

An $su(1, 1)$ algebraic method for the hydrogen atom

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Abstract

An algebraic solution for the hydrogen atom analogous to the one recently proposed to solve the relativistic version of the system is presented. We add to the usual radial description of the problem an additional angular variable and an associated operator which can be considered as part of an $su(1, 1)$ Lie algebra. The operators of the algebra define radial ladder operator relating the eigenfunctions of the system in unit steps of the principal quantum number. We conclude that the radial bound states of the hydrogen atom in our extended configuration space can be regarded as spanning the minimal M representation of the $su(1, 1)$ Lie algebra. The method can also be extended to solve the s-wave Morse problem and the three-dimensional harmonic oscillator.

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1. Introduction

Algebraic methods are widely used in physics, especially for studying the hydrogen atom in both the relativistic and non-relativistic descriptions [1–20]. In the non-relativistic case, the history of algebraic methods is particularly long, probably beginning with the 1926 paper by Pauli [1]. Today there are many works devoted to the symmetries of the non-relativistic Coulomb problem described by means of $O(4)$, $SU(2) \otimes SU(2)$ or even $SO(2, 1)$ group representations [21–23]. Also, there are some works based in non-compact (de Sitter) group representations, such as [24–27]. Comparison of the technique used in this paper with that in [21] is interesting, because they use shift operators of the angular

momentum l for the radial hydrogen atom wavefunctions with fixed principal quantum number N , whereas we use shift operators of the radial wavefunctions with fixed angular momentum l .

As is known, in the hydrogen atom the spherical symmetry of the problem accounts for the magnetic quantum number, m , degeneracy of its energy spectrum but offers no clue on the degeneracy in the angular momentum quantum number, l . Such an extra degeneracy is explained by the dynamical $SO(4)$ symmetry of the bound problem as discovered by Fock [2]. In the Dirac relativistic description the system possesses an $SO(2, 1)$ symmetry [15] which explains, on taking into account the Johnson–Lippmann constant [20], all the degeneracies of the spectrum.

Also in classical mechanics the remarkable symmetries of the Kepler orbits completely determine the Newtonian gravitational potential as Bertrand's theorem makes evident [28, 29]. Symmetries, even partial or approximate ones, are crucial for understanding the spectrum and properties of hydrogen-like or Rydberg atoms, and for devising approximation techniques for the corresponding perturbed systems [29–32].

The purpose of this work is to present an algebraic method for solving the bounded part of the non-relativistic hydrogen atom. Our approach is based on the $su(1, 1)$ symmetry of the extended radial part of the problem—we call it extended because we add an angular variable, a phase, to the usual description. The method is analogous to the spectrum generating algebra used for solving certain quantum problems [23]. We can summarize the approach as follows. We write the radial part of the Schrödinger equation as an eigenvalue equation for the Casimir operator of the Cartan Lie algebra of $su(1, 1)$. The radial Hamiltonian of the problem is then transformed in such a way that the eigenvalues of the resulting operator are the same as those of the squared angular momentum $l(l + 1)$. So, the radial part of the Schrödinger equation is related to the quantum number l instead of to the principal quantum number, N , as is customarily done [21]. The realization of the elements of the algebra is done in terms of two linear first-order differential operators acting on $\mathcal{R} \times S^1$. The space \mathcal{R} is related to the radial coordinate whereas the eigenvalues of the operator acting over S^1 are related with the discrete energy eigenvalues of the Hamiltonian.

We further remark that we use a two-dimensional realization of the $su(1, 1)$ Lie algebra instead of the more common one-dimensional one [33]. This algebra is shown to be spanned by two shift operators \mathfrak{E}_{\pm} , plus an additional phase-related operator \mathfrak{E}_3 (see equation (7)), both of which add an extra angular variable to the system and close the two-dimensional algebra [14, 33, 34]. The operators \mathfrak{E}_{\pm} are then shown to be ladder operators for the problem, which, after fixing the Casimir eigenvalue, (which turns out to be $l(l + 1)$ the same as the eigenvalues of the angular momentum \mathbf{J}^2), and finding the base states of the algebra, allows us to obtain both the energy spectrum and the bound state radial eigenfunctions of the non-relativistic hydrogen atom. We thus conclude that the radial bound states of the hydrogen atom in the extended configuration space we use span the so-called minimal M representation of the aforementioned algebra [34].

