



Is Dirichlet the physical boundary condition for the one-dimensional hydrogen atom?

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ABSTRACT

It is argued that Dirichlet is the physical boundary condition at the origin for the one-dimensional hydrogen atom: The three-dimensional hydrogen atom is confined to a tube, and the limit as the diameter of the tube cross section goes to zero is taken. It is shown that the energy expectations are finite only in case of Dirichlet boundary condition.

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When a quantum Hamiltonian have more than one self-adjoint extension, it is natural to ask which of such extensions is physically reasonable (if any) among the admissible ones. Sometimes, physicists take one self-adjoint extension for granted, usually guided by their expectations about a particular boundary condition they suspect will occur. But one must think of effective ways to justify each choice, and be aware that different boundary conditions will reflect different physical conditions and dynamics.

According to quantum mechanics, the allowable boundary conditions are those for which the corresponding Hamiltonians are self-adjoint. In some cases the initial Hamiltonian operator has just one self-adjoint extension, and so the modeling is clear; a prominent example is the three-dimensional (3D) hydrogen atom Hamiltonian ($0 \neq \kappa \in \mathbb{R}$)

$$H_H = -\Delta - \frac{\kappa}{|x|}, \quad \text{dom } H_H = \mathcal{H}^2(\mathbb{R}^3),$$

which is the unique self-adjoint extension of the operator with the same action but domain $C_0^\infty(\mathbb{R}^3)$ (see details in [1]); \mathcal{H}^2 is a usual Sobolev space of functions in L^2 whose first and second derivatives are also square integrable. This is in fact the textbook Hamiltonian of the hydrogen atom or, more precisely, of the electron motion under a Coulomb potential. However, the same model in one dimension (1D) has infinitely many self-adjoint extensions [2,3], and one reason is that in 1D one is forced to start with the domain $C_0^\infty(\mathbb{R} \setminus \{0\})$ (smooth functions of compact support that vanish in

a neighborhood of the origin), and so appropriate boundary conditions at the origin are necessary in order to get self-adjoint extensions. Denote such initial 1D Hamiltonian by \dot{H} , that is,

$$\dot{H} = -\frac{d^2}{dx^2} - \frac{\kappa}{|x|}, \quad \text{dom } \dot{H} = C_0^\infty(\mathbb{R} \setminus \{0\}). \quad (1)$$

We will refer to this operator, and its self-adjoint extensions as well, as the “one-dimensional hydrogen atom” (despite this name might refer to potentials obtained through fundamental solutions of the Laplace equation; see Section 5 in [3]).

In Ref. [3] there is a description of all self-adjoint extensions of \dot{H} ; here we describe in detail only the Dirichlet extension \dot{H}_D , since it will be the relevant one to this work. Shortly, \dot{H}_D is the extension of \dot{H} whose function in its domain vanish at the origin; precisely, \dot{H}_D has the same action as \dot{H} but with domain

$$\text{dom } \dot{H}_D = \left\{ \phi \in L^2(\mathbb{R} \setminus \{0\}) : \phi, \phi' \in \text{AC}(\mathbb{R} \setminus \{0\}), \right. \\ \left. \left(-\phi'' - \frac{\kappa}{|x|} \phi \right) \in L^2(\mathbb{R}), \phi(0^+) = 0 = \phi(0^-) \right\},$$

with ϕ' indicating the derivative of ϕ and $\text{AC}(\mathbb{R} \setminus \{0\})$ denoting the set of absolutely continuous functions on the subset $\mathbb{R} \setminus \{0\}$.

Since the publication of a work by Loudon [4] of 1959, there were interesting discussions about this 1D hydrogen atom, with different approaches and interpretations; one of the main points was the right choice of boundary conditions at the origin, including whether the origin is permeable or not (that is, if the electron could travel from one side of the origin to the other side [5–8,3]). Due to the Coulomb singularity (very strong in 1D, but mild in

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3D), the vanishing of the wave functions at the origin in 1D, the so-called Dirichlet boundary condition, has been assumed in most works (see, for instance, [4,9–13], references therein), so that the origin becomes impermeable. It is worth mentioning that, besides Dirichlet, there are other boundary conditions that turn the origin impermeable [3].

A result in [14] indicates that the Dirichlet condition is the relevant one for such 1D hydrogen model; it was shown that if the Coulomb potential is softened at the singularity in the form

$$-\frac{d^2}{dx^2} - \frac{\kappa}{|x| + a}, \quad a > 0,$$

then the Dirichlet boundary condition emerges in the limit $a \rightarrow 0$. It is the main goal of this work to present another argument, one we consider more physically appealing, to exclude boundary conditions different from Dirichlet; we will consider a dimension reduction from 3D to 1D in such model. Before going into details, let us briefly recall some facts of the history of the one-dimensional hydrogen atom.

Apparently this model was first considered by Vrkljan [15] in 1928, but Loudon's work [4] motivated a long controversial discussion through a series of publications by different authors. Loudon stated that the 1D hydrogen atom was twofold degenerate with even and odd eigenfunctions for each eigenvalue, except for the ground state with an infinite binding energy. Since it is expected that 1D systems should have no degenerate eigenvalues, the double degeneracy was justified in terms of the severe 1D Coulomb singularity. Andrews [5] questioned the existence of a ground state with infinite binding energy, and later on Haines and Roberts [16] have analyzed Loudon's arguments, found even wave functions with continuous eigenvalues, which were complementary to some odd functions; however, Andrews [17] disapproved these results by not accepting the continuous eigenvalues. Gomes and Zimmerman [18] argued that the even states with finite energy should be excluded. Spector and Lee [19] presented a relativistic treatment of this model with the advantage of excluding the ground state infinite binding energy; recently, careful studies of the bound-state energies for Klein–Gordon particles in a 1D cutoff Coulombian potential have been reported [20,21]. The classification of all boundary conditions at the origin compatible with quantum mechanics, as well as the question of permeability of the origin, are discussed in [2,3]. A particular self-adjoint extension was mathematically selected in [6] by employing tools of distribution theory, but this “selection of the physical boundary condition” was criticized in [22] by arguing that such a selection cannot be performed by mathematical considerations of self-adjoint extensions alone; see the response to the critics in [23]. Other works that have discussed this model include [24–32], and this list is far from comprehensive.

