx = \kappa^2 \int_0^\infty dr \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi |\psi(r, \theta, \varphi)|^2 < \infty.$$

The Kato-Rellich Theorem [23, 24] applies to this case, since $V_C \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, and H has just one self-adjoint extension whose domain is the Sobolev space $\mathcal{H}^2(\mathbb{R}^3)$. Thus, the Schrödinger operator is well established in this case, so the quantum dynamics, and this is the standard operator discussed in textbooks on quantum mechanics (usually with less mathematical details).

It is worth mentioning that in \mathbb{R}^n , $n \geq 4$, Kato-Rellich Theorem implies unique self-adjointness for potentials $V \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ with $p > n/2$; so in dimensions $n \geq 4$ the Schrödinger operators H with potential V_C and domain $C_0^\infty(\mathbb{R}^n)$ are always essentially self-adjoint.

However, in 1D and 2D the condition $\|V_C\psi\|^2 < \infty$ for all $\psi \in C_0^\infty(\mathbb{R}^3)$ requires $\psi(0) = 0$ for x in a neighbourhood of the origin, that is, $\psi \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$, $n = 1, 2$. The self-adjoint extensions in such cases will be discussed in other sections; for question of comparison with other dimensions, now we consider what happens if the origin is removed also in \mathbb{R}^3 , that is, if the initial hermitian operator is

$$\dot{H} = -\frac{\hbar^2}{2m}\Delta + V_C(x), \quad \text{dom } \dot{H} = C_0^\infty(\mathbb{R}^3 \setminus \{0\}).$$

Write $\xi = (\theta, \varphi)$ for the angular variables in the unit sphere S^2 and $d\xi = \sin \theta d\theta d\varphi$. Let \mathcal{D} denote the set of linear combinations of products

$f(r)w(\xi)$ with $f \in C_0^\infty(0, \infty) \subset L^2((0, \infty), r^2 dr)$ and $w \in L^2(S^2, d\xi)$. Due to the decomposition in spherical coordinates

$$L^2(\mathbb{R}^3) = L^2((0, \infty), r^2 dr) \otimes L^2(S^2, d\xi),$$

\mathcal{D} is a dense set in $L^2(\mathbb{R}^3)$. For functions $\phi(r, \xi) = f(r)w(\xi) \in \mathcal{D}$ the operator \dot{H} takes the form

$$\dot{H}f(r)w(\xi) = \left[-\frac{\hbar^2}{2m} \left(\partial_r^2 + \frac{2}{r} \partial_r \right) f(r) - \frac{\kappa}{r} f(r) \right] w(\xi) + \frac{\hbar^2}{2m} \frac{f(r)}{r^2} \mathcal{B}w(\xi),$$

where \mathcal{B} is the Laplace-Beltrami operator [25]

$$(\mathcal{B}w)(\xi) = -\frac{1}{\sin \theta} \left[\partial_\theta (\sin \theta \partial_\theta w) + \frac{1}{\sin \theta} \partial_\varphi^2 w \right]$$

acting in $L(S^2, d\xi)$. \mathcal{B} with domain $C_0^\infty(S^2)$ is essentially self-adjoint and its eigenfunctions are the spherical harmonics $Y_{l,m}(\xi)$, which constitute an orthonormal basis of $L(S^2, d\xi)$; recall that

$$(\mathcal{B}Y_{l,m})(\xi) = l(l+1)Y_{l,m}(\xi), \quad l \in \mathbb{N}, \quad -l \leq m \leq l.$$

Denote by \mathcal{J}_l the subspace spanned by $\{Y_{l,m} : -l \leq m \leq l\}$, that is, the subspace corresponding to the eigenvalue $l(l+1)$ and $L_l := L^2((0, \infty), r^2 dr) \otimes \mathcal{J}_l$; thus

$$L^2(\mathbb{R}^3) = L^2((0, \infty), r^2 dr) \otimes L^2(S^2, d\xi) = \bigoplus_{l=0}^{\infty} L_l.$$

If I_l is the identity operator on \mathcal{J}_l , the restriction of \dot{H} to $\mathcal{D}_l = \mathcal{D} \cap L_l$ is given by $\dot{H}|_{\mathcal{D}_l} = \dot{H}_l \otimes I_l$, with

$$\dot{H}_l = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right) - \frac{\kappa}{r},$$

and our task is reduced to finding the self-adjoint extensions of \dot{H}_l with domain $C_0^\infty(0, \infty)$. It is convenient to introduce the unitary transformation $U : L^2((0, \infty), r^2 dr) \rightarrow L^2(0, \infty)$, $(U\phi)(r) = r\phi(r)$, which maps $C_0^\infty(0, \infty)$ to itself and

$$h_l := U\dot{H}_l U^{-1} = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) - \frac{\kappa}{r},$$

with domain $\text{dom } H_l = C_0^\infty(0, \infty)$. Standard arguments gives that the adjoint h_l^* has the same action as h_l but with domain

$$\text{dom } h_l^* = \{ \phi \in L^2(0, \infty) : \phi, \phi' \in \text{AC}(0, \infty), h_l^* \phi \in L^2(0, \infty) \}.$$

If Ω is an open subset of \mathbb{R} , $\text{AC}(\Omega)$ indicates the set of absolutely continuous functions in every bounded and closed subinterval of Ω .

By adapting the analysis of the free hamiltonian in \mathbb{R}^3 with the origin removed, which was performed in [26], one proves the following result:

Theorem 1. h_0 has deficiency indices equal to 1, while h_l , $l \neq 0$, is essentially self-adjoint.

Hence, for $l \neq 0$ the unique self-adjoint extension of h_l is h_l^* , while h_0 has infinitely many self-adjoint extensions. In order to find such extensions in case $l = 0$, we will make use of the following lemma [27, 28, 29], whose proof we adapt and reproduce.

Lemma 1. If $\phi \in \text{dom } h_0^*$, then the lateral limits $\phi(0^+) := \lim_{r \rightarrow 0^+} \phi(r)$ and

$$\tilde{\phi}(0^+) := \lim_{r \rightarrow 0^+} \left(\phi'(r) + \frac{2m\kappa}{\hbar^2} \phi(r) \ln(\kappa r) \right)$$

exist (and are finite).

Proof. For $\phi \in \text{dom } h_0^*$ one has

$$-h_0^* \phi = \frac{\hbar^2}{2m} \frac{d^2 \phi}{dr^2} + \frac{\kappa}{r} \phi := u \in L^2(0, \infty),$$

and one can write $\phi = \phi_1 + \phi_2$ with $\frac{\hbar^2}{2m} \phi_1'' = u$, $\phi_1(0^+) = 0$ and $\frac{\hbar^2}{2m} \phi_2'' + \kappa/r \phi = 0$. Since $\phi_j \in \mathcal{H}^2(\varepsilon, \infty)$, $j = 1, 2$, for all $\varepsilon > 0$, and $u \in L^2$, it follows that these functions are of class $C^1(0, \infty)$.