The method discussed here can be applied to other quantum systems such as the three-dimensional oscillator, the Morse potential and the relativistic hydrogen atom [4] and allows making contact with developments in quantum optics and in the study of squeezed and coherent states of hydrogenic atoms and all of their applications [33, 35–38]. As the theory of hydrogen-like atoms is useful in condensed matter [39, 40] our results could be of interest there. On the other hand, they can help making contact with dynamical symmetry group techniques which are useful in atomic and molecular physics calculations [10, 41], and it may, possibly, be also applied to the study of ionization states [42] by using non-discrete representations of the $su(1, 1)$ algebra.

2. The $su(1, 1)$ Lie algebra of a hydrogen atom

The Schrödinger equation for a hydrogen-like atom with nuclear charge Z and eigenenergy E can be written as ($\hbar = m_e = q_e = 1$)

$$\left[-\frac{1}{2}\nabla^2 - \frac{Z}{r} - E \right] \Psi(\mathbf{r}) = 0. \quad (1)$$

After separating the angular contributions in (1) and rearranging, it can be written as

$$\left[\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{d}{d\rho} \right) + \frac{2\lambda}{\rho} - \frac{l(l+1)}{\rho^2} - 1 \right] R(\rho) = 0 \quad (2)$$

where we used $\Psi(\mathbf{r}) = R(r)Y(\theta, \phi)$, $r \equiv |\mathbf{r}|$, $\lambda \equiv 2Z/k$ and $l = 0, 1, 2, \dots$, is the orbital angular momentum quantum number; we have introduced the non-dimensional variable $\rho = kr/2$, and $k \equiv \sqrt{-8E}$ (note that ρ has been defined with an extra $1/2$ factor not used in the analogous variable usually employed in this problem). We are describing bound states, thus, $E < 0$ always.

Introducing the transformed radial eigenfunctions

$$R(\rho) = \frac{F(\rho)}{\rho^{1/2}}, \quad (3)$$

we obtain the expression

$$\left[\rho^2 \frac{d^2}{d\rho^2} + \rho \frac{d}{d\rho} + 2\lambda\rho - \rho^2 - \frac{1}{4} \right] F(\rho) = l(l+1)F(\rho). \quad (4)$$

Changing to the variable x defined through $\rho \equiv e^x$, we can finally write (2) in the form

$$\left[\frac{d^2}{dx^2} + 2\lambda e^x - e^{2x} - \frac{1}{4} \right] F(x) = l(l+1)F(x). \quad (5)$$

This equation is an eigenvalue equation with eigenvalues $l(l+1)$, $l = 0, 1, 2, 3, \dots$, which are fixed by the spherical symmetry of the problem. As we show in what follows, it can be used to obtain the bound radial eigenfunctions and the energy spectrum of the hydrogen atom. This is accomplished using the properties of the $su(1, 1)$ Lie algebra which stems from it.

The algebra we are going to construct is exactly the same as the one needed to solve for the bound states of the relativistic hydrogen atom in Dirac's description [4]. One probable reason for such behaviour is the fact that both in the relativistic and in the non-relativistic problems the solution can be expressed in terms of Laguerre polynomials [20, 43]; in the former case the Laguerre polynomials are labelled by a non-integer index s related to the total angular momentum as $s = \sqrt{(j+1/2)^2 - Z^2\alpha_F^2}$ where $\alpha_F = 1/c \simeq 1/137$ is the fine structure constant [4, 11, 12, 43]. When the non-relativistic limit is taken, α_F becomes negligible and s becomes an integer, transforming the non-integer polynomials into the more usual non-relativistic ones [29, 44]. Of course, in the relativistic case we have to deal with two independent radial equations instead of only one. But we have shown that, in this Dirac case, we just need to deal with two eigenvalue equations which differ from each other in one unit [4]. Such, at first sight, surprising algebraic parallelism between the relativistic and the non-relativistic problems may be explained by an already known parameter map relating these two problems; the map in question is [45]

