Relativistic one-dimensional hydrogen atom in momentum representation

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Abstract. The solution of the one-dimensional relativistic Klein–Gordon equation in the momentum representation for a particle in the H atom potential is presented. The eigenfunctions and the energy levels of bound states are found. In the non-relativistic limit, the energy of the particle is given by the Balmer formula. The eigenfunctions are found to be finite sums over poles along the imaginary axis in the complex plane.

Resumen. Se resuelve la ecuación de Klein–Gordon monodimensional para una partícula relativista moviéndose en el potencial del atomó de hidrógeno. Se han encontrado las autofunciones y los niveles de energía de los estados ligados. En el límite no relativista, la energía de la partícula viene dada mediante la fórmula de Balmer. Las autofunciones se pueden expresar como sumas finitas de polos, que se encuentran en el eje imaginario del plano complejo.

1. Introduction

Physics in one dimension (1D) may be used as a guide to more complex three-dimensional (3D) problems. Frequently 1D quantum mechanical problems allow analytical solutions, while the corresponding 3D equations have to be solved by numerical methods, as occurs for instance in the Kronig–Penney and Ising models. One of the more relevant 1D problems is that of the hydrogen atom (Loudon 1959) because of its numerous physical applications, i.e. impurities and excitons in semiconductors, quantum well structures and hydrogen atoms in strong magnetic fields. Nevertheless this problem, that could be thought of as easy, has become polemic due to the possible existence of degenerate levels and of a ground state with an infinite binding energy (Moss 1987, Hammer and Weber 1988).

Recently, it has been proved (Núñez Yepes *et al* 1987) that the ground state energy is finite and it is not possible to find states with definite parity, in spite of the symmetry of the potential $-1/|x|$. They claim that the discontinuity at $x \to 0$ plays the role of an infinite barrier, which breaks the space into two independent regions. Thus, an electron moving in the right (or left) region will remain there indefinitely.

The 1D hydrogen atom has also been studied using the relativistic treatment (Spector and Lee 1985, Moss 1987) with the Klein–Gordon equation in the position representation. Spector and Lee have found states with definite parity and a ground-state energy of the same order as the particle rest mass energy; however, Moss has shown that the corresponding solution is unacceptable. On the other hand, Lapidus (1983b) has used the Dirac equation with a delta-function potential, and obtained a finite energy for the only bound state. Nevertheless, the relativistic treatment of the delta potential exhibits some ambiguities, as Calkin *et al* (1987) have pointed out in a recent work. Moreover, no bound state solutions of the 1D Dirac equation for the Coulomb potential are found (Moss 1987, Domínguez-Adame 1990).

The momentum representation can be very useful in quantum mechanics, although it has been used almost exclusively in scattering problems. The 3D non-relativistic Coulomb problem was originally solved in the momentum representation by Podolsky and Pauling (1929), taking the Fourier transform of the eigenfunctions in the position representation. Six years later, Fock (1935) found the solution by solving the Schrödinger equation directly in momentum representation. In both cases, the momentum eigenfunctions were expressed in terms of Gegenbauer polynomials. The Dirac equation was also solved in momentum representation for the 3D hydrogen atom (Rubinowicz 1948, Lévy 1950). Recently, Lombardy has reviewed and discussed this problem in both non-relativistic (Lombardy 1980) and relativistic

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(Lombardy 1983) cases. He has found that the radial functions are finite sums over poles in the complex plane.

The non-relativistic 1D hydrogen atom was first studied in the momentum representation by Lapidius (1983a), assuming a δ interaction potential. Lately, the potential $-1/|x|$ has been analysed in an elegant way by Núñez Yepes *et al* (1987), solving the integral Schrödinger equation in momentum representation. As far as we know the analogous relativistic problem remains open in the literature.

In this paper the eigenfunctions of a relativistic particle in the potential $-1/|x|$ are found, solving the Klein–Gordon equation directly in the momentum representation. The particle energy is the same as that reported by Moss (1987). Also we calculate the non-relativistic limit in agreement with the results from Núñez Yepes *et al*.

2. Klein–Gordon equation in momentum representation

Let us consider a relativistic particle without spin, moving under the action of the potential

$$V(x) = -Ze^2/|x| \tag{1}$$

so the particle satisfies the 1D Klein–Gordon equation (Schiff 1965)

$$\frac{d^2\psi(x)}{dx^2} + \left\{-\lambda^2 + \frac{2EZ\alpha}{\hbar c}\frac{1}{|x|} + \frac{Z^2\alpha^2}{x^2}\right\}\psi(x) = 0. \tag{2}$$

The parameters appearing in this equation are $\alpha = e^2/\hbar c$, $\lambda = (mc/\hbar)(1-\varepsilon^2)^{1/2}$ and $\varepsilon = E/mc$. We are looking for the bound states, thus we have the condition $\varepsilon < 1$, and then λ is a real parameter.

