The one-dimensional hydrogen atom in momentum representation

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Abstract A momentum representation treatment of the one-dimensional hydrogen atom with Coulomb interaction is presented. We obtain the energy levels and bound-state eigenfunctions for the problem and discuss the general properties of the solution. The energy spectrum is discrete and given by the Balmer formula. We show that, despite the symmetry of the potential, it is impossible to find eigenfunctions with definite parity for the system.

Resumen El problema del átomo de hidrógeno unidimensional con interacción Coulombiana se resuelve en la representación de momentos. Se obtienen los niveles de energía, las eigenfunciones de los estados ligados del problema y se discuten sus principales propiedades. El espectro de energías es discreto y se calcula de la fórmula de Balmer. Demostramos que, a pesar de la simetría del potencial, no hay eigenestados con paridad definida en el sistema.

1. Introduction

The one-dimensional hydrogen atom with Coulomb interaction

$$V(x) = -e^2/|x| \qquad (1)$$

has been the subject of various discussions (Loudon 1959, Andrews 1966, 1976, 1981, Haines and Roberts 1969, Gomes and Zimerman 1980, 1981) since the solution given by Loudon (1959). The interest generated by this problem stems not only from the peculiar features of its solution or its possible pedagogical value but also by its diverse physical applications; for example in the theory of excitons (Elliot and Loudon 1960) or atoms (Landau and Lifschitz 1977) in high magnetic fields, or for modelling the interaction of electrons with the surface of liquid helium (Cole and Cohen 1969).

Loudon (1959) claimed that the ground state of the one-dimensional hydrogen atom is a strongly localised even state of infinite binding energy, and that the energy spectrum of the excited states is given by the Balmer formula, as in the three-dimensional case. Andrews (1966) has questioned the existence of the infinite-energy ground state and has proved that it is unobservable. Loudon also claimed that the Balmer energy levels of the system are twofold degenerate and he associated with each level an eigenfunction of even parity and another of odd parity. This result contradicts the well known theorem of the nondegeneracy of the energy levels in the discrete spectrum of a one-dimensional system (for a proof see Landau and Lifschitz (1977)). In fact, in Loudon's treatment the degeneracy of the levels appears to be a necessary consequence of the parity of the Coulomb potential.

Loudon's conclusions have been challenged by Haines and Roberts (1969) who obtained instead nondegenerate energy levels, with odd eigenfunctions (the same as Loudon's) belonging to the discrete Balmer spectrum but with even eigenfunctions (different from Loudon's) associated with a continuum of negative-energy eigenvalues. These results have been criticised by Andrews (1976) on the basis of general considerations on the admissible eigenfunctions for one-dimensional potentials with non-integrable singularities, as is the case of the Coulomb potential. Gomes and Zimerman (1980, 1981) also have questioned the validity of the even solutions of Haines and Roberts. More recently Spector and Lee (1985) have suggested that the

infinite-energy ground state obtained by Loudon might still exist since – they argue – there is not a definitive proof to the contrary. Spector and Lee (1985) solved the Klein–Gordon version of the relativistic one-dimensional hydrogen atom; they found a ground state with an energy of the order of the rest-mass energy of the electron. Therefore they concluded that a relativistic treatment removes the infinite binding energy for the ground state of the system.

In this paper we give a solution for the bound states of the nonrelativistic one-dimensional hydrogen atom using the momentum representation. This treatment gives some insights into the unusual features of the solution to the problem. In contrast to previous treatments, we show that the only acceptable eigenstates of the system are those corresponding to the finite-energy Balmer levels.

The origin of all the peculiarities in the behaviour of the system is the singularity of the potential at $x = 0$. As we shall see the singularity acts as an impenetrable barrier for the electrons. This property will lead us to the conclusion that, despite the overall symmetry of the problem, the one-dimensional hydrogen atom does not admit eigenstates of definite parity. This surprising result is a strong argument against the validity of the previously reported solutions to the problem. It happens as if the singularity in the one-dimensional Coulomb potential has produced a 'spontaneous breaking' of the reflection symmetry of the system.

Finally we shall also briefly discuss the apparent breakdown of the nondegeneracy theorem in this and similar one-dimensional systems.