Consider an interval $[r, c]$, $0 < r < c < \infty$. Since

$$\phi_1'(r) - \phi_1'(c) = \frac{2m}{\hbar^2} \int_r^c u(s) ds,$$

$\phi_1'(r)$ has a lateral limit

$$\phi_1'(0^+) = \phi_1'(c) + \frac{2m}{\hbar^2} \int_0^c u(s) ds.$$

On integrating successively twice over the interval $[r, c]$ one gets

$$\phi_2'(c) - \phi_2'(r) = -\frac{2m\kappa}{\hbar^2} \int_r^c \frac{\phi(s)}{s} ds,$$

and then

$$\begin{aligned} \phi_2(r) &= \phi_2(c) - (c-r)\phi_2'(c) - \frac{2m\kappa}{\hbar^2} \int_r^c dv \int_v^c ds \frac{\phi(s)}{s} \\ &= \phi_2(c) - (c-r)\phi_2'(c) - \frac{2m\kappa}{\hbar^2} \int_r^c ds \phi(s) \frac{s-r}{s}, \end{aligned}$$

and since $0 \leq (s-r)/s < 1$, by dominated convergence the last integral converges to $\int_0^1 \phi(s)$ as $r \rightarrow 0^+$. Therefore $\phi_2(0^+)$ exists and

$$\phi_2(0^+) = \phi_2(c) - c\phi_2'(c) - \frac{2m\kappa}{\hbar^2} \int_0^c \phi(s) ds.$$

Now,

$$|\phi_2(r) - \phi_2(0^+)| \leq r|\phi_2'(c)| + \frac{2m\kappa}{\hbar^2} \int_0^r |\phi(s)| ds + \frac{2m\kappa}{\hbar^2} r \int_r^c ds \frac{|\phi(s)|}{s}.$$

Taking into account that ϕ is bounded, say $|\phi(r)| \leq C, \forall r$, Cauchy-Schwarz in L^2 implies

$$\int_0^r |\phi(s)| ds = \int_0^r 1 |\phi(s)| ds \leq C\sqrt{r},$$

and so, for r small enough and fixing $c = 1$,

$$\int_r^c ds \frac{\phi(s)}{s} \leq C(c|\ln c| + r|\ln r|) \leq \tilde{C}\sqrt{r},$$

for some constant \tilde{C} . Such inequalities imply $\phi(r) = \phi(0^+) + O(\sqrt{r})$, and on substituting this into

$$\phi'(r) = \phi'(1) + \frac{2m\kappa}{\hbar^2} \int_r^1 \frac{\phi(s)}{s} ds$$

(recall that $\phi_1'(0^+)$ is finite) it is found that there is b so that, as $r \rightarrow 0^+$,

$$\phi'(r) = \phi'(1) - \frac{2m\kappa}{\hbar^2} \phi(0^+) \ln(\kappa r) + b + o(1);$$

thus, the derivative ϕ' has a logarithmic divergence as $r \rightarrow 0$ and the statement in the lemma also follows. \square

For $\phi, \psi \in \text{dom } h_0^*$ integration by parts gives

$$\langle h_0^* \psi, \phi \rangle - \langle \psi, h_0^* \phi \rangle = \Gamma(\psi, \phi),$$

where

$$\Gamma(\psi, \phi) := -\frac{\hbar^2}{2m} \lim_{r \rightarrow 0^+} \left(\psi(r) \overline{\phi'(r)} - \psi'(r) \overline{\phi(r)} \right)$$

is called a *boundary form* for h_0 [22]. Note that although $\Gamma(\psi, \phi)$ is finite, the lateral limit $\phi'(0^+)$ can diverge; however, by Lemma 1 it is readily verified that

$$\Gamma(\psi, \phi) = -\frac{\hbar^2}{2m} \left(\psi(0^+) \overline{\tilde{\phi}(0^+)} - \tilde{\psi}(0^+) \overline{\phi(0)} \right)$$

and now all lateral limits are finite. The self-adjoint extensions of h_0 are restrictions of h_0^* to suitable subspaces D so that $\text{dom } h_0 \subset D \subset \text{dom } h_0^*$ and $\Gamma|_D = 0$, that is, $\Gamma(\psi, \phi) = 0$ for all $\phi, \psi \in D$.

We introduce the unidimensional vector spaces $X = \{\rho_1(\psi) := \psi(0^+) + i\tilde{\psi}(0^+) : \psi \in \text{dom } h_0^*\}$ and $Y = \{\rho_2(\psi) := \psi(0^+) - i\tilde{\psi}(0^+) : \psi \in \text{dom } h_0^*\}$ and note that

$$\frac{4mi}{\hbar^2} \Gamma(\psi, \phi) = \langle \rho_1(\psi), \rho_1(\phi) \rangle_X - \langle \rho_2(\psi), \rho_2(\phi) \rangle_Y,$$

with inner products in X, Y , as indicated. Hence, the subspaces D for which Γ vanishes are related to maps that preserve inner products, that is, unitary maps from X to Y (see details in [22]), and since these vector spaces are unidimensional such maps are multiplication by the complex numbers $e^{i\theta}$, $0 \leq \theta < 2\pi$. Therefore, for each θ a self-adjoint extension of h_0 is characterized by the functions $\psi \in \text{dom } h_0^*$ so that $\rho_2(\psi) = e^{i\theta} \rho_1(\psi)$, that is,

$$(1 - e^{i\theta})\psi(0^+) = i(1 + e^{i\theta})\tilde{\psi}(0^+).$$

If $\theta \neq 0$ this condition reduces to

$$\psi(0^+) = \lambda \tilde{\psi}(0^+), \quad \lambda = i \frac{1 + e^{i\theta}}{1 - e^{i\theta}} \in \mathbb{R},$$

and writing $\lambda = \infty$ in case $\theta = 0$, the desired self-adjoint extensions h_0^λ are described by

$$\text{dom } h_0^\lambda = \left\{ \psi \in \text{dom } h_0^* : \psi(0^+) = \lambda \tilde{\psi}(0^+) \right\}, \quad \lambda \in \mathbb{R} \cup \{\infty\},$$

and $h_0^\lambda \psi = h_0^* \psi$. The Dirichlet boundary condition corresponds to $\lambda = 0$. With such results at hand, we have

Theorem 2. *The self-adjoint extensions of \dot{H} in 3D are*

$$H^\lambda = \left(U^{-1} h_0^\lambda U \otimes I_0 \right) \bigoplus_{l=1}^{\infty} \left(U^{-1} h_l^* U \otimes I_l \right), \quad \lambda \in \mathbb{R} \cup \{\infty\}.$$

This should be compared with the case without removing the origin, for which there is just one self-adjoint extension. The eigenvalue equation for the Dirichlet case $\lambda = 0$ can be exactly solved in terms of Whittaker functions, and the negative eigenvalues are

$$E_n^0 = -\frac{\kappa^2 m}{2\hbar^2} \frac{1}{n^2}, \quad n = 1, 2, 3, \dots,$$

each one with multiplicity n^2 . For $\lambda \neq 0$ the manipulations become more involved and numerical procedures must be employed to find roots of implicit functions, and so the eigenvalues.