Solutions of equation (2) in momentum representation are given by the Fourier transform

$$\varphi_\pm(p) = (2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty} dx \exp(-ipx/\hbar)\psi_\pm(x)$$

where the upper (lower) sign refers to $x > 0$ $(x < 0)$, i.e. ψ_+ (ψ_-) vanishes for $x \leqslant 0$ $(x \geqslant 0)$. This is consistent with the fact mentioned above that the left and the right regions are independent. To determine the Klein–Gordon equation governing $\varphi_+(p)$, we make the following operator replacements,

$$\frac{\hat{1}}{x} \to -\frac{i}{\hbar}\int_{-\infty}^{p} dp'$$

and

$$\frac{\hat{1}}{x^2} \to -\frac{1}{\hbar}\int_{-\infty}^{p} dp' \int_{-\infty}^{p'} dp''$$

so equation (2) becomes

$$(p^2/\hbar^2 + \lambda^2)\varphi_\pm(p) \pm (2iZ\alpha E/\hbar^2 c)\int_{-\infty}^{p} dp'\varphi_\pm(p')$$
$$+ (Z^2\alpha^2/\hbar^2)\int_{-\infty}^{p} dp'\int_{-\infty}^{p'} dp''\varphi_\pm(p') = 0. \tag{3}$$

For the sake of simplicity, we introduce the notation $q = pa_0/Z\varepsilon\hbar$, $a_0 = \hbar^2/me^2$ being the Bohr radius, and $v = Z\varepsilon/\lambda a_0$. By differentiating twice with respect to the new variable q, we get the following second-order differential equation

$$\left\{(1 + v^2q^2)\frac{d^2}{dq^2} + 2v^2(2q \pm i)\frac{d}{dq} + v^2(2 + Z^2\alpha^2)\right\}\varphi_\pm(q) = 0. \tag{4}$$

In order to find the regular solutions of this equation, it is convenient to replace q by the variable $\xi = 2/(1 \pm ivq)$ so that

$$\left\{(\xi - 1)\xi^2\frac{d^2}{d\xi^2} + (2 - v\xi)\xi\frac{d}{d\xi} - (2 + Z^2\alpha^2)\right\}\varphi_+(\xi) = 0.$$

Using the series solution

$$\varphi_\pm(\xi) = \sum_{k=0}^{\infty} a_k \xi^{k+s+1} \qquad a_0 \neq 0$$

where s is a parameter to be determined, we obtain the following recurrence relation

$$a_k = [(k+s)(k+s-v-1)/k(k+2s-1)]a_{k-1}$$

choosing $s = \frac{1}{2} \pm (\frac{1}{4} - Z^2\alpha^2)^{1/2}$. As Moss has pointed out, the corresponding solution for the smaller value of s is unacceptable, so we must take the upper sign. The general expression for the expansion coefficients is found by successive use of the recurrence relation

$$a_k = \frac{(s+1)_k(s-v)_k}{k!\,(2s)_k}a_0 \tag{5}$$

where the Pochhammer's symbol is defined $(a)_0 = 1$ and $(a)_k = \Gamma(a+k)/\Gamma(a) = a(a+1)\ldots(a+k-1)$.

The quantum condition $v - s = n$, being a non-negative integer, arises from the requirement that $\varphi_\pm(q) \to 0$ as $p \to 0$. Thus remembering the relation between v and ε, we obtain the energy of the particle as

$$E_n = mc^2[1 + Z^2\alpha^2/(n+s)^2]^{-1/2}$$
$$n = 0, 1 \ldots. \tag{6}$$

The eigenfunctions of the relativistic particle in momentum representation are

$$\varphi_\pm(p) = A_\pm \sum_{k=0} \frac{(-n)_k(s+1)_k}{k!\,(2s)_k}\left(\frac{2}{1 \pm ip/\lambda\hbar}\right)^{k+s+1} \tag{7}$$

where $A_\pm$ are the normalisation constants. Similar expressions are found for the relativistic 3D hydrogen atom in momentum representation by Lombardi (1983) with the aid of the Dirac equation.

3. Non-relativistic limit

It is interesting to look for the limiting case $c \to \infty$ of our previous results, so that $Z^2\alpha^2 \ll 1$. For this situation, we can set $s = 1$ and $\nu = n + 1 = 1, 2 \ldots$. Taking into account the well known result (Abramowitz and Stegun 1964)

$$\sum_{k=0}^{\nu-1} \frac{(1-\nu)_k}{k!} z^k = (1-z)^{\nu-1}$$

and the expression (7), the non-relativistic eigenfunctions become

$$\varphi_\pm(q) = \frac{A_\pm}{(1+\nu^2 q^2)} \left(\frac{1 \mp i\nu q}{1 \pm i\nu q} \right)^\nu \qquad \nu = 1, 2 \ldots$$

which is the solution obtained by Núñez Yepes *et al* (1987). In this case, the energy of the particle can be found by expanding equation (6) to first order in $Z^2\alpha^2$, and then we get the usual Balmer formula

$$E - mc^2 \simeq -mc^2 Z^2 \alpha^2 / 2\nu \qquad \nu = 1, 2 \ldots.$$

This result is in contradiction to that of Spector and Lee (1985) who find a ground-state energy of the order of the rest mass energy of the particle. However, our expression (6) for the particle energy, with $s = \frac{1}{2} + (\frac{1}{4} - Z^2\alpha^2)^{1/2}$, gives the correct non-relativistic limit.

4. Conclusions

The relativistic 1D hydrogen atom can be solved directly in momentum representation, by means of the Klein–Gordon equation. The ground-state energy is found to be finite and is given by $E = mc^2 - \frac{1}{2}mc^2 Z^2\alpha^2 + O(\alpha^4)$. The Schrödinger equation results are recovered in the non-relativistic limit. The eigenfunctions in momentum representation have poles $\pm imc(1 - \varepsilon^2)^{1/2}$ along the imaginary axis, and can be expressed as sums over poles up to order $n + s + 1$ in the complex plane.

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