2. Solution in momentum representation

The Schrödinger equation in coordinate representation for an electron moving in the one-dimensional Coulomb potential has the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - \frac{e^2}{|x|}\psi(x) = E\psi(x). \tag{2}$$

To transform equation (2) to momentum space, we must recall that in this representation the operator $\hat{x}^{-1}$ is given by (Constantinescu and Magyari 1971)

$$\frac{\hat{1}}{x} \rightarrow \frac{i}{\hbar}\int_{-\infty}^{p} \ldots dp' \tag{3}$$

as can be seen almost directly from the p-space correspondence

$$\hat{x} \rightarrow i\hbar\, d/dp. \tag{4}$$

If we write equation (2) for the regions $x > 0$ and $x < 0$ separately then, using equation (3), we can write the Schrödinger equation in the momentum representation as a pair of Volterra integral equations:

$$\frac{p^2}{2m}\varphi_+(p) + \frac{ie^2}{\hbar}\int_{-\infty}^{p} \varphi_+(p')dp' = E\varphi_+(p) \tag{5a}$$

and

$$\frac{p^2}{2m}\varphi_-(p) - \frac{ie^2}{\hbar}\int_{-\infty}^{p} \varphi_-(p')dp' = E\varphi_-(p). \tag{5b}$$

The momentum-space wavefunctions φ_- and φ_- are related to the coordinate-space wavefunctions by

$$\psi_\pm(x) = (2\pi\hbar)^{-1/2}\int_{-\infty}^{+\infty} \exp(ipx/\hbar)\varphi_\pm(p)dp, \tag{6}$$

where the coordinate-space function $\psi_+(x)$ $(\psi_-(x))$ corresponds to the solution of the eigenvalue problem equation (2) to the right (left) of the origin. In other words ψ_- (ψ_-) is defined only for $x \geqslant 0$ $(x \leqslant 0)$, while the functions φ_+ and φ_- are defined in the entire range of p values, from $-\infty$ to $+\infty$. The main problem encountered in previous treatment of the problem (Loudon 1959, Haines and Roberts 1969, Gomes and Zimerman 1980, 1981, Andrews 1981) has been how to join ψ_+ and ψ_- at $x = 0$. The solutions proposed to this by different authors are the origin of the disagreements on whether the system has only odd eigenfunctions or whether it also has even eigenfunctions with the same energy. One of the advantages of working in momentum representation is that it is not necessary to worry about the appropriate value which ψ or its derivative must have at the origin to obtain the energy eigenvalues and eigenfunctions of the problem.

Note that under complex conjugation, equation (5a) is transformed into equation (5b) and vice versa. This is equivalent to saying that the replacement

$$\varphi_\pm(p) \rightarrow \varphi_\mp^*(p) \tag{7}$$

leaves the Schrödinger equation unchanged.

We are interested in the negative-energy eigenvalues of equations (5) so, following Loudon, we introduce a dimensionless real parameter α through the relation

$$E = -\hbar^2/2ma_0^2\alpha^2, \tag{8}$$

where a_0 is the Bohr radius ;

$$a_0 = \hbar^2/me^2. \tag{9}$$

We also define a dimensionless momentum variable k by

$$k = pa_0/\hbar. \tag{10}$$

Using the new variables, equations (5) become

$$(1 + \alpha^2 k^2)\varphi_\pm(k) \pm i2\alpha^2\int_{-\infty}^{k} \varphi_\pm(k')dk' = 0. \tag{11}$$

According to the above equation, the only solutions for $\alpha = 0$ vanish identically: $\varphi_\pm(k) = 0$, which means that Loudon's infinite-energy ground state is not allowed. To solve those equations we differentiate them and we get for $\varphi_\pm$ two very simple differential equations

$$\frac{d\varphi_\pm}{dk} + \frac{2(k \pm i)}{k^2 + \alpha^{-2}}\varphi_\pm = 0. \tag{12}$$

The solutions of these differential equations may be written as

$$\varphi_{\pm}^{\alpha}(k) = \frac{\alpha^2 A_{\pm}}{(1 + \alpha^2 k^2)} \left(\frac{1 \mp i\alpha k}{1 \pm i\alpha k} \right)^{\alpha}, \qquad (13)$$

where the $A_{\pm}$ are integration constants.

As they stand in equation (13), φ_{+}^{α} and φ_{-}^{α} are in general multiple-valued functions of k and thus they are unsuitable as eigenfunctions for the problem. It is only when α takes integer values that the functions $\varphi_{\pm}^{\alpha}$ become single-valued (Churchill 1960). But the $\alpha = 0$ value is not allowed because the functions vanish identically in such a case as we said above, while negative integer values of α merely interchange the roles of φ_{+}^{α} and φ_{-}^{α}, and it is not necessary to take those values into account separately. It is apparent then, that appropriate bound-state eigenfunctions can be formed only when α is a positive integer

$$\alpha = n, \qquad n = 1, 2, 3, \ldots . \qquad (14)$$

The energy eigenvalues are then given by the Balmer formula

$$E_n = -\frac{1}{2} \frac{e^2}{a_0} \frac{1}{n^2}, \qquad (15)$$

and the normalised eigenfunctions corresponding to the nth energy level are

$$\varphi_{+}^{n}(p) = (2a_0 n/\pi\hbar)^{1/2} [1 + (npa_0/\hbar)^2]^{-1}$$
$$\times \left(\frac{1 - i(npa_0/\hbar)}{1 + i(npa_0/\hbar)} \right)^{n}, \qquad (16a)$$

