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Classical and quantum space splitting: the one-dimensional hydrogen atom

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Abstract

The one-dimensional (1D) hydrogen atom with potential energy $V(q) = -e^2/|q|$, with e the electron charge and q its position coordinate, has been a source of discussion and controversy for more than 55 years. A number of incorrect claims have been made about its spectrum; for example, that its ground state has infinite binding energy, that bound states associated with a continuum of negative energy values exist, or that anomalous non-Balmer energy levels are present in the system. Given such claims and the ongoing controversy, we have re-analysed the 1D hydrogen atom, first from a classical and then from a quantum perspective both in the coordinate and in the momentum representations. This work exhibits that certain classical properties of the system may serve to clarify the properties of the quantum problem. Using the Dirichlet boundary condition, we show that the singularity of the potential prevents any relation between the right and left sides of the origin. Hence we prove that the attractive potential $V(q)$ acts in that case as an impenetrable barrier splitting the coordinate space into two independent regions. We show that such splitting appears both in the classical and in the quantum descriptions of the system. The analysis presented in this paper may serve as a pedagogical tool for the comparison between classical and quantum problems, as well as an illustrative example of a problem involving a singular potential that can be approached both from its position and momentum representations.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The one-dimensional (1D) hydrogen atom has been a subject of attention since the early works of Vrkljan [1, 2] in the dawn of quantum theory and from Loudon's celebrated paper [3]. It is from the discussions which followed Loudon's work that most of the misunderstandings plaguing this problem have arisen. Even the term 'one-dimensional Coulomb problem' may be a cause of confusion since the Coulomb (or Kepler) potential in one dimension does not correspond to the potential term traditionally used in the system under consideration. The potential energy that should appear in any Hamiltonian describing the problem must be the solution to the one-dimensional Poisson equation with a point charge; that is, should be $V_C(q) = -2\pi e|q|$ and not the potential energy given in equation (1). In his pioneering papers Vrkljan has referred to it using the analogous term quantum 1D Kepler problem. However, in spite of such minor qualms, in this work we use the standard terminology with the (so-called) 1D Coulomb potential

$$V(q) = -\frac{e^2}{|q|}, \qquad -\infty < q < \infty, \tag{1}$$

with e the electron's charge and q its position along a straight line. We should emphasize the highly singular nature, of the potential at $q = 0$ which makes the solution of the Schrödinger equation with potential as in equation (1) problematic, as difficulties may arise when a singular potential is used in the Schrödinger equation [4, 5]. However, despite its use in various settings and its great pedagogical interest, the problem has been a source of discussions and disagreements for more than 55 years [3, 6–11].

The importance of the 1D hydrogen atom with the potential given in equation (1) stems not only because it is an interesting example in 1D quantum mechanics or by the surprising features of its solutions but also for its very diverse physical applications. For instance, Loudon's interest in the problem arose from a study of the light-absorption properties of semiconductor hole–electron pairs in a magnetic field B. In this setting, one needs to solve the Schrödinger equation for an atom in such a field in the approximation (valid for high B fields) in which the electric field affects only the motion along B [12]. This approximation also serves for describing the behavior of atomic systems in super-strong magnetic fields [13] and for describing, albeit approximately, the bound spectrum of electrons hovering above a helium surface [14].

The 1D hydrogen atom proves to be a rather useful tool when modeling a system restricted to move on a line—as in dealing with nanotubes and other reduced dimensional systems [12, 15]—because it still takes into account that the Universe is 3D though the system is confined to move on a line. Therefore, this model has various uses in diverse areas of physics [7, 15–35]. Moreover, features of the motion under this potential have been used for studying chaos in periodically driven atoms [36], for modeling excited states of hydrogen in electric fields [37, 38], and even for imagining quantum computing devices [39, 40]. It has been used for analysing processes leading to the formation of 1D hydrogen hydrates in nanotubes [41], and for illustrating techniques in quantum phase space [42]. The 1D hydrogen atom has also been studied in the presence of a minimal length uncertainty [43, 44], and in interaction with electromagnetic fields [32, 45]. We should also mention that the two-dimensional hydrogen atom (with a

potential energy term given by $U_{2D} = -k/\sqrt{x^2 + y^2}$, with $k > 0$) has also been used in various important applications; for example, in studying electron motion in highly anisotropic crystals, for investigating atom cooling processes, and in semiconductor spectroscopy [46–48].

In this work we will show how a careful assessment of the mathematical tools needed for describing the classical 1D Coulomb problem provides good insight into the most remarkable features of the quantum problem. Thus, we intend to analyze the classical behavior and relate it with the corresponding quantum one. In particular, we find that the space splitting is a common property of both the classical and the quantum cases of the problem. Such analysis might be useful for other singular problems in low dimensions. The paper is organized as follows: we begin in section 2 with the discussion of the classical problem. We carry out here a study of the bound classical 1D problem in the framework of Hamiltonian mechanics. Then, in section 3, we straightforwardly solve for the bound states of the quantum 1D hydrogen atom trying to correct along the way some of the erroneous beliefs held on the problem. To complete the discussion in the quantum setting, we found the bound states of the problem again but this time in the momentum representation. As pointed out in reference [49], momentum space is a natural setting for potentials represented by equation (1) due to the fact that the 3D Schrödinger equation in the momentum representation for the Kepler problem may be interpreted as an integral equation on the group space of O(3). Such feature also applies to the description of the 1D hydrogen atom, see also reference [26].

2. Motion in a classical one-dimensional Coulomb—or Kepler—potential

We deal with the classical 1D hydrogen atom with Hamiltonian

$$H = \frac{p^2}{2m} - k\frac{e^2}{|q|}, \quad -\infty < q < \infty \tag{2}$$

where k is the Coulomb's constant, m and e are, respectively, the mass and the electric charge of the electron, q its position coordinate, and p the corresponding conjugate momentum. Hamilton's equations of motion follow immediately:

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \text{and} \quad \dot{p} = -\frac{\partial H}{\partial q} = -ke^2\frac{|q|}{q^3}, \quad q > 0 \text{ or } q < 0. \tag{3}$$

Note that these equations are singular at $q = 0$ and thus one has to be cautious when dealing with them. But a glance at the phase portrait of the problem in figure 1 suffices to exhibit that, in spite of the attractive nature of the potential, the classical motion avoids the singularity completely. That is, the phase flow never crosses the vertical line passing through the origin. Moreover, from the time independence of its Hamiltonian the energy, E, is a constant of motion and, as it is strongly suggested by the phase plot, the sign of the q-coordinate should be another constant of the motion. Such constant may be written with the help of the sign function as $s = \text{sgn}(q)$. The constancy of s means that the particle can never go through the origin neither from the region with $q > 0$ to the region with $q < 0$ nor the other way round.