$$\begin{aligned} Z &\rightarrow Z\mathcal{E}, \\ l &\rightarrow \begin{cases} s, \\ -s - 1, \end{cases} \\ E &\rightarrow \frac{1}{2}(\mathcal{E}^2 - c^4), \end{aligned} \quad (6)$$

where E is the non-relativistic energy and \mathcal{E} is the relativistic one, and helps explain the connection found between the relativistic and non-relativistic problems.

2.1. Defining the algebra

Let us introduce an additional angular variable $\varphi \in [0, 2\pi]$ into the problem's description through the operator

$$\Xi_3 \equiv -i \frac{\partial}{\partial \varphi}, \quad (7)$$

and try to associate the discrete energy eigenvalues of the Hamiltonian with the discrete eigenvalues of this operator. Let us also introduce the operators

$$\Xi_{\pm} \equiv i e^{\pm i\varphi} \left(\frac{\partial}{\partial x} \mp e^x \mp i \frac{\partial}{\partial \varphi} + \frac{1}{2} \right), \quad (8)$$

which depend both on φ and x . We can show that these three operators satisfy an $su(1, 1)$ Lie algebra [14, 33, 34], that is

$$[\Xi_3, \Xi_{\pm}] = \pm \Xi_{\pm}, \quad (9)$$

and

$$[\Xi_+, \Xi_-] = -2\Xi_3. \quad (10)$$

We can alternatively define the two operators Ξ_1 and Ξ_2 as

$$\Xi_1 = \frac{1}{2}(\Xi_+ + \Xi_-), \quad \Xi_2 = \frac{1}{2i}(\Xi_+ - \Xi_-), \quad (11)$$

in terms of (10) and (11), the $su(1, 1)$ algebra takes the form

$$[\Xi_1, \Xi_2] = -i\Xi_3, \quad [\Xi_2, \Xi_3] = i\Xi_1, \quad [\Xi_3, \Xi_1] = i\Xi_2. \quad (12)$$

The Casimir operator of the algebra is [14, 33, 34]

$$\Xi_c = -\Xi_1^2 - \Xi_2^2 + \Xi_3^2 = \frac{\partial^2}{\partial x^2} - e^{2x} - 2i e^x \frac{\partial}{\partial \varphi} - \frac{1}{4}, \quad (13)$$

satisfying $[\Xi_c, \Xi_i] = 0$, for $i = 1, 2, 3$.

To obtain the complete set of eigenvalues and of simultaneous eigenfunctions of Ξ_c and Ξ_3 , let us write their eigenfunctions as $V_{\xi}^{\lambda'}(x, \varphi)$, using λ' for the eigenvalue of Ξ_3 and ξ for the eigenvalue of Ξ_c ; we set

$$\Xi_3 V_{\xi}^{\lambda'}(x, \varphi) = \lambda' V_{\xi}^{\lambda'}(x, \varphi), \quad (14)$$

$$\Xi_c V_{\xi}^{\lambda'}(x, \varphi) = \xi V_{\xi}^{\lambda'}(x, \varphi). \quad (15)$$

From the definition of Ξ_3 , we find

$$V_{\xi}^{\lambda'}(x, \varphi) = e^{i\lambda'\varphi} F_{\xi}^{\lambda'}(x). \quad (16)$$

From equation (7) we conclude that we can cast equation (15) precisely in the form of the radial equation for the hydrogen atom, equation (5). If we then set $\lambda' = \lambda$ and identify the eigenfunctions of the algebra as

$$F(x) \equiv F_{\xi}^{\lambda}(x) \quad \text{with} \quad R(x) = e^{-x/2} F_{\xi}^{\lambda}(x) = \frac{1}{\rho^{1/2}} F_{\xi}^{\lambda}(\rho), \quad (17)$$

the eigenvalues ξ are necessarily

$$\xi = l(l+1). \quad (18)$$

We have thus written the radial problem of the non-relativistic hydrogen atom as the eigenvalue problem for the Casimir operator of a $su(1, 1)$ algebra with eigenvalues $\xi = l(l+1)$. Note the clear analogy with the angular momentum algebra and thence with the Legendre polynomials; we thus expect that the $F_{\xi}^{\lambda}(x)$ functions defined here depend on ξ and λ eigenvalues as happens in the angular momentum case.