Figure 1 Plots of the real and imaginary parts of the momentum-space wavefunctions: Re $\varphi_{-}^{1}(p)/\varphi_{+}^{1}(0)$ (broken curve), Im $\varphi_{+}^{1}(p)/\varphi_{+}^{1}(0)$ (dotted curve), Re $\varphi_{+}^{2}(p)/\varphi_{+}^{1}(0)$ (chain curve), and Im $\varphi_{+}^{2}(p)/\varphi_{+}^{1}(0)$ (full curve) plotted against $k = pa_0/\hbar$, where $\varphi_{+}^{1}(0) = (2a_0/\pi\hbar)^{1/2}$. Note the relations Re φ_{+}^{n} = Re φ_{-}^{n} and Im φ_{+}^{n} = Im φ_{-}^{n}.
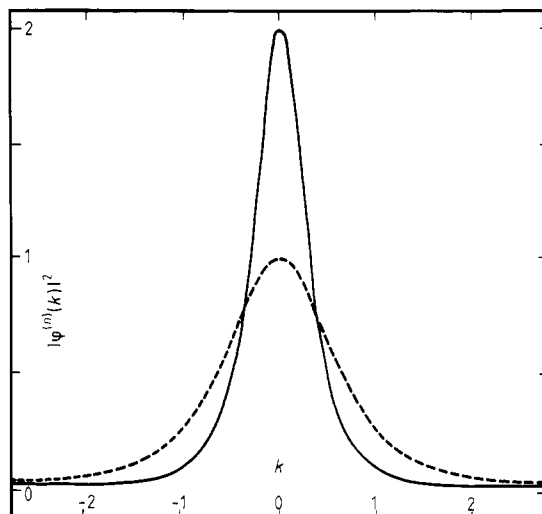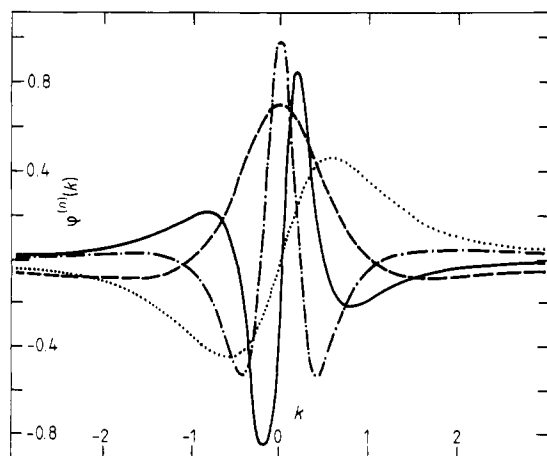
Figure 2 Plots of the probability densities in momentum-space against $k = pa_0/\hbar$: $|\varphi_{+}^{1}/\varphi_{+}^{1}(0)|^2$ (broken curve), $|\varphi_{-}^{2}/\varphi_{+}^{1}(0)|^2$ (full curve). The relation $|\varphi_{+}^{n}(p)|^2 = |\varphi_{-}^{n}(p)|^2$, which is valid for all n, is one of the manifestations of the 'broken reflection symmetry' in the system.

and

$$\varphi_{-}^{n}(p) = (2a_0 n/\pi\hbar)^{1/2} [1 + (npa_0/\hbar)^2]^{-1}$$
$$\times \left(\frac{1 + i(npa_0/\hbar)}{1 - i(npa_0/\hbar)} \right)^{n}. \qquad (16b)$$

The real and imaginary parts of the first two momentum-space eigenfunctions are shown in figure 1, and the corresponding probability densities in figure 2.

It can be argued that φ_{+} or φ_{-} alone do not describe completely the stationary states of the one-dimensional hydrogen atom. For φ_{+} describes an electron moving to the right of the singularity whereas φ_{-} describes its motion only to the left of it. Nevertheless since the motion of an electron in one of those regions is not affected by what happens in the other region, the functions φ_{+} and φ_{-} must be regarded as complete eigenfunctions of the system. This will be shown in § 4.