Let us show explicitly that the sign of the particle's coordinate never changes; that is, that the following equation holds:

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{\partial s}{\partial q}\dot{q} + \frac{\partial s}{\partial p}\dot{p} = \frac{\partial s}{\partial q}\dot{q} = 0. \tag{4}$$

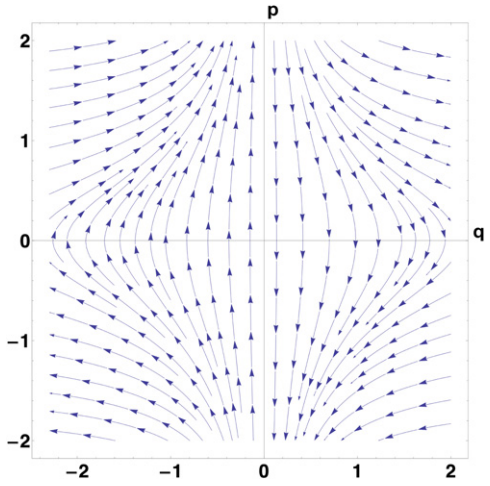

Figure 1. Phase diagram, p vs q, for the classical 1D hydrogen atom in arbitrary units. Notice that no phase trajectory is able to cross from the $q > 0$ region to the $q < 0$ region nor the other way around.

A result which is valid because s does not depend on p and because it has a piecewise constant value as a function of q. Also notice that equation (4) might have been written as

$$\frac{\mathrm{d}s}{\mathrm{d}t} = 2\delta(q)\dot{q} \tag{5}$$

suggesting that it vanishes in the whole q-axis, except at $q = 0$.

In order to analyze what happens near the origin, let us suppose first that $p \geqslant 0$, the case when $p \leqslant 0$ is completely similar. From equation (2) we have that

$$p = +\sqrt{2m\left(H + k\frac{e^2}{|q|}\right)}. \tag{6}$$

So, when $|q| \to 0$ we have that $p \to \infty$ for any H. Now equation (6) is zero when $|q| = -(ke^2/H)$, attained for bound sates only, and since p should remain real we must conclude that $H + (ke^2/|q|) \geqslant 0$. We have then two possibilities, either $-(ke^2/H) \geqslant q > 0$ or $0 > q \geqslant (ke^2/H)$. From equation (6) we can calculate the slope of p as a function of q for these two cases; that is, for a vicinity around the origin:

$$\frac{\mathrm{d}p}{\mathrm{d}q} = \begin{cases} -mke^2/pq^2 & \text{if } -(ke^2/H) \geqslant q > 0, \\ +mke^2/pq^2 & \text{if } \quad 0 > q \geqslant (ke^2/H). \end{cases} \tag{7}$$

Then for the right part of the coordinate axis, when p grows q diminishes, and vice versa, if p diminishes q grows. For the left part of the axis we have the opposite behavior. But the 1D electron cannot go from $q > 0$ to $q < 0$, because the q coordinate cannot change its sign. In other words, if the electron is approaching the origin the potential drive backwards its incoming trajectory just precisely in $q = 0$; consequently we can say that the origin acts effectively as an impenetrable barrier for the electron. This is the same behavior that we would obtain in the case of elastic collision between two particles in the limit when the mass of one of the particles

goes to infinity. That is, as in the case of an infinite mass wall when the finite mass particle bounces back after a frontal collision.

Additionally, since classical quantities may never be interpreted as distributions [50], we simply take $\mathrm{d}s/\mathrm{d}t = 0$. Let us note that these arguments are equally applicable to the classical analysis reported in reference [20], where an unwarranted repulsive Dirac delta interaction is added to the classical force obtained from the 1D Coulomb potential, thus casting doubts on their analysis.

The constancy of s is quite surprising because we do not expect an attractive potential, such as the one we use in the Hamiltonian of equation (2), to behave as an impenetrable barrier as the previous discussion exhibits. In fact, as has been argued in Boya *et al* [26], the sign of q can be regarded as the 1D remnant of the conserved Laplace–Runge–Lenz vector that exists in the classical three-dimensional (3D) problem. Therefore, regardless of the initial conditions, the particle is going to avoid the origin [26, 51, 52]. That is, the 1D potential appearing in equation (2) effectively divides the classical coordinate space into two independent regions, one to the right and another to the left of the singularity. We call this feature a *classical space splitting* or a *classical space separation* [53, 54].

The system's equations of motion (3) lead to

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} \pm \frac{k^2 e^2}{m q^2} = 0, \tag{8}$$

where the $+$ sign is used for $q > 0$ and the $-$ sign for $q < 0$. The solutions of equation (8) are of the form $q = q_{\pm}(t)$, where $q_{+}(t)$ describes the motion of a particle to the right of the singularity and $q_{-}(t)$ its motion to the left. Therefore, each of the classical solutions describe separately the particle motion at each side of the singularity at $q = 0$. That is, they explicitly show the classical space splitting occurring in the system. Such splitting can be more clearly exhibited analytically for the bound case, $E < 0$, as we show in the following. We first change variables by performing a counterclockwise rotation by $\pi/2$ in phase space; that is, $q \to p$ and $p \to -q$ (which is indeed a canonical transformation [26, 55])

$$H = \frac{q^2}{2m} - k\frac{e^2}{|p|} \tag{9}$$

and taking into account that the energy E, i.e. the value of the Hamiltonian, is constant. After this transformation the units of q become momentum units and those of p become the same as q.

We can rewrite equation (9) to get

$$\frac{|p|}{ke^2}\left(\frac{q^2}{2mE} - 1\right) = \frac{1}{E}. \tag{10}$$

Then, squaring the result, we obtain

$$\frac{Ep^2}{2k^2e^4}\left(\frac{q^2}{2mE} - 1\right)^2 = \frac{1}{2E} \tag{11}$$

and after performing the change from the variable q to the angle θ through the stereographic transformation

$$q = 2R\ \tan(\theta/2), \tag{12}$$

where $-\pi \leqslant \theta < \pi$ is defined on a circle of radius R, we get the new Hamiltonian

$$H' = \frac{p_\theta^2}{2\mu R^2}, \tag{13}$$

where p_θ is the new momentum canonically conjugated to θ. The parameters μ and R can be identified with the charge and mass of the electron via the relations

$$\mu = \frac{ke^2}{E^2}, \qquad R = \sqrt{\frac{m|E|}{2}}. \tag{14}$$

The details of the stereographic transformation equation (12) are given in appendix A.