3 Self-adjoint extensions: 2D

Although our main interest is in the 1D and 3D cases, we say something about the Coulomb system in 2D. As already mentioned, the origin must be excluded from the domain of the Coulomb potential in 2D and the initial hermitian operator is

$$\dot{H} = -\frac{\hbar^2}{2m} \Delta + V_C(x), \quad \text{dom } \dot{H} = C_0^\infty(\mathbb{R}^2 \setminus \{0\}).$$

To find its self-adjoint extensions, introduce polar coordinates (r, φ) so that

$$L^2(\mathbb{R}^2) = L^2((0, \infty), r dr) \otimes L^2(S^1, d\varphi),$$

(S^1 is the usual unit circle in \mathbb{R}^2) and the set \mathcal{D} of linear combinations of the products $f(r)g(\varphi)$, $f \in C_0^\infty(0, \infty)$ and $g \in C_0^\infty(S^1)$, is dense in $L^2(\mathbb{R}^2)$. Now

$$\dot{H}f(r)g(\varphi) = \left[-\frac{\hbar^2}{2m} \left(\partial_r^2 + \frac{1}{r} \partial_r \right) f(r) - \frac{\kappa}{r} f(r) \right] g(\varphi) - \frac{\hbar^2}{2m} \frac{f(r)}{r^2} \mathcal{B}g(\varphi),$$

where $\mathcal{B} = \partial_\varphi^2$ is the Laplace-Beltrami operator acting in $L^2(S^1, d\varphi)$. This operator with domain $C_0^\infty(S^1)$ is essentially self-adjoint, its eigenvectors $g_l(\varphi) = e^{il\varphi}/\sqrt{2\pi}$ constitute an orthonormal basis of $L^2(S^1, d\varphi)$ and

$$(\mathcal{B}g_l)(\varphi) = -l^2 g_l(\varphi), \quad l \in \mathbb{Z}.$$

Let $[g_l]$ denote the subspace spanned by g_l and $L_l = L^2((0, \infty), r dr) \otimes [g_l]$; thus

$$L^2(\mathbb{R}^2) = \bigoplus_{l \in \mathbb{Z}} L_l,$$

and if I_l is the identity operator on $[g_l]$, the restriction of \dot{H} to $\mathcal{D}_l = \mathcal{D} \cap L_l$ is given by $\dot{H}|_{\mathcal{D}_l} = \dot{H}_l \otimes I_l$, with

$$\dot{H}_l = -\frac{\hbar^2}{2m} \left(\partial_r^2 + \frac{1}{r} \partial_r - \frac{l^2}{r^2} \right) - \frac{\kappa}{r},$$

with domain $C_0^\infty(0, \infty)$, and the question is to find the self-adjoint extensions of such restrictions. By using the unitary operator $U : L^2((0, \infty), r dr) \rightarrow L^2(0, \infty)$, $(U\phi)(r) = r^{1/2}\phi(r)$, one has

$$h_l := U\dot{H}_l U^{-1} = -\frac{\hbar^2}{2m} \left(\partial_r^2 + \left(\frac{1}{4} - l^2 \right) \frac{1}{r^2} \right) - \frac{\kappa}{r}$$

with $\text{dom } h_l = C_0^\infty(0, \infty)$ (since this set is invariant under U). By standard results it follows that the adjoint h_l^* has the same action as h_l but with domain

$$\text{dom } h_l^* = \left\{ \phi \in L^2(0, \infty) : \phi, \phi' \in \text{AC}(0, \infty), h_l^* \phi \in L^2(0, \infty) \right\}.$$

Theorem 3. *The operators h_l are essentially self-adjoint if, and only if, $l \neq 0$, whereas h_0 has deficiency indices equal to one.*

Proof. Weyl's limit point-limit circle criterion will be used [23]. Thus we consider the solutions of $h_l^* \phi = i\phi$, that is,

$$-\frac{\hbar^2}{2m} \phi'' - \left[\frac{\hbar^2}{2m} \left(\frac{1}{4} - l^2 \right) \frac{1}{r^2} + \frac{\kappa}{r} + i \right] \phi = 0, \quad \phi \in \text{dom } h_l^*.$$

By writing $p = \frac{2m\kappa}{\hbar^2}$, $q = \frac{2mi}{\hbar^2}$ and performing the change of variable $y = (-4q)^{1/2}r$, one gets

$$\phi'' + \left[\left(\frac{1}{4} - l^2 \right) \frac{1}{y^2} + \frac{\tau}{y} - \frac{1}{4} \right] \phi = 0,$$

with $\tau = p/(-4q)^{1/2}$. This equation has two linearly independent solutions given by the Whittaker functions [30, 31]

$$\phi_1(y) = \mathcal{M}_{\tau,|l|}(y) \quad \text{e} \quad \phi_2(y) = \mathcal{W}_{\tau,|l|}(y),$$

whose asymptotic behaviors as $|y| \rightarrow \infty$ are

$$\phi_1(y) \sim e^{y/2}(-y)^{-\tau} \quad \text{e} \quad \phi_2(y) \sim e^{-y/2}y^\tau.$$

Since there is no $c \in \mathbb{R}$ so that $\phi_2 \in L^2(c, \infty)$, it follows that h_l is limit point at ∞ . Note that the above asymptotic behaviors as $|y| \rightarrow \infty$ do not depend on l ; however, at the origin we need to separate the cases $l = 0$ and $l \neq 0$.

For $l = 0$ [30, 31],

$$\phi_1(0^+) = 0 \quad \text{and} \quad \phi_2(0^+) = 0.$$

In this case there is $c > 0$ so that $\phi_1, \phi_2 \in L^2(0, c)$ and h_0 is limit circle at 0. Therefore, h_0 is not essentially self-adjoint but has deficiency indices equal to 1.

For $l \neq 0$, $\phi_1(0^+) = 0$ while $\phi_2(y)$ diverges as

$$\sum_{k=0}^{2|l|-1} \frac{\Gamma(2|l| - k)}{k!} \Gamma(k - |l| - \tau + 1/2) (-y)^{-2|l|+k},$$

for $y \rightarrow 0^+$ (here Γ denotes the well-known Gamma function). Therefore, h_l ($l \neq 0$) is limit point at 0. By Weyl criterion, h_l is essentially self-adjoint if $l \neq 0$. \square

Since h_l , $l \neq 0$, is essentially self-adjoint, its unique self-adjoint extension is exactly h_l^* . According to the proof of Theorem 3, the deficiency subspace $K_-(h_0)$ is spanned by $\phi_-(r) = \mathcal{M}_{\tau,0}((-4q)^{1/2}r)$ and the deficiency subspace $K_+(h_0)$ spanned by $\phi_+(r) = \overline{\phi_-(r)}$. The von Neumann theory of self-adjoint extensions [32, 24] characterizes them by unitary maps from, say, K_- to K_+ , and since such subspaces are unidimensional these unitary maps are just multiplication by $e^{i\theta}$, $0 \leq \theta < 2\pi$. Thus there is a self-adjoint extension h_0^θ of h_0 , for each θ , and if $\overline{h_0}$ denotes the closure of h_0 , it is given by

$$\text{dom } h_0^\theta = \left\{ \psi + c \left(\phi_+ - e^{i\theta} \phi_- \right) : \psi \in \text{dom } \overline{h_0}, c \in \mathbb{C} \right\},$$

$$h_0^\theta \psi = h_0^* \psi, \quad \psi \in \text{dom } h_0^\theta.$$

In summary:

Theorem 4. *The self-adjoint extensions of \dot{H} in 2D are*

$$H^\theta = \left(U^{-1} h_0^\theta U \otimes I_0 \right) \bigoplus_{l \in \mathbb{Z}, l \neq 0}^{\infty} (U^{-1} h_l^* U \otimes I_l), \quad \theta \in [0, 2\pi).$$

4 Hydrogen atom: 1D

In the unidimensional case the initial hermitian operator is

$$\dot{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{\kappa}{|x|}, \quad \text{dom } \dot{H} = C_0^\infty(\mathbb{R} \setminus \{0\}),$$

and the origin naturally decomposes the space

$$L^2(\mathbb{R} \setminus \{0\}) = L^2(-\infty, 0) \oplus L^2(0, \infty),$$

and also the domain of \dot{H} into $C_0^\infty(-\infty, 0)$ and $C_0^\infty(0, \infty)$; let \dot{H}_+ and \dot{H}_- denote the restriction of \dot{H} to these subspaces, respectively. Thus, we have

$$\dot{H} = \dot{H}_- \oplus \dot{H}_+.$$

From the physical point of view, an important question is about the behavior of the system at the origin, e.g., is it impermeable, so that the system actually decomposes into a right one and a left one, or is it permeable? In the latter possibility, what do happen with wavefunctions at the transition point (the origin)? As discussed ahead, there are plenty of possibilities, due to infinitely many self-adjoint extensions.

4.1 Self-adjoint extensions

The adjoint operator \dot{H}_+^* has the same action as \dot{H} but with domain

$$\text{dom } \dot{H}_+^* = \{ \phi \in L^2(0, \infty) : \phi, \phi' \in \text{AC}(0, \infty), H_+^* \phi \in L^2(0, \infty) \},$$

and an analogous expression for \dot{H}_-^* and its domain.

To find the deficiency subspace $K_+(\dot{H}_+)$ we look for solutions of

$$-\frac{\hbar^2}{2m} \phi'' + \left(-\frac{\kappa}{x} + i \right) \phi = 0$$

that belong to $\text{dom } \dot{H}_+^*$. Write $p = \frac{2m\kappa}{\hbar^2}$, $q = -\frac{2mi}{\hbar^2}$ and perform the change of variable $y = (-4q)^{1/2}x$, so that this equation takes the form

$$\phi''(y) + \left(\frac{\tau}{y} - \frac{1}{4} \right) \phi(y) = 0,$$

with $\tau = p/(-4q)^{1/2}$, which has exactly two linearly independent solutions [30, 31]

$$\phi_{1+}(y) = \mathcal{W}_{\tau,1/2}(y), \quad \phi_{2+}(y) = \mathcal{M}_{\tau,1/2}(y).$$

These solutions have finite limites as $y \rightarrow 0$. The asymptotic behaviors for $|y| \rightarrow \infty$ are

$$\phi_{1+}(y) \sim y^\tau e^{-y/2} \quad \text{and} \quad \phi_{2+}(y) \sim (-y)^{-\tau} e^{y/2}.$$

Hence, in the original variable the deficiency subspace $K_+(\dot{H}_+)$ is unidimensional and spanned by $\phi_{1+}(x) = \mathcal{W}_{\tau,1/2}((-4q)^{1/2}x)$. A similar analysis implies that $K_-(\dot{H}_+)$ is also unidimensional and spanned by $\overline{\phi_{1+}(x)}$. Therefore \dot{H}_+ has both deficiency indices equal to 1.

Similarly one finds that the deficiency subspaces $K_+(\dot{H}_-)$ and $K_-(\dot{H}_-)$ of \dot{H}_- are spanned, respectively, by $\phi_{1-}(x) = \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|)$ and $\overline{\phi_{1-}(x)}$. Therefore \dot{H}_- also has both deficiency indices equal to 1.

Now, due to the above results, the adjoint operator \dot{H}^* has the same action as \dot{H} but domain (write $\mathcal{H} = L^2(\mathbb{R} \setminus \{0\})$)

$$\text{dom } H^* = \left\{ \phi \in \mathcal{H} : \phi, \phi' \in \text{AC}(\mathbb{R} \setminus \{0\}), -\frac{\hbar^2}{2m} \phi'' - \frac{\kappa}{|x|} \phi \in \mathcal{H} \right\},$$

and both deficiency subspaces $K_\pm(\dot{H})$ have dimension 2; $K_+(\dot{H})$ is spanned by

$$\psi_1(x) = \begin{cases} \phi_{1+}(x) & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases} \quad \text{and} \quad \psi_2(x) = \begin{cases} 0 & \text{if } x > 0 \\ \phi_{1-}(x) & \text{if } x < 0 \end{cases},$$

and $K_-(\dot{H})$ by $\overline{\psi_1}$ and $\overline{\psi_2}$.

Therefore, \dot{H} has both deficiency indices equal to 2 and it has infinitely many self-adjoint extensions. A boundary form will be used in order to get such extensions. The following lemma will be needed, whose proof is similar to the proof of Lemma 1 (note the difference of signs in the definitions of $\tilde{\phi}(0^+)$ and $\tilde{\phi}(0^-)$ below).

Lemma 2. *If $\phi \in \text{dom } \dot{H}^*$, then the lateral limits $\phi(0^\pm) := \lim_{x \rightarrow 0^\pm} \phi(x)$ and*

$$\tilde{\phi}(0^\pm) := \lim_{x \rightarrow 0^\pm} \left(\phi'(x) \pm \frac{2m\kappa}{\hbar^2} \phi(x) \ln(\pm \kappa x) \right)$$

exist and are finite.

For $\psi, \phi \in \text{dom } \dot{H}^*$ one has, upon integrating by parts,

$$\langle \dot{H}^* \psi, \phi \rangle - \langle \psi, \dot{H}^* \phi \rangle = \Gamma(\psi, \phi),$$

where

$$-\frac{2m}{\hbar^2} \Gamma(\psi, \phi) = \left[\lim_{x \rightarrow 0^+} \left(\psi(x) \overline{\phi'(x)} - \psi'(x) \overline{\phi(x)} \right) + \lim_{x \rightarrow 0^-} \left(-\psi(x) \overline{\phi'(x)} + \psi'(x) \overline{\phi(x)} \right) \right]$$

and, using Lemma 2, straightforward computation gives

$$\Gamma(\psi, \phi) = \frac{-\hbar^2}{2m} \left(\psi(0^+) \overline{\tilde{\phi}(0^+)} - \tilde{\psi}(0^+) \overline{\phi(0^+)} - \psi(0^-) \overline{\tilde{\phi}(0^-)} + \tilde{\psi}(0^-) \overline{\phi(0^-)} \right),$$

and now each lateral limit is finite.