2.2. The relationship with the relativistic hydrogen atom

We have shown [4] that the radial equations for the big $F(\rho)/\rho$ and small components $G(\rho)/\rho$, where $\rho = kr$ and $k = \sqrt{c^4 - \mathcal{E}^2}$, \mathcal{E} being the relativistic energy, can also be casted in the form of equation (5), using again the variable $\rho = e^x$ and defining

$$F(\rho(x)) = \sqrt{c^2 + \mathcal{E}}[\psi_-(x) + \psi_+(x)], \tag{19}$$

$$G(\rho(x)) = \sqrt{c^2 - \mathcal{E}}[\psi_-(x) - \psi_+(x)], \tag{20}$$

It is then possible to show that the equations for $\psi_{\pm}(x)$ are the same as (5) but with a parameter $\lambda \rightarrow \lambda_{\text{rel}}$ and the eigenvalue of the Casimir operator changed as $l(l + 1) \rightarrow (j + 1/2)^2 - Z^2\alpha^2 - 1/4$, where for $\psi_+(x)$ we have

$$\lambda_{\text{rel}} = \frac{(Z\alpha)\mathcal{E}}{\sqrt{c^4 - \mathcal{E}^2}} + \frac{1}{2}, \tag{21}$$

and the same equation for $\psi_-(x)$ changing only $\lambda_{\text{rel}} \rightarrow \lambda_{\text{rel}} - 1$ [4]. In the non-relativistic limit we have that $s \approx (j + 1/2)$ becomes an integer and $\sqrt{c^4 - \mathcal{E}^2} \approx \sqrt{-2E}$. The non-relativistic limit can be established using

$$\begin{aligned} \psi_+(x) &\rightarrow \psi_-(x), \\ \lambda_{\text{rel}} &\rightarrow \frac{Z}{\sqrt{-2E}} + \frac{1}{2} = \lambda + \frac{1}{2}, \\ e^{-x/2}\psi_+(x) &\rightarrow F(x). \end{aligned} \tag{22}$$

With the above limit and using the coupled, first-order differential equations that follow from the radial Dirac equation [4], we obtain precisely equation (5).

3. The algebraic solution

The operators Ξ_{\pm} play the role of ladder operators as follows from equation (9); since

$$\Xi_3 \Xi_{\pm} V_{\xi}^{\lambda}(x, \varphi) = (\Xi_{\pm} \Xi_3 \pm \Xi_{\pm}) V_{\xi}^{\lambda}(x, \varphi) = (\lambda \pm 1) \Xi_{\pm} V_{\xi}^{\lambda}(x, \varphi), \tag{23}$$

the Ξ_{\pm} operators shift λ to $\lambda \pm 1$,

$$\Xi_{\pm} V_{\xi}^{\lambda}(x, \varphi) \propto V_{\xi}^{\lambda \pm 1}(x, \varphi). \tag{24}$$

Let us define the inner product

$$(g, f) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \int_{-\infty}^{\infty} g^*(\varphi, x) f(\varphi, x) dx, \tag{25}$$

where $g(\varphi, x)$ and $f(\varphi, x)$ are periodic functions on the interval $\varphi \in [0, 2\pi]$ and tend to zero as $x \rightarrow \pm\infty$; we can now show that $\Xi_i, i = 1, 2, 3$, are all Hermitian, $\Xi_i^{\dagger} = \Xi_i$. Therefore, we can find a complete orthogonal basis of simultaneous eigenfunctions of Ξ_c and Ξ_3 which can be written as $V_{\xi}^{\lambda}(x, \varphi) \equiv |\xi \lambda\rangle$ and it is assumed to be orthonormalized, i.e. $\langle \xi' \lambda' | \xi \lambda \rangle = \delta_{\xi, \xi'} \delta_{\lambda, \lambda'}$.