You can see now that H' has the form of the Hamiltonian of a particle moving freely on a circle of radius R. Thus, we have not only transformed the problem to free motion on a circle but we have also managed to remove from sight the problematic singularity at $q = 0$. In classical mechanics this kind of singularity-removing transformation is termed a regularization. Moreover, the equivalence to geodesic motion is in fact valid for the Kepler problem in arbitrary dimensions, and can be established mathematically either by considering a geometrical regularization in which motion under the potential equation (2) transforms into geodesic curves on a sphere—in this case a circle, as we show in appendix A. The D-dimensional general result is due to Moser [51, 52, 56]. Notice also that we have two essentially different ways of traversing the circle: clockwise and counterclockwise. Such ways correspond to the classical electron coming towards the singularity from the right of it in one case, and from the left of it in the other. Notice that these motions are described by $q_+(t)$ and $q_-(t)$ respectively.

The important point to grasp is that both circular motions are totally independent from one another so that you cannot go freely from one to the other. In the original coordinates, we would say that there is no way of going through the origin. The source of all these intriguing features is precisely the singularity of the potential. As we have shown, the singularity acts as a classical impenetrable barrier for the electron. This property leads us to the conclusion that, in spite of the overall symmetry of the potential function, the classical 1D Coulomb problem does not admit trajectories such that $q(t) = \pm q(-t)$. To see this, take a particle that starts at a specific initial position $q_0 = -k/E < 0$ with zero initial velocity. Then, by the effect of the interaction it starts moving towards the origin but, as it reaches the singularity, the electron suddenly changes its velocity from $-\infty$ to $+\infty$ bouncing back to its initial position q_0 in a certain finite time. This bouncing phenomenon, although striking at first glance, is a well studied effect in celestial mechanics known as *collision–ejection trajectories* (see for instance, section 13.4 in [57]). In the standard Kepler problem in 3D, this feature can be thought as arising when the limit as the impact parameter of an orbit approaches zero. Recall that in this case, according to Kepler's laws, such an orbit is highly elongated and the time it spends in the close fly-by around the singularity is very small compared to the orbital period. Hence, in the limit we expect to have a straight trajectory with an instantaneous bouncing at the singularity. As it turns out, this property can be also established by blowing up the singularity using a change of coordinates in which the new time parameter moves really slow with respect to the original one. This very powerful technique for analyzing singularities was developed in the context of celestial mechanics by McGehee [57, 58].

Hence, we have to conclude that the two regions, $q < 0$ and $q > 0$ are unreachable one from the other and, so, space is effectively separated in two completely disconnected regions. Most of the conclusions reached in this section can be corroborated by just taking a glance at the phase plot shown in figure 1 which corresponds to the vector field generated by the Hamiltonian of

equation (2). In the next section we show that a careful treatment of the singularity is the key for getting a proper solution to the quantum problem.

3. The quantum problem

In this section we solve the quantum 1D hydrogen atom problem first in coordinate space and then find its solution in momentum space. Such double effort will provide key elements for a complete understanding of the quantum solution and, in addition, could be used as an original pedagogical technique. This approach can fill a void in the literature, since it is hard to find instances in which a problem is solved, side-by-side, using these two complementary representations.

3.1. Coordinate space solution

Let us write down the Schrödinger equation for the problem

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}q^2}-\frac{e^2}{|q|}\psi=E\psi, \tag{15}$$

where m and e are the mass and the electron charge, respectively. The main issue with the quantum 1D hydrogen atom problem is, to state it clearly from the start, whether the Hamiltonian in equation (15) may be regarded as self-adjoint or not. Let us first explain in full detail what is understood by a self-adjoint operator—which is usually taken to be a synonym of Hermitian but it is actually not. An operator H is *self-adjoint* whenever it coincides with its adjoint: $H=H^\dagger$. The crucial point in this definition is that in the last equality the operators are understood as mathematical objects acting on an infinite dimensional vector space. As such, an equality between them will imply not only that their respective *actions* agree (in which case the operator is called *Hermitian* or *symmetric*) but also that their respective *domains* agree. That is, we would also need $D(H)=D(H^\dagger)$—where $D(O)$ stands for the domain of operator O.[7] To illustrate this, consider the following example [59–63]: take the 1D momentum operator $P=-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$ on the closed interval $[0,1]$ with domain

$$D(P)=\{\varphi:\varphi,\varphi'\in L^2([0,1])\ \text{ and }\ \varphi(0)=0=\varphi(1)\}. \tag{16}$$

A straightforward calculation shows that

$$\langle\psi,P\varphi\rangle-\langle-\mathrm{i}\hbar\psi',\varphi\rangle=-\mathrm{i}\hbar[\psi^*(1)\varphi(1)-\psi^*(0)\varphi(0)]=0, \tag{17}$$

thus showing that $P^\dagger=-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$; or in other words, that P is symmetric. However, it is clear that equation (17) holds *regardless* of any boundary conditions imposed on ψ. That is,

$$D(P^\dagger)=\{\psi:\psi,\psi'\in L^2([0,1])\}, \tag{18}$$

which clearly shows that $D(P)\neq D(P^\dagger)$. Notice that though P and $P^\dagger$ are formally defined by the same action (or transformation), the functions they operate on belong to different functional spaces, and thus, the operator *P is not* self-adjoint. Very good pedagogical explanations of the important differences between Hermitian and self-adjoint operators together with a detailed examination of the quantum troubles caused by not recognizing this distinction have been discussed before [64, 65].

[7] Recall that the domain of an operator is defined as the class of functions in which it operates.

As the above example illustrates, it is often the case that the class of functions in which the adjoint $H^\dagger$ operates is *strictly larger* than $D(H)$. Thus, conditions on the admissible states need to be carefully tailored in order to guarantee that $D(H) = D(H^\dagger)$. Such requirements usually translate into matching or boundary conditions [59–65]. For instance, in our example of the momentum operator, the choice of a boundary condition of the form $\varphi(1) = \mathrm{e}^{\mathrm{i}\theta}\varphi(0)$, with θ a fixed phase, would result in a self-adjoint operator, as can be easily established from equation (17). That is,

$$D(P) = \{\psi : \psi, \psi' \in L^2([0,1]) \quad \text{and} \quad \psi(1) = \mathrm{e}^{\mathrm{i}\theta}\psi(0)\} = D(P^\dagger), \tag{19}$$

Furthermore, notice that the domain in equation (19) contains our first choice of domain for the momentum operator, equation (16). In the language of functional analysis, we say that equation (19) describes a *self-adjoint extension* of the momentum operator.