Introduce two linear maps $\rho_1, \rho_2 : \text{dom } \dot{H}^* \rightarrow \mathbb{C}^2$:

$$\rho_1(\psi) = \begin{pmatrix} \tilde{\psi}(0^+) + i\psi(0^+) \\ \tilde{\psi}(0^-) - i\psi(0^-) \end{pmatrix} \quad \text{and} \quad \rho_2(\psi) = \begin{pmatrix} \tilde{\psi}(0^+) - i\psi(0^+) \\ \tilde{\psi}(0^-) + i\psi(0^-) \end{pmatrix},$$

so that

$$\langle \rho_1(\psi), \rho_1(\phi) \rangle_{\mathbb{C}^2} - \langle \rho_2(\psi), \rho_2(\phi) \rangle_{\mathbb{C}^2} = -\frac{4m}{\hbar^2} i \Gamma(\psi, \phi), \quad \forall \psi, \phi \in \text{dom } \dot{H}^*.$$

As in Section 2, the self-adjoint extensions of \dot{H} are restrictions of \dot{H}^* to suitable subspaces D so that $\text{dom } \dot{H} \subset D \subset \text{dom } \dot{H}^*$ and $\Gamma|_D = 0$, that is, $\Gamma(\psi, \phi) = 0$ for all $\phi, \psi \in D$ [22].

Vanishing of Γ on domains D is equivalent to the preservation of the inner products in \mathbb{C}^2 , and so it corresponds to unitary 2×2 matrices \hat{U} , and each of such matrices characterizes a self-adjoint extension $\dot{H}_{\hat{U}}$ of \dot{H} , so that $\text{dom } \dot{H}_{\hat{U}}$ is composed of $\psi \in \text{dom } \dot{H}^*$ so that $\rho_2(\psi) = \hat{U} \rho_1(\psi)$; also $\dot{H}_{\hat{U}} \psi = \dot{H}^* \psi$ for $\psi \in \text{dom } \dot{H}_{\hat{U}}$.

The condition $\rho_2(\psi) = \hat{U} \rho_1(\psi)$ is then written

$$(I - \hat{U}) \begin{pmatrix} \tilde{\psi}(0^+) \\ \tilde{\psi}(0^-) \end{pmatrix} = -i(I + \hat{U}) \begin{pmatrix} -\psi(0^+) \\ \psi(0^-) \end{pmatrix},$$

and we have explicitly got the boundary conditions characterizing the desired self-adjoint extensions.

In case $(I - \hat{U})$ is invertible (similarly if $(I + \hat{U})$ is invertible) it is possible to write the above boundary conditions in the form

$$\begin{pmatrix} \tilde{\psi}(0^+) \\ \tilde{\psi}(0^-) \end{pmatrix} = A \begin{pmatrix} -\psi(0^+) \\ \psi(0^-) \end{pmatrix},$$

with $A = -i(I - \hat{U})^{-1}(I + \hat{U})$ being a 2×2 self-adjoint matrix.

In [18] the authors have got this form for the self-adjoint extensions, and it was claimed that by allowing the entries of A taking infinity all self-adjoint extensions are found; we think it is a hard task to cover all possibilities above (i.e., via \hat{U}) with this representation via self-adjoint matrices A .

Particular choices of the matrix \hat{U} (I is the identity matrix)

$$\text{a) } I, \quad \text{b) } -I, \quad \text{c) } \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{d) } \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix},$$

impose, respectively, the boundary conditions: a) $\psi(0^-) = 0 = \psi(0^+)$ (Dirichlet); b) $\tilde{\psi}(0^-) = 0 = \tilde{\psi}(0^+)$ (“Neumann”); c) $\psi(0^-) = \psi(0^+)$ and $\tilde{\psi}(0^-) = \tilde{\psi}(0^+)$ (periodic); d) $\psi(0^-) = -\psi(0^+)$ and $\tilde{\psi}(0^-) = -\tilde{\psi}(0^+)$ (antiperiodic).

Recall that the general form of a 2×2 unitary matrix is

$$\hat{U} = e^{i\theta} \begin{pmatrix} a & -\bar{b} \\ b & \bar{a} \end{pmatrix}, \quad \theta \in [0, 2\pi), \quad a, b \in \mathbb{C}, |a|^2 + |b|^2 = 1.$$

This form will be used ahead.

4.2 Negative eigenvalues

In this subsection we discuss the negative eigenvalues of some self-adjoint extensions $\hat{H}_{\hat{U}}$. The main goal is to remark that the eigenvalues, their multiplicities and parity of eigenfunctions depend on the boundary conditions. This becomes important since in the past some authors have assumed particular hypotheses on the eigenfunctions (see references in the Introduction), but without specifying the self-adjoint extension they were working with; this was the main source of controversies in the studies of the unidimensional hydrogen atom.

Our first analysis is for $\hat{U} = I$, i.e., Dirichlet boundary condition, and denote by H_D the operator

$$H_D = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{\kappa}{|x|}, \quad \text{dom } H_D = \{\phi \in \text{dom } \hat{H}^* : \phi(0^+) = 0 = \phi(0^-)\}.$$

As in [18] we consider the Green function of $(H_D - E)^{-1}$, denoted by $G(x, y)$, that is

$$(H_D - E)^{-1}u(x) = \Theta(x) \int_0^x G(x, y)u(y)dy + \Theta(-x) \int_x^0 G(x, y)u(y)dy.$$

Here $\Theta(x) = 1$ if $x > 0$ and vanishes if $x < 0$.

If $u \in \text{rng}(H_D - E)$, we search for solutions ϕ of

$$(H_D - E)\phi = u, \tag{1}$$

and the discussion is for $(-\infty, 0)$ and $(0, \infty)$ separately.

For $x \in (0, \infty)$, by the method of variation of parameters, one finds the solution

$$\phi(x) = \phi_1(x) \int_0^x -\frac{\phi_2(y)u(y)}{W_x(\phi_1, \phi_2)}dy + \phi_2(x) \int_0^x \frac{\phi_1(y)u(y)}{W_x(\phi_1, \phi_2)}dy,$$

where ϕ_1 and ϕ_2 are independent solutions of the homogeneous equation $(H_D - E)\phi = 0$, that is,

$$-\frac{h^2}{2m}\phi'' - \left(\frac{\kappa}{x} + E\right)\phi = 0, \quad (2)$$

and $W_x(\phi_1, \phi_2)$ the corresponding Wronskian.