The Casimir operator Ξ_c is not positive definite, as $\Xi_c = -\Xi_1^2 - \Xi_2^2 + \Xi_3^2$, but the operator $\Xi^2 = (\Xi_1^2 + \Xi_2^2 + \Xi_3^2)$ is indeed positive. From the relation

$$\Xi^2 = \Xi_1^2 + \Xi_2^2 + \Xi_3^2 = 2\Xi_3^2 - \Xi_c, \tag{26}$$

we directly obtain

$$2\lambda^2 \geq \xi. \tag{27}$$

Thus $|\lambda|$ must be bounded by below. Let us call $|\lambda|_{\min}$, the minimum value of it. We can choose either $\lambda > 0$ or $\lambda < 0$; then, respectively, λ is bounded by below or λ is bounded by above. The relevant representation we are constructing is thus the lowest weight representation. Let us consider first $\lambda > 0$, and define $N \equiv \lambda_{\min}$. Therefore, $\Xi_+ \Xi_- |\xi N\rangle = 0$. From

$$\Xi_+ \Xi_- = -\Xi_c + \Xi_3^2 - \Xi_3 \quad (28)$$

we get

$$-\xi + N^2 - N = 0 \quad \text{or} \quad \xi = l(l+1) = N(N-1); \quad (29)$$

with solutions $N = l+1$ or $N = -l$. So, the positive solution is then

$$N = l+1. \quad (30)$$

Thence $N = 1, 2, 3, \dots$; in other words, λ is just the principal quantum number N of the hydrogen atom problem. Once with the eigenvalues of the algebra, we can rename the eigenfunctions as $|\xi\lambda\rangle \rightarrow |Nl\rangle$, where we interchanged the order of the labels of the eigenvalues in order to rewrite them in the usual order of the wavefunctions of the hydrogen atom. From the point of view of the $su(1, 1)$ algebra, the label l stands for the Casimir eigenvalue of the algebra, $l(l+1)$, whereas N is the eigenvalue of the operator Ξ_3 .

The representation we are working out here is called the two-mode bosonic representation of $su(1, 1)$, because the operators (7) and (11) can be constructed using two bosonic creation operators [33]. Since λ is the principal quantum number because $\lambda_{\min} = l+1$, the representation becomes what Bargmann calls *minimal M*, (λ has a minimal value), D_λ^+ , where λ takes the values $1/2, 1, 3/2, \dots$ [34]. In our non-relativistic case the semi-integer representations are excluded.

3.1. The energy eigenstates

The energy spectrum of the hydrogen atom follows immediately from the definition of λ ,

$$E = -\frac{1}{2} \frac{Z^2}{N^2} \quad N = 1, 2, 3, \dots, \quad (31)$$

which is the standard Balmer formula [44].

To obtain the wavefunctions of the hydrogen, let us start with the ground state $|10\rangle$; applying Ξ_- to such state,

$$e^{-i\varphi} \left(\frac{\partial}{\partial x} + e^x + i \frac{\partial}{\partial \varphi} + \frac{1}{2} \right) e^{i\varphi} F_1^0(x) = 0, \quad (32)$$

we obtain

$$F_1^0(x) = C_1^0 e^{x/2} \exp(-e^x) \quad \text{or} \quad F_1^0(\rho) = C_1^0 \rho^{1/2} e^{-\rho}, \quad (33)$$

where C_1^0 is a normalization constant. So, the ground state radial eigenfunction can be written as

$$R_1^0(r) = C_1^0 e^{-Zr}, \quad (34)$$

with $C_1^0 = 2Z^{3/2}$. Once with the base state for a given l , we can obtain the whole series of states with l fixed for all $N = l+1, l+2, \dots$ from $\Xi_+ |Nl\rangle \sim |N+1l\rangle$.