The requirement that in the 1D hydrogen atom problem the wave functions should vanish at the origin,

$$\psi(0) = 0, \tag{20}$$

limits the domain of definition of the Hamiltonian [66], and the choice is dictated by the previously conclusion that the electron cannot cross the origin. This (Dirichlet) condition has been shown to be sufficient—although not necessary—in order to guarantee the self-adjointness of the Hamiltonian operator of the 1D hydrogen atom [67–69]. In terms of the above discussion, we can say that the choice of the Dirichlet boundary condition singles out a particular self-adjoint extension of the Hamiltonian given by equation (15). We can solve directly for the energy eigenstates that follow from the Schrödinger equation (15) and apply the previous matching condition, as this procedure is sure to guarantee the self-adjointness of the Hamiltonian. We point out from the start that the eigensolutions to the Schrödinger equation of the 1D hydrogen atom are going to be of the form calculated by Loudon [3].

To find the bound states with negative energy, $E < 0$, define

$$\alpha^2 \equiv -\frac{\hbar^2}{2mEa_{\mathrm{B}}^2}, \tag{21}$$

where

$$a_{\mathrm{B}} \equiv \frac{\hbar^2}{me^2} \tag{22}$$

is the Bohr radius. We now change the variable to

$$z = \frac{2q}{a_{\mathrm{B}}\alpha} \tag{23}$$

and substitute in equation (15) to obtain

$$\frac{\mathrm{d}^2\psi(z)}{\mathrm{d}z^2} + \left(\pm\frac{\alpha}{z} - \frac{1}{4}\right)\psi(z) = 0, \tag{24}$$

where the sign $(+)$ is only valid for $z > 0$ and likewise $(-)$ for $z < 0$.

In the limit $z \to \pm\infty$ equation (24) transforms to

$$\frac{\mathrm{d}^2\psi_{\mathrm{asy}}}{\mathrm{d}z^2} - \frac{\psi_{\mathrm{asy}}}{4} = 0 \tag{25}$$

whose solutions are

$$\psi^{\pm}_{\text{asy}}(z) = B_{\pm} \ \exp\ (\mp z/2). \tag{26}$$

To take advantage of the asymptotic behavior described above, we write

$$\psi^{\pm}(z) = \exp\ (\mp z/2) G(z) \tag{27}$$

for the eigenfunctions of the 1D hydrogen atom, where $G(z)$ is an unknown function to be determined. Thus we can separate the study of the exponential asymptotic behavior for $z \to \pm\infty$ from the near-to-the-origin behavior described by the function $G(z)$. We note that $\psi(z) \equiv \psi^{+}(z)$ is the solution for the region $z > 0$, while $\psi^{-}(z)$ describes the solution in the region $z < 0$. After finding $\psi^{+}(z)$ and $\psi^{-}(z)$, the standard procedure consists in piecing them together for getting the complete eigenfunctions valid in all coordinate space, from $-\infty$ to ∞. But, as we demonstrate below, it is not possible to perform such matching without obtaining inconsistent results.

We confine our analysis of the problem to the positive case $z > 0$ only since a completely analogous analysis can be made for the region $z < 0$.

Using the relation (27) in equation (24), we get

$$z\frac{\mathrm{d}^2 G(z)}{\mathrm{d}z^2} - z\frac{\mathrm{d}G(z)}{\mathrm{d}z} + \alpha G(z) = 0 \tag{28}$$

and introduce $g(z)$ through

$$G(z) = z g(z); \quad z > 0. \tag{29}$$

This substitution guarantees the vanishing of $G(z)$, hence of $\psi(z)$, at $z = 0$. In this way, we finally obtain

$$z\frac{\mathrm{d}^2 g(z)}{\mathrm{d}z^2} + (2 - z)\frac{\mathrm{d}g(z)}{\mathrm{d}z} + (\alpha - 1) g(z) = 0, \tag{30}$$

which is the confluent hypergeometric differential equation whose solution, regular at $z = 0$ for any value of α, is

$$g(z) \sim C_1 F_1(1 - \alpha; 2; z), \quad z > 0, \tag{31}$$

the confluent hypergeometric function of the first kind [70, 71]. To see the implications of our selection, we may try a series solution for equation (30). The series would diverge if we let z go to infinity because, as we can see in (30), if z is very large we may neglect both the constant 2 appearing in the second term and the term proportional to $(\alpha - 1)$. In this limit then the solution becomes a divergent exponential unless we cut the series off. Therefore, proceeding step by step, exactly as one proceeds in the 3D hydrogen atom case, we find that the series converges only if we take $\alpha = n$, with n being a positive integer. In such a case the solution becomes an associated Laguerre polynomial $L^{1}_{n-1}(z)$ and behaves as a possible eigenfunction—this should be clear because both the equations and the procedure are the same as for the radial eigenstates of the 3D case. These considerations yield the energy eigenvalues

$$E_n = -\frac{e^2}{2n^2 a_{\text{B}}}, \tag{32}$$

which is the Balmer formula, as in the 3D case—a result already pointed out by Andrews in 1966 [6]. Note that no trace of the infinite energy ground state [3], nor of the continuum

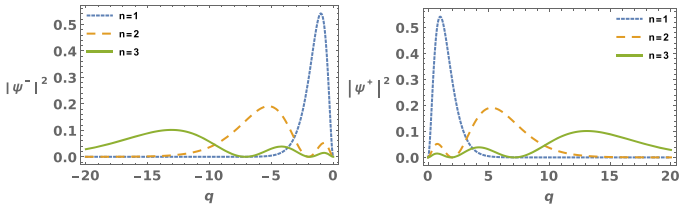

Figure 2. Probability distributions for the first three eigenstates in the q-representation, showing $|\psi_n^-(q)|^2$ to the left and $|\psi_n^+(q)|^2$ to the right. These eigenfunctions vanish, respectively, for $q > 0$ ($\psi_n^-(q)$) and for $q < 0$ ($\psi_n^+(q)$). Notice also that the variance $\sigma_q = \sqrt{\langle q^2\rangle - \langle q\rangle^2}$ increases with n.