Writing $p = \frac{2m\kappa}{h^2}$, $q = \frac{2mE}{h^2}$, $\tau = p/(-4q)^{1/2}$ and $z = (-4q)^{1/2}x$, the last equation takes the form

$$\phi'' + \left(\frac{\tau}{z} - \frac{1}{4}\right)\phi = 0,$$

whose independent solutions are

$$\phi_1(z) = \mathcal{W}_{\tau,1/2}(z) \quad \text{and} \quad \phi_2(z) = \mathcal{M}_{\tau,1/2}(z).$$

Recall that $\mathcal{W}_{\tau,1/2}(z) \sim e^{-z/2}z^\tau$ and $\mathcal{M}_{\tau,1/2}(z) \sim e^{z/2}(-z)^{-\tau}$, as $z \rightarrow \infty$. In the original variable

$$W_x(\phi_1, \phi_2) = -\frac{(-4q)^{1/2}}{\Gamma(1-\tau)},$$

and the unique solution satisfying $\phi(0^+) = 0$ is

$$\begin{aligned} \phi(x) = \int_0^x \frac{\Gamma(1-\tau)}{(-4q)^{1/2}} & \left(\mathcal{W}_{\tau,1/2}((-4q)^{1/2}x) \mathcal{M}_{\tau,1/2}((-4q)^{1/2}y) - \right. \\ & \left. \mathcal{M}_{\tau,1/2}((-4q)^{1/2}x) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}y) \right) u(y) dy. \end{aligned}$$

Similarly, for $x \in (-\infty, 0)$, the unique solution satisfying $\phi(0^-) = 0$ is

$$\begin{aligned} \phi(x) = \int_x^0 \frac{\Gamma(1-\tau)}{(-4q)^{1/2}} & \left(\mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|) \mathcal{M}_{\tau,1/2}((-4q)^{1/2}|y|) - \right. \\ & \left. \mathcal{M}_{\tau,1/2}((-4q)^{1/2}|x|) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|y|) \right) u(y) dy. \end{aligned}$$

Summing up, the Green function of the resolvent operator $(H_D - E)^{-1}$ is given by

$$\begin{aligned} G(x, y) = \Theta(xy) \frac{\Gamma(1-\tau)}{(-4q)^{1/2}} \\ \times \left[\Theta(|x| - |y|) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|) \mathcal{M}_{\tau,1/2}((-4q)^{1/2}|y|) - (x \leftrightarrow y) \right]. \end{aligned}$$

The values E for which $(H_D - E)^{-1}$ does not exist constitute the eigenvalues of H_D , and they are obtained from the points for which the Gamma

function $\Gamma(1 - \tau)$ is not defined, that is, $1 - \tau$ is a negative integer number. By recalling the expressions of p , q and τ , the condition $1 - \tau = -n$, $n = 0, 1, 2, 3, \dots$, gives

$$E_n = -\frac{\kappa^2 m}{2\hbar^2} \frac{1}{n^2} \quad n = 1, 2, 3, \dots,$$

which coincide with the eigenvalues of the usual 3D hydrogen atom model.

These eigenvalues are twofold degenerated and a basis $\{\phi_{n,1}, \phi_{n,2}\}$ of the subsequent eigenspace is

$$\phi_{n,k}(x) = \Theta((-1)^k x) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|), \quad k = 1, 2.$$

The negative eigenvalues of other extensions $\hat{H}_{\hat{U}}$ are harder to get and numerical computation should be employed. In the following particular cases of interest are selected. Let $\Psi(x) := \frac{d}{dx}(\ln \Gamma(x))$ and define

$$\omega(E) := \frac{2m\kappa}{\hbar^2} \left[\ln \left(\frac{\hbar^2}{2m} \tau \right) + 2\Psi(1) - \Psi(1 - \tau) - 1 \right] - \frac{(-2Em)^{1/2}}{\hbar}$$

with $[\Gamma(1 - \tau)]^{-1}$ and $\pm\omega(E)[\Gamma(1 - \tau)]^{-1}$ denoting, respectively, the values of the lateral limits $\lim_{x \rightarrow 0^\pm} \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|)$ and

$$\lim_{x \rightarrow 0^\pm} \left(\frac{d}{dx} \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|) \pm \frac{2m\kappa}{\hbar^2} \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|) \ln(\pm\kappa x) \right).$$

Given a unitary matrix \hat{U} , the candidates for eigenfunctions of $\hat{H}_{\hat{U}}$ must satisfy the corresponding boundary conditions.

Example 1. Let's take $\theta = \frac{\pi}{2}$, $a = 1$ and $b = 0$ so that

$$\hat{U} = i \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and the values of E for which $\omega(E) = -1$ are the eigenvalues of $\hat{H}_{\hat{U}}$ and with multiplicity two; the corresponding eigenspace is spanned by

$$\phi_k(x) = \Theta((-1)^k x) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|), \quad k = 1, 2.$$

Example 2. Consider another case: $\theta = \frac{\pi}{2}$, $a = i$ and $b = 0$ so that

$$\hat{U} = i \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

and the values of E for which $\omega(E) = 0$ are found to be nondegenerate eigenvalues of $\hat{H}_{\hat{U}}$, and for each eigenvalue the corresponding eigenspace is spanned by

$$\phi(x) = \Theta(x) \mathcal{W}_{\tau,1/2}((-4q)^{1/2}|x|).$$

These two cases illustrate that the behavior of eigenfunctions are not related only to the parity of the potential $V_C(x)$, since there are cases for which the eigenfunctions do not have a definite parity and cases with eigenvalues simple as well as with multiplicity two. These different possibilities are directly related to the singularity of the potential and depend on the selected self-adjoint extension.

4.3 Permeability of the origin

Another question that has been discussed in the literature is about the permeability of the origin in the unidimensional hydrogen atom; see, for instance [8, 7, 27, 28, 29, 33, 34]. Some authors consider the origin an impermeable barrier, while others assume it is permeable. Again the answer strongly depends on the self-adjoint extension considered (see also [33]), as illustrated ahead. Here the definition of permeability is through the probability current density; for simplicity we assume $\hbar = 1$ and $m = 1$.

Recall that the probability current density $j(x)$ in 1D is given by

$$j(x) = \frac{i}{2} \left(\phi(x)\overline{\phi'(x)} - \phi'(x)\overline{\phi(x)} \right), \quad \phi \in \text{dom } \dot{H}_{\hat{U}},$$

and it satisfies the continuity equation

$$\frac{\partial}{\partial t} |\phi(t, x)|^2 + \frac{\partial}{\partial x} j(t, x) = 0.$$

Our previous results in Subsection 4.1 show that $\lim_{x \rightarrow 0^\pm} j(x)$ do exist (see ahead).