Although at first glance the one-dimensional hydrogen atom seems to be a question of purely academic interest, one should note that such model has been used as approximations in theoretical and numerical studies of more realistic 3D models [33–35], particularly describing atoms in very strong magnetic fields [36]; in the description of electrons hovering above superfluids [37,12,38]; in investigations of the threshold ionization of atoms under very intense laser fields [39]; in applications to condensed matter [40,37]; electrons trapped in one-dimensional hydrogenic levels have been suggested as a possible device for quantum computing [41]; it was noted that the electronic distribution of atoms, in excited states under time-periodically electric fields, can be modelled by the one-dimensional hydrogen atom [42,43]. Furthermore, some experimental evidences for the 1D hydrogen atom [12,44] have been reported and, recently, in [11] the authors present a discussion against the assertion that the 1D Coulomb potential “does not properly exist.”

The above remarks reinforce the motivation for arguments towards a selection of physical self-adjoint extensions of this model, and this is our main goal in this work. We propose a mathematical mechanism that is not restricted to the sole classification of self-adjoint extensions: we discuss a way of getting the 1D model from the familiar 3D hydrogen atom while keeping track of the behaviour of the energy expectations. In the first step we assume that the Coulombian center of force is kept fixed at the origin, but we restrict the electron motion to a tube Ω^ϵ whose cross section has diameter 2ϵ ; the second step is to take the limit $\epsilon \rightarrow 0$, so that the tube reduces to a straight line (the x -axis), and we shall argue that only the Dirichlet boundary condition gives rise to finite (i.e., different from both $\pm\infty$) energy expectations during the confining process. The energy expectations, described by means of quadratic forms of the relevant Hamiltonian operators, will be our physical guides to the selection of the physically reasonable boundary condition.

Consider an electron, under the influence of a Coulomb potential with center of force located at the origin, and restricted to a tube with cross section $\emptyset \neq S \subset \mathbb{R}^2$ along the x -axis. S is an open, connected, bounded subset of \mathbb{R}^2 . As usual, denote by \mathbf{i} , \mathbf{j} , \mathbf{k} the unit vectors pointing towards the positive directions of the axes x , $y_1 = y$, $y_2 = z$, respectively. Assume that the point with coordinates $y_1 = 0 = y_2$ belongs to S (in case S is an open disk we get the usual infinitely long cylinder). For each $\epsilon > 0$, denote

$$f^\epsilon(x, y_1, y_2) = x\mathbf{i} + \epsilon y_1\mathbf{j}(x) + \epsilon y_2\mathbf{k}(x),$$

which defines a tube given by

$$\Omega^\epsilon := \{(x, y, z) \in \mathbb{R}^3 : (x, y, z) = f^\epsilon(x, y_1, y_2), (y_1, y_2) \in S\}.$$

Our initial Hilbert space is $L^2(\Omega^\epsilon)$, but it is necessary to restrict the calculation of the energy to suitable subspaces. For instance, some derivatives are required and we also assume that the functions vanish at the tube border $\partial\Omega^\epsilon$, as a way to restrict the electron motion to the tube.

Instead of the usual expression for the energy expectation

$$\left\langle \psi, \left(-\Delta - \frac{\kappa}{|(x, y)|} \right) \psi \right\rangle, \quad (2)$$

we shall use another one that requires a weaker condition on the wave function and reduces to (2) in case ψ is smooth, that is, we define the energy expectation for functions in $\mathcal{H}_0^1(\Omega^\epsilon)$ (recall that the subscript “0” in $\mathcal{H}_0^1(\Omega^\epsilon)$ indicates that the elements of this space vanish at $\partial\Omega^\epsilon$) by writing

$$\mathcal{E}^\epsilon(\psi) := \int_{\Omega^\epsilon} \left(|\nabla\psi|^2 - \kappa \frac{|\psi|^2}{|(x, y)|} \right) dx dy, \quad \psi \in \mathcal{H}_0^1(\Omega^\epsilon),$$

so that only the first derivatives of ψ are required to belong to $L^2(\Omega^\epsilon)$ (that is the meaning of the superscript “1” in \mathcal{H}_0^1); ∇ is the usual gradient in Cartesian coordinates $(x, y) = (x, y_1, y_2)$, $dy = dy_1 dy_2$. The gradient in the cross section variables $y = (y_1, y_2)$ will be denoted by ∇_\perp , and the prime ' will indicate derivative with respect to the 1D variable x .

After a properly regularized $\mathcal{E}^\epsilon(\psi)$ (regularizations are unavoidable since there is a reduction of dimension of the system [45,46]), we will show that the condition of the energy to be finite in the singular limit $\epsilon \rightarrow 0$, that is, when the tube approaches a straight line, requires Dirichlet boundary condition at the origin in the corresponding 1D model.

When the tube is compressed, there are divergent energies due to terms (at least) of the form λ_0/ϵ^2 related to transverse oscillations in the tube, where $0 < \lambda_0$ is the least eigenvalue of the

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