of negative energy states [7], and neither of the so-called anomalous solutions with energy eigenvalues $E_n = -e^2/((n+1/2)^2 a_{\mathrm{B}})$ found in the analysis of Abramovici and Avisai [24] are found in the energy spectrum equation (32). Let us note that the solution for the case $z < 0$ is similar to the one already found, the only difference being that z is necessarily less than zero. This condition define the functions

$$g(z) \sim {}_1F_1(1-\alpha; 2; z), \quad z < 0, \tag{33}$$

for building the $z < 0$ part of the eigenfunctions. However, let us remark that—as shown below—it is not possible to match the positive and negative parts of the q axis in any consistent way in order to obtain meaningful eigenfunctions valid in all coordinate space. So, acknowledging the previous impossibility we may write the eigenfunctions of the Schrödinger equation (15) as

$$\begin{aligned}
\psi_n^+(q) &= \begin{cases} 0 & \text{if} \quad q \leqslant 0, \\ 2(n^5 a_{\mathrm{B}}^3)^{-1/2}|q|\ \exp(-q/(na_{\mathrm{B}}))L_{n-1}^1(2q/(na_{\mathrm{B}})) & \text{if} \quad q > 0, \end{cases} \\
\psi_n^-(q) &= \begin{cases} 2(n^5 a_{\mathrm{B}}^3)^{-1/2}|q|\ \exp(q/(na_{\mathrm{B}}))L_{n-1}^1(-2q/(na_{\mathrm{B}})) & \text{if} \quad q < 0. \\ 0 & \text{if} \quad q \geqslant 0. \end{cases}
\end{aligned} \tag{34}$$

Here $\psi_n^-(q)$, that we call the left eigenfunctions, are the solutions valid for $q < 0$ (or equivalently, $z < 0$) while $\psi_n^+(q)$, called the right eigenfunctions, are valid for $q > 0$ ($z > 0$). Further notice that $\psi_n^+(q) = 0 = \psi_n^-(q)$, in agreement with the intuition developed from the Kepler problem in section 2. The probability distributions corresponding to the first three right and three left eigenfunctions are shown in figure 2.

We now proceed to clarify in detail the role the matching condition equation (20) plays in tackling the erroneous claims about the existence of an infinite negative energy state and of the even and odd solutions. First notice that the eigenfunctions equation (34) might be extended to functions defined on the whole q axis, but this can only be done at the expense of requiring the vanishing of such functions on a semi-axis [9, 31, 72]. In other words, we cannot piece together the functions ψ^+ and ψ^- in order to obtain a non-vanishing eigenfunction defined for $-\infty < q < \infty$.

First, we rule out the possibility that an eigenfunction of even parity, say $\psi = (\psi^+ + \psi^-)/\sqrt{2}$, can be defined over the whole real axis $-\infty < q < \infty$. Notice that a direct calculation

from equation (34) shows that

$$\psi'(0^+) - \psi'(0^-) = \left(\frac{2}{na_{\mathrm{B}}}\right)^{2/3} \tag{35}$$

and hence the derivative ψ' has a finite jump discontinuity at $q = 0$, while the Dirac δ function cancels out in this last result. Thus the derivatives of the solutions of the quantum 1D Coulomb potential will not match when approaching the singularity—a feature also observed in the classical 3D Coulomb problem—thus preventing any possible matching at $q = 0$. Nonetheless, this fact alone is not strong enough to discard ψ as a proper eigenstate since the matching condition for a singular (but not Dirac type) potential can be obtained by integrating Schrödinger equation (15) directly:

$$\psi'(0^+) - \psi'(0^-) = -\frac{2me^2}{\hbar^2}\int_{0^-}^{0^+} \frac{\psi(q)}{|q|}\mathrm{d}q. \tag{36}$$

However, from equation (34) we conclude that $\psi(q)/|q|$ is bounded near $q = 0$ and thus

$$\int_{0^-}^{0^+} \frac{\psi(q)}{|q|}\mathrm{d}q = 0, \tag{37}$$

thus violating condition (35). As a consequence, ψ cannot be considered as a *bona-fide* solution. We have thus shown that no even eigenfunctions may exist.

On the other hand, considering only odd eigenfunctions would imply that the matrix elements of both the position operator $\hat{q}$, and of the momentum operator $\hat{p}$, between any two eigenfunctions ψ_1 and ψ_2 would necessarily vanish:

$$\int_{-\infty}^{\infty} \psi_1^* q \psi_2 \mathrm{d}q = 0 \quad \text{and} \quad -\mathrm{i}\hbar\int_{-\infty}^{\infty} \psi_1^* \frac{\mathrm{d}\psi_2}{\mathrm{d}q}\mathrm{d}q = 0. \tag{38}$$

Thus, the odd eigenfunctions cannot be considered proper solutions either. For, if we do so, any quantum operator defined in terms of the operators $\hat{q}$ and $\hat{p}$ need to be identically zero. Hence, we cannot assume the existence of any eigenfunction defined in the whole q-interval $-\infty < q < \infty$ as such assumption leads directly to absurd results. Therefore, the only valid eigenfunctions of the system should describe states confined in one or the other of the two disconnected regions $-\infty < q < 0$ or $0 < q < \infty$. Furthermore, as one may ascertain from the condition $\psi(0) = 0$, the electron is forbidden to get to the singularity at the origin. Even the quantum flux

$$j = \frac{\mathrm{i}\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial q} - \psi^*\frac{\partial\psi}{\partial q}\right)_{q=0} = 0 \tag{39}$$

should vanish at the origin in any state of the system. This property of the quantum solutions may also be termed as space-splitting or space-separation phenomenon and is related to the classical property of the conservation of the sign of the q-coordinate $s = \mathrm{sgn}(q)$ and thus to the space splitting we have classically established in section 2 [53, 54]. Therefore, in the quantum setting, the splitting means that no parity eigenstates may occur in the 1D hydrogen atom subject to the Dirichlet condition $\psi(0) = 0$. Let us note that our discussion has also some bearings on the non-penetrability of the 1D Coulomb potential at positive energies as pointed out a long time ago [6, 73].