For each $\phi \in \text{dom } \dot{H}_{\hat{U}}$, on integrating by parts we get

$$0 = \langle \dot{H}_{\hat{U}} \phi, \phi \rangle - \langle \phi, \dot{H}_{\hat{U}} \phi \rangle = i \lim_{\varepsilon \rightarrow 0} [j(\varepsilon) - j(-\varepsilon)].$$

Hence, the function $j(x)$ can be continuously defined at the origin $j(0)$ via lateral limits. Physically this relation means that the current density is isotropic at the origin, in spite of the strong singularity there. A simple observation shows that

$$j(x) = \text{Im} (\phi'(x)\overline{\phi(x)}), \quad \phi \in \text{dom } \dot{H}_{\hat{U}},$$

where Im indicates imaginary part, so that

$$j(0) = \lim_{x \rightarrow 0^+} \text{Im} (\phi'(x)\overline{\phi(x)}) = \lim_{x \rightarrow 0^-} \text{Im} (\phi'(x)\overline{\phi(x)}).$$

Since $\phi'(0^+)$ and $\phi'(0^-)$ can be divergent, we use using Lemma 2 to obtain

$$j(0) = \lim_{x \rightarrow 0^+} \text{Im} (\tilde{\phi}(x)\overline{\phi(x)}) = \lim_{x \rightarrow 0^-} \text{Im} (\tilde{\phi}(x)\overline{\phi(x)}).$$

Note that it is exactly this relation that guaranties that $j(0)$ is well defined and finite.

We are now in position of giving a rigorous definition of permeability: If $j(0) = 0, \forall \phi \in \text{dom } \dot{H}_{\hat{U}}$, the electron is completely reflected when approaching the origin, and so we say the origin is not permeable (or is impermeable), so that the regions $x < 0$ and $x > 0$ are kept separated by the singularity. If $j(0) \neq 0$ we say the origin is permeable.

Next we study the current density related to $\dot{H}_{\hat{U}}$ in three cases.

Case 1. $(I - \hat{U})$ is invertible. Since $A = -i(I - \hat{U})^{-1}(I + \hat{U})$ is a self-adjoint matrix, the boundary conditions of $\dot{H}_{\hat{U}}$ become

$$\begin{pmatrix} \tilde{\phi}(0^+) \\ \tilde{\phi}(0^-) \end{pmatrix} = \begin{pmatrix} u & z \\ \bar{z} & v \end{pmatrix} \begin{pmatrix} -\phi(0^+) \\ \phi(0^-) \end{pmatrix}, \quad u, v \in \mathbb{R}, z \in \mathbb{C},$$

and u, z and v are functions of the entries of \hat{U} . The boundary conditions become

$$\lim_{x \rightarrow 0^+} \tilde{\phi}(x) = -u \lim_{x \rightarrow 0^+} \phi(x) + z \lim_{x \rightarrow 0^-} \phi(x) \quad (3)$$

$$\lim_{x \rightarrow 0^-} \tilde{\phi}(x) = -\bar{z} \lim_{x \rightarrow 0^+} \phi(x) + v \lim_{x \rightarrow 0^-} \phi(x) \quad (4)$$

Multiply the first equation (before taking limits) by $\overline{\phi(x)}$ to get

$$\lim_{x \rightarrow 0^+} \tilde{\phi}(x) \overline{\phi(x)} = -u \lim_{x \rightarrow 0^+} |\phi(x)|^2 + z \lim_{x \rightarrow 0^+} \phi(-x) \overline{\phi(x)},$$

and so

$$j(0) = \lim_{x \rightarrow 0^+} \text{Im}(\tilde{\phi}(x) \overline{\phi(x)}) = \lim_{x \rightarrow 0^+} \text{Im}(z \phi(-x) \overline{\phi(x)}).$$

Therefore, if $z = 0$ then $j(0) = 0, \forall \phi \in \text{dom } \dot{H}_{\hat{U}}$, and we have found a family of self-adjoint extensions for which the origin is not permeable. Example 1 above corresponds to the self-adjoint matrix

$$-i(I - \hat{U})^{-1}(I + \hat{U}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and the origin is not permeable in this case.

Case 2. $(I + \hat{U})$ is invertible. The matrix $A = i(I + \hat{U})^{-1}(I - \hat{U})$ is also self-adjoint and the boundary conditions of $\dot{H}_{\hat{U}}$ take the form

$$\begin{pmatrix} u & z \\ \bar{z} & v \end{pmatrix} \begin{pmatrix} \tilde{\phi}(0^+) \\ \tilde{\phi}(0^-) \end{pmatrix} = \begin{pmatrix} -\phi(0^+) \\ \phi(0^-) \end{pmatrix}, \quad u, v \in \mathbb{R}, z \in \mathbb{C},$$

and u, z and v are functions of the entries of \hat{U} . Table 1 shows the current density at the origin for various values of u, z and v .

Table 1: Current density for invertible $(I + \hat{U})$.

$u, z, v \neq 0$	$j(0) = \text{Im} \left(-\frac{z}{u} \lim_{x \rightarrow 0^-} \tilde{\phi}(x) \overline{\phi(-x)} \right)$
$z = 0$	$j(0) = 0$
$z \neq 0$ and $u = 0$	$j(0) = \text{Im} \left(-\frac{1}{z} \lim_{x \rightarrow 0^+} \phi(x) \overline{\phi(-x)} \right)$
$z \neq 0$ and $v = 0$	$j(0) = \text{Im} \left(\frac{1}{z} \lim_{x \rightarrow 0^-} \phi(x) \overline{\phi(-x)} \right)$

Note that Dirichlet boundary condition (so $\hat{U} = I$) is a particular case with $z = 0$ (the matrix $A = 0$), and since this case can not be an extension of another self-adjoint extension of \dot{H} , we conclude that the current density vanishes for all $\phi \in \text{dom } \dot{H}_{\hat{U}}$ if, and only if, $z = 0$. In other words, if $(I + \hat{U})$ is invertible, the origin is impermeable precisely if $z = 0$. As expected, Dirichlet boundary condition implies the origin is impermeable.

Case 3. Both $(I + \hat{U})$ and $(I - \hat{U})$ are not invertible. This case amounts to

$$\det(I + \hat{U}) = 0 = \det(I - \hat{U}),$$

which turns out to be equivalent to the following matrix representation

$$\hat{U} = \begin{pmatrix} -u & v \\ \bar{v} & u \end{pmatrix}, \quad u \in \mathbb{R}, v \in \mathbb{C}, \quad |u|^2 + |v|^2 = 1.$$

The current density always vanishes at the origin if, and only if, $v = 0$, that is, the matrix \hat{U} equals

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

If $v \neq 0$, we have

$$j(0) = \text{Im} \left(\frac{v}{1+u} \lim_{x \rightarrow 0^-} \tilde{\phi}(x) \overline{\phi(-x)} - \frac{iv}{(1+u)} \lim_{x \rightarrow 0^-} \phi(x) \overline{\phi(-x)} + i \frac{1-u}{1+u} \lim_{x \rightarrow 0^+} |\phi(x)|^2 \right).$$

Example 3. Consider the self-adjoint extension $\dot{H}_{\hat{U}}$ which corresponds to the unitary matrix

$$\hat{U} = i \begin{pmatrix} \sqrt{2}/2 & -\sqrt{2}/2 \\ \sqrt{2}/2 & \sqrt{2}/2 \end{pmatrix}.$$

The domain of $\dot{H}_{\hat{U}}$ constitutes of the $\psi \in \text{dom } \dot{H}^*$ so that

$$\begin{pmatrix} \tilde{\psi}(0^+) \\ \tilde{\psi}(0^-) \end{pmatrix} = \begin{pmatrix} \sqrt{2} & -i \\ i & \sqrt{2} \end{pmatrix} \begin{pmatrix} -\psi(0^+) \\ \psi(0^-) \end{pmatrix},$$

and such conditions imply

$$j(0) = \lim_{x \rightarrow 0^+} \operatorname{Im}(-i\psi(-x)\overline{\psi(x)}).$$

The values of E for which $\omega(E) = -\sqrt{2}$ are eigenvalues of $\dot{H}_{\hat{U}}$ of multiplicity two, and the corresponding eigenfunctions are

$$\phi_k(x) = \Theta((-1)^k x) \mathcal{W}_{\tau, 1/2}((-4q)^{1/2}|x|), \quad k = 1, 2.$$

By taking the linear combination $\psi(x) = \phi_1(x) + \phi_2(x)$, and the asymptotic behavior of such eigenfunctions near zero, discussed in Subsection 4.2, we obtain

$$j(0) = -\Gamma(1 - \tau)^{-2} \neq 0,$$

that is, if the electron is in this eigenstate it is transmitted through the origin.