3. Properties of the eigenfunctions

The results we obtained in § 2 show that neither Loudon's ground state nor the even-parity wavefunctions of Haines and Roberts appear in the momentum-space solution. The reason for the inadequacy of such functions for describing eigenstates of the system is the presence of the pole in the Coulomb potential, as we will show below.

Notice that the momentum-space eigenfunctions $\varphi_{\pm}^{n}$ are not parity eigenstates but 'mirror images' of each other. For, if $\hat{P}$ is the parity operator we have

$$\hat{P}\varphi_{\pm}^{n} = \varphi_{\mp}^{n}. \qquad (17)$$

We also can prove easily that the $\varphi_{\pm}^{n}$ satisfy

$$\int_{-\infty}^{+\infty} \varphi_{\pm}^{n}(p)\, dp = 0. \tag{18}$$

In the coordinate representation equation (18) means that all acceptable eigenfunctions must vanish at the origin, i.e.

$$\psi_{\pm}^{n}(x)\Big|_{x=0} = 0. \tag{19}$$

So the momentum-space solution has given us the correct boundary condition to be imposed in coordinate space. This is the boundary condition used by Loudon (1959).

In fact equation (18) (and hence equation (19)) turns out to be the only one compatible with the singular nature of the Coulomb potential. This point is rather delicate, for if these conditions are not satisfied then the Hamiltonian operator becomes non-hermitian with respect to its own set of eigenstates (Andrews 1976). In their solution to the problem Haines and Roberts did not recognise this fact and they were led to the erroneous conclusion of the existence of a continuum of negative-energy eigenvalues.

Equation (18) is very strong. For example it implies that if we have the system in an arbitrary (possibly non-stationary) state Φ, the net particle flux crossing through the origin from one side of the singularity to the other is always zero. For, as Φ can always be expressed as a linear combination of the eigenfunctions, and all of these vanish at the origin, Φ must vanish there too. So the flux

$$j = \frac{i\hbar}{m}\left(\Phi\frac{\partial\Phi^{*}}{\partial x} - \Phi^{*}\frac{\partial\Phi}{\partial x}\right)$$

must certainly vanish at $x=0$. Thus the singularity of the Coulomb potential at the origin acts as an impenetrable potential barrier for the electron. The mathematical expression of this fact is the boundary condition (19).

Physically, this means that if we have an electron moving on the right (left) of the singularity it will remain confined there forever. With this in mind we can proceed to calculate the coordinate-space counterparts of $\varphi_{\pm}^{n}$. Using equations (16) in equation (6) and evaluating the resulting integrals by contour integration, we get:

$\psi_{+}^{n}(x)$

$$= \begin{cases} \left(\dfrac{4}{a_0^3 n^3}\right)^{1/2}(-1)^{n-1}x L_{n-1}^{1}\left(\dfrac{2x}{na_0}\right)\exp\left(\dfrac{-x}{na_0}\right) & \text{if } x>0 \\ 0 & \text{if } x\leqslant 0 \end{cases}$$

$$\tag{20a}$$

$\psi_{-}^{n}(x)$

$$= \begin{cases} 0 & \text{if } x\geqslant 0 \\ \left(\dfrac{4}{a_0^3 n^3}\right)^{1/2}(-1)^{n}x L_{n-1}^{1}\left(\dfrac{2x}{na_0}\right)\exp\left(\dfrac{+x}{na_0}\right) & \text{if } x<0 \end{cases}$$

$$\tag{20b}$$

where $L_{n-1}^{1}(z)$ are the associated Laguerre polynomials (Ederlyi 1953). These are the coordinate-space eigenfunctions of the one-dimensional hydrogen atom.

It must be noted that the set of functions ψ_{+}^{n} form a basis for the 'right-states' of the system; any wavefunction vanishing on the left can be expanded using the eigenfunctions (20a). Similarly the ψ_{-}^{n} form a basis for the 'left-states' of the system (Higgins 1977).

At this point one may be tempted to try to match ψ_{+}^{n} with ψ_{-}^{n} at $x=0$ to obtain eigenfunctions valid in all coordinate space or to obtain parity eigenstates. However we shall prove in the next section that any such attempt is futile.

4. Parity and degeneracy

The reflection invariance of the Coulomb potential may lead us to expect the existence of a complete set of simultaneous eigenfunctions of both energy and parity for the problem. This conclusion is, however, wrong for the one-dimensional hydrogen atom as we will show in this section.