Finally, it is crucial to stress the fact that there is no *a priori* canonical choice of matching conditions that would ensure self-adjointness of the 1D Coulomb Hamiltonian. Let us recall the classical result that guarantees that all the eigenvalues of a self-adjoint operator are real. On the other hand, if an operator H is merely symmetric, it may have complex eigenvalues with non vanishing imaginary part. As it turns out, understanding how the corresponding eigenstates are spread throughout $D(H)$ is the key to classify all possible self-adjoint extensions of the symmetric operator H. Indeed, the deficiency indices defined by

$$n_+ = \dim\{\psi \in D(H) : \text{there is an eigenvalue of } H \text{ with } \operatorname{Im}(z) > 0\}, \tag{40}$$

$$n_- = \dim\{\psi \in D(H) : \text{there is an eigenvalue of } H \text{ with } \operatorname{Im}(z) < 0\}, \tag{41}$$

carry enough information to describe the space of all possible self-adjoint extensions of H. In fact, the fundamental theorem of von Neumann[8] establishes that a necessary and sufficient condition for the existence of self-adjoint extensions of H is that its deficiency indices satisfy $n_+ = n_1 < \infty$. In this case, the self-adjoint extensions require $n_+ \times n_+$ parameters for its descriptions. Such parameters can be further combined giving rise to $n_+ \times n_+$ unitary matrices (see for instance chapter X in [60] or chapter VII in [59] for detailed accounts of these facts). In the case of the 1D hydrogen atom, the deficiency indices of the Hamiltonian are equal to 2 and hence the full space of its self-adjoint extensions is parameterized by unitary 2×2 matrices U [67, 68]. Different choices of U lead to different matching conditions and hence to different domains for the 1D Coulomb Hamiltonian. In turn, each of these choices describes a different phenomenon both mathematically and physically. For instance, the Dirichlet condition $\lim_{q\to 0^-} \varphi(q) = 0 = \lim_{q\to 0^+} \varphi(q)$ we employ here, corresponds to an scenario where the eigenspaces are two dimensional and no parity eigenfunctions exist. On the other hand, if we choose instead the matching conditions $\lim_{q\to 0^-} \varphi(q) = \lim_{q\to 0^+} \varphi(q)$ and $\lim_{q\to 0^-} \varphi'(q) = \lim_{q\to 0^+} \varphi'(q)$—as was done by Palma and Raff [22]—we end up with a system with no degenerate eigenspaces and odd parity eigenfunctions. For a detailed account on how the choice of U influences the permeability of the origin and the degeneracy of the eigenspaces see references [68, 74].

3.2. Momentum space solution

Our conclusions on the quantum behavior of the 1D hydrogen atom can be made more transparent by working in the momentum representation since it is known that momentum space is a natural choice for the problem [49, 72]. We therefore turn to such p-representation to continue the quantum analysis of the system. To write the Schrödinger equation for the 1D hydrogen atom in the p-representation, we use the operator correspondence [72, 75]:

$$q^{-1} \to \frac{-\mathrm{i}}{\hbar}\int_{-\infty}^{p} \ldots \mathrm{d}p', \tag{42}$$

which follows directly from $q \to \mathrm{i}\hbar \mathrm{d}/\mathrm{d}p$. Using equation (42), the Schrödinger equation (15) is then written as the following integral equations in p-space:

$$\frac{p^2}{2m}\phi(p)^{\pm} \pm \mathrm{i}\frac{e^2}{\hbar}\int_{-\infty}^{p} \phi^{\pm}(p')\mathrm{d}p' = E\phi^{\pm}(p), \tag{43}$$

where $\phi^+(p)$ and $\phi^-(p)$ are the momentum space eigenfunctions for the regions $q > 0$ and $q < 0$ respectively. Notice that from equation (42) the coordinate wave function evaluated at

[8] We have included a statement of von Neumann's theorem in appendix B.

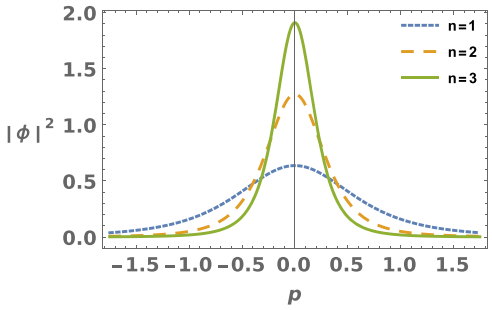

Figure 3. Probability distributions for the first three eigenstates in the p-representation. The variance, $\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$, diminishes as n increases in accord with Heisenberg's principle.

the origin $\psi(x = 0)$, is equal to the action of q^{-1} in $p = \infty$, $\hat{q}^{-1}[\phi]|_{p\to\infty} = \psi(0) = 0$, which in turn means that the action of q^{-1} is always bounded, and so equation (42) is well defined for any value of p [63]. Therefore the self-adjointness of the Hamiltonian operator is assured in the p-representation [9, 18, 72, 75–77]. If $a_B \equiv \hbar^2/(me^2)$ stands for the Bohr radius and $k \equiv pa_B/\hbar$, we may write the Schrödinger equation (43) in non-dimensional form as

$$(1 + \alpha^2 k^2)\phi^{\pm}(k) \pm 2i\alpha^2 \int_{-\infty}^{k} \phi^{\pm}(k')dk' = 0, \tag{44}$$

differentiating the last equations leads to the differential equations

$$\frac{d\phi^{\pm}}{dk} + \frac{2\alpha^2(k \pm i)}{1 + \alpha^2 k^2}\phi_{\pm} = 0, \tag{45}$$

whose solutions in terms of the original variables are

$$\phi_{\pm}(p) = \sqrt{\frac{2\alpha a_B}{\pi\hbar}} \left(\frac{1}{1 + (\alpha p a_B/\hbar)^2}\right) \left(\frac{1 - i\alpha p a_B/\hbar}{1 + i\alpha p a_B/\hbar}\right)^{\pm\alpha}. \tag{46}$$

The solutions (46) do not necessarily correspond to single valued functions and thus they are not very appropriate as eigenfunctions for the problem, but when α takes integer values the expressions become single valued. This condition determines the energy eigenvalues of the system through equation (21) as $E_n = -e^2/(2n^2 a_B)$; with $n = 1, 2, 3, \ldots$, which is the Balmer formula as in equation (32) [8, 9, 72]. Notice that equation (46) immediately tells us that the value $\alpha = n = 0$ is forbidden, otherwise the wave function $\phi_0^{\pm}(p)$ would vanish everywhere. Therefore, the supposed infinite energy ground state cannot exist (figure 3).

We should note the simplicity of the momentum space solution as compared with the coordinate space one, clearly illustrating the convenience of the p-representation for analysing the problem [9, 72].

3.3. Quantum properties

We have demonstrated that the energy eigenvalues of the 1D hydrogen atom are given by the Balmer formula equation (32) and that the principal quantum number takes values $n = 1, 2, 3, \ldots$, therefore the ground state of the system is $E_1 = -e^2/2a_B$. With these conclusions we have gotten rid of the supposed negative infinite energy ground state of the problem, of the

continuum of even negative energy states reported in reference [7] and also of the so-called anomalous states predicted in a recent work [24, 25]. This also means that any conclusion reached using as part of the argument the existence of such negative infinite energy states is probably wrong. For instance, in a recent analysis [11] a proof was given of the non-existence of critical dipole moment in one dimension based on the existence of an infinite binding-energy ground state, however this assumption was proven wrong by the explicit calculation of such moment [78, 79]. Previously, other studies have pointed out the inadequacy of the supposed ground state with infinite energy [6, 10].