We conclude that there are extensions for which the origin is permeable and for others it is impermeable. Andrews [8] defines $j(x) = i[\overline{F'(x)}F(x) - \overline{F(x)}F'(x)]$ but computes $j(0)$ only for eigenfunctions; it is clear that j vanishes if the eigenvalue is nondegenerate, since the corresponding eigenfunction can be taken real. Andrews mentioned the possibility of zero current in case of degenerated eigenvalues. In our Example 1 the eigenvalues have multiplicity two and the current density is zero, whereas for the operator in Example 3 the eigenvalues have multiplicity two and the origin is permeable; therefore both possibilities are allowed in case of multiple eigenvalues.

We note that the analysis of Moshinsky [29], although interesting, considers the ‘‘eigenfunctions’’ $\mathcal{W}_\lambda(-z)$ and $\mathcal{W}_\lambda(z)$ that do not belong to $L^2(\mathbb{R} \setminus \{0\})$.

5 Potentials Via Laplace Equation

This brief section deals with Schrödinger operators with potentials V along the fundamental solutions of Laplace equation

$$\Delta V = 0.$$

As mentioned in the Introduction, in physics sometimes one assumes that in each dimension the potential describing the Coulomb interaction is the fundamental solutions of Laplace equation [35, 36]; recall that these solutions are (take $\kappa > 0$)

$$V_1(x) = \kappa|x|, \quad V_2(x) = \kappa \ln|x|, \quad V_3(x) = -\frac{\kappa}{|x|},$$

in 1D, 2D and 3D, respectively.

The case of V_3 in 3D is standard and was recalled in Section 2; we underline that the operator

$$H = -\frac{\hbar^2}{2m}\Delta + V_3(x), \quad \text{dom } H = C_0^\infty(\mathbb{R}^3),$$

is essentially self-adjoint and its unique self-adjoint extension has the same action but domain $\mathcal{H}^2(\mathbb{R}^3)$; this extension has nonempty discrete and essential spectra.

The case of potential V_2 was analyzed by Gesztesy and Pittner [37] and they state the following result:

Theorem 5. *The operator*

$$H = -\frac{\hbar^2}{2m}\Delta + \kappa \ln |x|, \quad \text{dom } H = C_0^\infty(\mathbb{R}^2),$$

is essentially self-adjoint, and its unique self-adjoint extension has empty essential spectrum.

Now we consider the unidimensional Schrödinger operator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \kappa|x|, \quad \text{dom } H = C_0^\infty(\mathbb{R}),$$

whose adjoint H^* has the same action as H but domain

$$\text{dom } H^* = \{\phi \in L^2(\mathbb{R}) : \phi, \phi' \in AC(\mathbb{R}), H^*\phi \in L^2(\mathbb{R})\}.$$

Since V_1 is a bounded from below and continuous potential, with

$$\lim_{|x| \rightarrow \infty} V_1(x) = \infty,$$

the following theorem follows from general results [23, 24].

Theorem 6. *The above unidimensional operator H is essentially self-adjoint, its unique self-adjoint extension H^* is bounded from below and has empty essential spectrum.*

By solving the eigenvalue equation

$$-\frac{\hbar^2}{2m}\phi'' + (\kappa|x| - E)\phi = 0$$

in terms of Airy functions we have found the eigenvalues E_n are simple and with asymptotic behavior

$$E_n \sim \frac{\hbar^2}{2m} \left[\frac{m\kappa}{\hbar^2} \frac{3\pi}{4} (4n - 3) \right]^{2/3}, \quad n \rightarrow \infty.$$

Hence, for Schrödinger operators H with potentials along the fundamental solutions of the Laplace equation, we have:

1. H is essentially self-adjoint in $C_0^\infty(\mathbb{R}^3)$ and its self-adjoint extension has both nonempty discrete and essential spectra.
2. H is essentially self-adjoint in $C_0^\infty(\mathbb{R}^n)$ and its self-adjoint extension has purely discrete spectrum for $n = 1, 2$.

However, for Schrödinger operators whose potential is the Coulomb one, i.e., $V_C(x)$, we have:

1. The deficiency indices are equal to 0 in $C_0^\infty(\mathbb{R}^3)$.
2. The deficiency indices are equal to 1, 1 and 2 in $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$, $C_0^\infty(\mathbb{R}^2 \setminus \{0\})$ and $C_0^\infty(\mathbb{R} \setminus \{0\})$, respectively.

6 Conclusions

Although the 3D usual model hamiltonian H with Coulomb potential V_C , $\text{dom } H = C_0^\infty(\mathbb{R}^3)$, is essentially self-adjoint, in \mathbb{R}^n the $1/|x|$ singularity imposes the initial domain must be $C_0^\infty(\mathbb{R}^n \setminus \{0\})$, $n = 1, 2$, and the corresponding operators \dot{H} have deficiency indices equal to 2 and 1, respectively; hence with infinitely many self-adjoint extensions. For the sake of comparison, we have also considered the origin removed in \mathbb{R}^3 , that is, \dot{H} with domain $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$: the deficiency indices are equal to 1 in this case. In each case, all self-adjoint extensions have been found.

In 1D the question of permeability of the origin was analyzed and the answer depends strongly on the self-adjoint extension considered. Due to particular examples discussed, we conclude that the multiplicity two of the eigenvalues does not determine the permeability.

We have paid particular attention to the 1D case, since there are many papers in the literature about this model and occasionally with conflicting conclusions. We have found that these conflicting positions have been originated from boundary conditions imposed mainly on “physical basis” that can fail for strong singularities, as is the case of V_C in one-dimension. We expect to have clarified the situation, and the next step could be presenting arguments to select the extension(s) to be considered natural, with the consequent implications as, for instance, the permeability of the origin.

Finally, we have found remarkable that, for potentials in \mathbb{R}^n , $n = 1, 2, 3$, given by fundamental solutions of Laplace equation, the corresponding initial hermitian operators with domain $C_0^\infty(\mathbb{R}^n)$ are always essentially self-adjoint.

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