From the eigenfunctions $\varphi_{\pm}^{n}$ we can easily construct parity eigenstates:

$$\begin{aligned} \varphi_{e}^{n} &= 2^{-1/2}(\varphi_{+}^{n} + \varphi_{-}^{n}) \\ \varphi_{o}^{n} &= 2^{-1/2}(\varphi_{+}^{n} - \varphi_{-}^{n}). \end{aligned} \tag{21}$$

The coordinate-space counterparts of φ_{e}^{n} and φ_{o}^{n} are easily seen to be

$$\begin{aligned} \psi_{e}^{n} &= 2^{-1/2}(\psi_{+}^{n} + \psi_{-}^{n}) \\ \psi_{o}^{n} &= 2^{-1/2}(\psi_{+}^{n} - \psi_{-}^{n}). \end{aligned} \tag{22}$$

Equations (22) correspond to the finite-energy eigenfunctions obtained by Loudon (1959).

However equations (21) and (22) do not represent physically realisable states of the system. In fact, φ_{e}^{n} and φ_{o}^{n} are not even solutions of the eigenvalue problem. The reason for this result is very clear, as equations (11) and (12) are first-order equations and, for a given n value, they admit only one independent solution. Any linear combination of the φ_{+}^{n} with the φ_{-}^{n} is not a solution to the problem. Physically the reason can be traced back to the impenetrability of the Coulomb potential. It is interesting to see how this result can be proved in the coordinate representation. Since, except for ψ_{e}^{n} at $x=0$, both ψ_{e}^{n} and ψ_{o}^{n} satisfy the Schrödinger equation of the problem and it is not readily apparent why ψ_{e}^{n} and ψ_{o}^{n} are not valid eigenstates for the system.

Suppose we accept ψ_{e}^{n} and ψ_{o}^{n} as two distinct realisable states of the one-dimensional hydrogen atom, then those states must be independent. However it is easy to see that the Wronskian determinant

$$W(\psi_{e}^{n}, \psi_{o}^{n}) = \psi_{e}^{n\prime}\psi_{o}^{n} - \psi_{o}^{n\prime}\psi_{e}^{n} \tag{23}$$

always vanishes. This implies that the functions ψ_{e}^{n} and ψ_{o}^{n} are not independent and therefore that, contrary to our assumption, they cannot describe different states of the system.

Viewed from another angle, the vanishing of $W(\psi_e^n, \psi_o^n)$ implies that we cannot distinguish between the states ψ_e^n and the states ψ_o^n. It is clear then that the relative phase of the components along the left and right eigenstates of the state described by ψ_e^n or ψ_o^n, is intrinsically irrelevant. Any form of matching ψ_+^n with ψ_-^n is therefore entirely devoid of physical meaning.

The conclusion is then unavoidable: the one-dimensional hydrogen atom has no eigenstates with definite parity. The singularity of the potential produces a 'spontaneous symmetry breaking'. The symmetry of the potential is reflected in the invariance properties expressed by equations (7) or (17), not in the parity of the eigenfunctions.

As we have seen, the eigenfunctions ψ_+^n and ψ_-^n both correspond to the same energy spectrum, the energy levels appear to be twofold degenerate. But the above discussion also accounts for the apparent degeneracy of the energy levels. For it allows us to consider the right and left regions of the problem as independent. We may say then that we are dealing with two one-dimensional problems simultaneously and since in each of them not all energy eigenstates are degenerate, we cannot say that there is a strict violation of the nondegeneracy theorem. It is only if we insist on thinking of both systems as parts of a larger system that 'degeneracy' appears.

Notice that the previous argument is applicable equally well to all the symmetric one-dimensional systems with 'degenerate' bound states, for the general characteristic of such systems is to have the coordinate space available to the particles very constrained, either by infinite barriers, as in the well known example of a pair of infinitely deep square wells of finite width, or by a singular potential that has the effect of an impenetrable barrier, as in the problem dealt with here.

5. Summary

The momentum-space solution for the one-dimensional hydrogen atom given in this paper has provided very interesting insights which help one to understand the origin of the characteristic difficulties associated with this system. The singularity at the origin in the one-dimensional Coulomb potential is the cause of these difficulties. The existence of this singularity imposes severe restrictions on the eigen-functions of the system. The allowed eigenfunctions must vanish at the origin. Both the one-dimensional and three-dimensional hydrogen atoms have the same energy spectrum.

We have shown that the previously reported solutions cannot be considered as correct. All of them are based on the untenable assumption that the eigenfunctions of the system can be chosen as parity eigenstates. We have here a curious example of a symmetric Hamiltonian for which the stationary states cannot be classified according to parity. Parity is not a good quantum number for the one-dimensional hydrogen atom. This is a consequence of the restrictions in the domain of hermiticity of the Hamiltonian imposed on the system by the singular nature of the Coulomb potential. A more complete explanation of this result will be published elsewhere (Núñez Yépez *et al* 1987).

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