Notice that equation (34) are essentially the solutions found by Loudon [3], although they are not matched to form states of definite parity defined along the whole q axis. The structure of the eigenfunctions, expressing a clear separation between the right and the left sides of the singularity at $q = 0$, can be thought of as a quantum manifestation of the classical impenetrability derived in section 2, preventing—even in the quantum realm—the electron from traversing from one side of the singularity to the other. So, the 1D Coulomb potential $-e^2/|q|$ acts, both classically and quantum mechanically, as an impenetrable potential barrier of zero width [33]. Therefore, the 1D Coulomb potential appearing in equation (15) divides the space available to the electron into two independent regions, one to the right and another to the left of the singularity at $q = 0$. We have interpreted such phenomenon as a manifestation of a superselection rule in the problem [29, 72, 77]. No parity eigenstates may occur in the 1D hydrogen atom.

4. Conclusions

In this paper, we have re-analyzed the negative energy classical motions or quantum eigenstates of the 1D hydrogen atom trying to emphasize its most important feature. Namely, that *both in the classical and in the quantum case a separation exists between the* $q > 0$ *and the* $q < 0$ *regions of coordinate space which prevents any passage between the two*. In this regard, the attractive 1D hydrogen atom potential behaves as an impenetrable potential barrier. In the classical description, we reached this conclusion by converting the dynamics to free motion on a circle. This regularization of the problem clearly exhibits that the only possible circular motions are completely unrelated.

The quantum impenetrability may be explained as the manifestation of a superselection rule [29, 72, 77]. Note that this impenetrability is directly related to the particular self-adjoint extension of the Hamiltonian of the problem we choose to analyze, which is characterized by the Dirichlet boundary condition $\psi(0) = 0$. This condition is not the only choice that guarantees the self-adjointness of the Hamiltonian, but is the one used in most of the physical applications of the model; see the detailed discussions in references [67, 69] for a thorough explanation. We have solved for the bound states of the quantum problem both in the coordinate and in the momentum representations obtaining—as it should necessarily be—identical results in both representations. We have established the following.

- The non-existence of the infinite-energy ground state [9, 72].
- That all the energy levels of the system are given by Balmer's formula equation (32): $E_n = -e^2/(2n^2 a_{\mathrm{B}})$ with $n = 1, 2, 3, \ldots$. This excludes anomalous states as those claimed in reference [24] or in reference [7].
- The splitting of the coordinate space available to the system in two non-overlapping regions, one for $q > 0$ and the other for $q < 0$. This is a feature valid both in quantum and in classical mechanics and implies, as have been argued in different works [9, 33, 72], that there cannot be any physical connection between the left ($q < 0$) and the right

($q > 0$) sides of the singularity. This behavior is associated with the choice of the Dirichlet condition $\psi(0) = 0$.

- The non-existence of even or odd states; that is, the complete absence of parity eigenfunctions. Such states have been generally assumed in most of the previous analysis but, as we have shown here, the 1D hydrogen atom shows a sort of spontaneous breaking of parity. This feature is also related to the Dirichlet boundary condition we use.

Also notice that the violation of the non-degeneracy of the eigenspaces in this 1D system is only mathematical in nature. As we show, it is caused by conceiving the range of the spatial coordinate of the eigenfunctions as $-\infty < q < \infty$, even if $\psi_n^+(q)$ or $\psi_n^-(q)$ vanishes in a whole semi-axis. Rather, we have proved that inconsistent conclusions necessarily follow from assuming such range as valid for a function that does not vanish completely on a semi-axis. If despite such fact one insists on regarding both sides as comprising a single system then the 1D hydrogen atom could be regarded as degenerate. But even in this scenario, a close look at the assumptions used in the proof of the nondegeneracy theorem would reveal that it is not strictly applicable to the 1D Coulomb system [55, 80, 81].

We expect the analysis made on the properties of the negative energy eigenstates of the 1D hydrogen atom will prove useful in clarifying some of the misunderstandings that arose in the long-standing history of the problem. We also hope that our discussions will shed some light into the techniques and the mathematical intricacies associated with the solution of this fascinating model.

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Appendix A. Equivalence to free motion on a circle

We show, following Moser and Boya *et al* [26, 52], that the classical 1D Coulomb problem is equivalent to the motion of a free particle on a circle. We proceed by demonstrating that the Hamiltonian of the latter transforms to the Hamiltonian of the former via a stereographic projection and the appropriate change of coordinates. This equivalence exhibits that the two ways of traversing the circle, corresponding to initially moving towards or initially moving away from the singularity are necessarily unconnected. We cannot go smoothly from one to the other or viceversa. Therefore, it is not possible to go through the singularity at the origin.

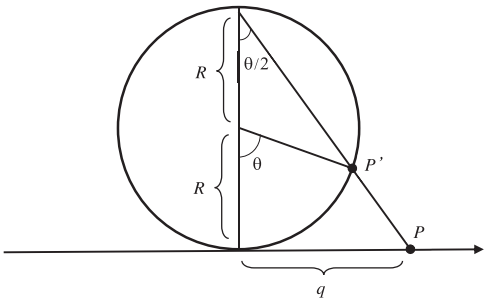

Figure A1. Stereographic projection corresponding to the transformation $q = 2R\tan(\theta/2)$.

The transformation process itself is of good pedagogical value, since it exhibits how various standard techniques and ingenuity play together in order to reach the goal. From our starting point, we first use the Legendre transform, then a rational transformation and finally a reparameterization; giving rise to a sequence of Hamiltonians $H_0 \to H_1 \to H_2$.

Let us start with the free Hamiltonian,

$$H' = \frac{p_\theta^2}{2\mu R^2}, \tag{A.1}$$

which describes the motion of a particle P' with mass μ moving with constant angular velocity $\dot{\theta} \equiv C$ in a circle of radius R. Notice that in this case the energy E' of the system satisfies

$$E' = \frac{\mu R^2 C^2}{2}. \tag{A.2}$$

Consider now the motion of a particle P on the q-axis whose movement is related to that of P' via the stereographic projection depicted in figure A1. Thus we have

$$\dot{q} = R\left(1 + \frac{q^2}{4R^2}\right)C, \tag{A.3}$$

In order to find the corresponding Hamiltonian in the variables (q, p_q) we apply first a Legendre transform $\mathcal{L} = \dot{\theta}p_\theta - H'$ and use equation (A.3) to find

$$\mathcal{L} = \frac{\dot{\theta}^2\mu R^2}{2} = \frac{(\dot{q})^2\mu}{2(1 + q^2/(4R^2))^2}. \tag{A.4}$$

Hence

$$p_q = \frac{\partial\mathcal{L}}{\partial\dot{q}} = \frac{\dot{q}\mu}{(1 + q^2/(4R^2))^2} = \frac{R\mu C}{1 + q^2/(4R^2)}, \tag{A.5}$$

and, by using the inverse Legendre transform $H_0 = \dot{q}p_q - \mathcal{L}$, we obtain

$$H_0 = \frac{(\dot{q})^2\mu}{2(1 + q^2/(4R^2))^2} = \frac{(p_q)^2(1 + q^2/(4R^2))^2}{2\mu}, \tag{A.6}$$

while equation (A.5) implies that $\mathrm{sgn}(p_q) = \mathrm{sgn}(C)$ and, as follows from Hamilton's equations:

$$-\dot{p}_q = \frac{\partial H_0}{\partial q} = \frac{\mu q C^2}{2(1+q^2/4R^2)} = \frac{p_q q C}{2R}. \tag{A.7}$$

We now consider the function

$$H_1 = \sqrt{2\mu R^2 C^2 H_0} - \mu R^2 C^2 = R(1+q^2/4R^2)p_q C - \mu R^2 C^2 \tag{A.8}$$

and observe that it defines a Hamiltonian for the variables (q, p_q) since Hamilton's equations are satisfied:

$$\frac{\partial H_1}{\partial q} = \frac{p_q q C}{2R} = -\dot{p}_q \tag{A.9}$$

$$\frac{\partial H_1}{\partial p_q} = R(1+q^2/4R^2)C = \dot{q}. \tag{A.10}$$

Next, consider the function

$$H_2 = \frac{H_1}{|p_q|} - R|C| \tag{A.11}$$

and recall that $\mathrm{sgn}(p_q) = \mathrm{sgn}(C)$, thus

$$H_2 = \frac{q^2|C|}{4R} - \frac{\mu R^2 C^2}{|p_q|}, \tag{A.12}$$

and notice that it is a Hamiltonian when we use the time variable

$$T = \int |p_q| \, \mathrm{d}t. \tag{A.13}$$

Indeed, under this change of variable we have $q' = \dot{q}/|p_q|$, $p_q{}' = \dot{p}_q/|p_q|$—where the symbol $'$ denotes a derivative with respect to T—and therefore Hamilton's equations hold:

$$\frac{\partial H_2}{\partial q} = \frac{q|C|}{2R} = \frac{1}{|p_q|}\frac{p_q q C}{2R} = -\frac{\dot{p}_q}{|p_q|} = -p_q{}' \tag{A.14}$$

$$\frac{\partial H_2}{\partial p_q} = \frac{\mu R^2 C^2}{|p_q|^2 \,\mathrm{sgn}(p_q)} = \frac{1}{|p_q|}\frac{\mu R^2 C^2}{|p_q|\,\mathrm{sgn}(C)} = \frac{R(1+q^2/4R^2)C}{|p_q|} \tag{A.15}$$

$$= \frac{\dot{q}}{|p_q|} = q'. \tag{A.16}$$

Finally, by taking the canonical transformation $p = q$, $q = -p_q$ we readily obtain from equation (A.12) the Hamiltonian

$$H = \frac{p^2|C|}{4R} - \frac{\mu R^2 C^2}{|q|}, \tag{A.17}$$

which is the 1D Coulomb Hamiltonian of equation (2) where m and e^2 are given by

$$m = \frac{2R}{|C|}, \qquad e^2 = \frac{\mu R^2 C^2}{k}. \tag{A.18}$$

In order to get the relations in equation (14), we notice that the value $E' = \mu R^2 C^2/2$ of the energy for Hamiltonian H' transforms to $E^1 = 0$ for Hamiltonian H_1 and then to $E = -R|C|$ for the 1D Coulomb Hamiltonian. Therefore, relations

$$\frac{m|E|}{2} = R^2, \qquad \frac{ke^2}{E^2} = \mu, \tag{A.19}$$

which are equation (14), follow.

Appendix B. Deficiency indices theorem

Given a symmetric operator H, consider the following subspaces:

$$K_+ = \{\psi \in D(H) : \text{there is an eigenvalue of } H \text{ with } \mathrm{Im}(z) > 0\}, \tag{B.1}$$

$$K_- = \{\psi \in D(H) : \text{there is an eigenvalue of } H \text{ with } \mathrm{Im}(z) < 0\}, \tag{B.2}$$

whose dimensions are the corresponding *deficiency indices* of H:

$$n_+ = \dim\ K_+, \qquad n_- = \dim\ K_-. \tag{B.3}$$

Since self-adjoint operators have only real eigenvalues, it is clear that the spaces $K^{\pm}$ give a measure of how much the operator H fails to be self-adjoint, hence the terms deficiency space and deficiency index. The precise statement that the fundamental theorem that relates deficiency indices and self-adjoint extensions is follows:

Theorem [82]: let H be a densely defined and closed symmetric (Hermitian) operator and $H^\dagger$ its adjoint. Then the following holds:

(a) If $n_+ = n_- = 0$ then H is self-adjoint.
(b) If $n_+ = n_- = n$, with $1 \leqslant n < \infty$, then H has infinitely many self-adjoint extensions H_U parameterized by $n \times n$ unitary matrix maps $U : K_+ \to K_-$.
(c) If $n_+ \neq n_-$, then H is not self-adjoint and it has no self-adjoint extensions.

Furthermore, if (b) holds then for each choice of U, $D(H) \subset D(H_U) \subset D(H^\dagger)$, where $D(H_U)$ is given by

$$D(H_U) = \{\phi + \psi_+ + U\psi_+ \ : \ \phi \in D(H) \text{ and } \psi_+ \in K^+\}. \tag{B.4}$$

In the case of the 1D Coulomb Hamiltonian discussed here, U is a 2×2 unitary matrix, and different choices of this matrix gives different self-adjoint extensions. The matrix U that corresponds to the Dirichlet boundary condition $\psi(0) = 0$ is the identity matrix $I_{2\times 2}$, as can be verified in [68].

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