To obtain the rest of the eigenfunctions, we first need to obtain the base state of the algebra for l fixed. Such a base state is given by the condition $\Xi_- |\lambda_{\min} l\rangle = 0$; the base state is precisely $|Nl-1\rangle$. The condition that the operator Ξ_- annihilates this state becomes

$$ie^{-i\varphi} \left(\frac{\partial}{\partial x} + e^x + i \frac{\partial}{\partial \varphi} + \frac{1}{2} \right) e^{iN\varphi} F_N^{l=N-1}(x) = 0, \quad (35)$$

and so

$$|NN - 1\rangle \sim e^{iN\varphi} e^{(N-1/2)x} e^{-e^x}. \tag{36}$$

Thus, $R_N^{N-1}(r) = C_N^{N-1} r^{N-1} e^{-(2Z/a_0 N)r}$, with $C_N^{N-1} = 2^N (Z/a_B N)^{(N+1/2)} (N\Gamma(2N))^{-1/2}$ to be properly normalized. The radial wavefunctions for any value of $l = 0, 1, 2, \dots$ are obtained applying successively the operator Ξ_+ to (36).

There is only one more thing to address, the case where $\lambda < 0$. In this instance, we should have that $\lambda_{\max} \equiv M < 0$ is the largest eigenvalue. Consequently $\Xi_+|\xi M\rangle = 0$ for this state, or $\Xi_- \Xi_+|\xi M\rangle = 0$. The solutions to this equation are $M = l$, or $M = -(l + 1)$. Taking the negative solution, we find by successive applications of Ξ_- to the ket $|\xi M\rangle$, that

$$|\xi M\rangle \sim e^{iM\varphi} e^{-(M+1/2)x} e^{e^x} = e^{iM\varphi} \rho^{-(M+1/2)} e^\rho, \tag{37}$$

state which diverges as $\rho \rightarrow \infty$. Thus, to describe physically realizable states, we have to select just the positive set of λ eigenvalues. To summarize, we have from equation (28) $N = l + 1$ or $N = -l$. The former is associated with the regular representation, whereas the latter with the irregular one. They behave near the origin as r^{l+1} and r^{-l} respectively. Since we need to chose $\lambda > 0$, we keep only the regular representation which is the one that has the correct behaviour near the origin. On the other hand the representation just discussed above (case $\lambda < 0$) corresponds to either $M = l$ or $M = -l - 1$ which is an equivalent, though disconnected representation of the former. Since in this last case we are forced to take negative values for λ , we discard this representation. Thus, the only relevant representation is the minimal weight representation with $\lambda > 0$.

3.2. The extra variable and the Lie algebra of the problem

But now, what is the interpretation of the extra variable φ ? When we perform a rotation on the functions $V_\xi^\lambda(x, \varphi)$, using the Ξ_3 operator with parameter φ' , we get

$$V_\xi^\lambda(x, \varphi) \xrightarrow{\Xi_3} e^{i\Xi_3\varphi'} V_\xi^\lambda(x, \varphi) = e^{i\lambda\varphi'} V_\xi^\lambda(x, \varphi). \tag{38}$$

From equations (16) and (17), we conclude that the effect of a Ξ_3 rotation over the radial wavefunction is

$$R(\rho) \xrightarrow{\Xi_3} e^{i\lambda\varphi'} R(\rho); \tag{39}$$

the effect is thus only multiplying it by a global phase factor. In this sense, the present approach takes advantage of a basic property of quantum theory incorporating it into the basic features of our system. Namely, that the properties of any quantum system are unaffected by a global phase change in the wavefunctions describing the system.

What is the symmetry of the system implied by our approach? As the angular momentum operators, J_i and the Ξ_i , are completely independent of one another, we have $[\Xi_i, J_j] = 0$. So, together the six generators span a $SO(3) \otimes SU(1, 1)$ group. Let us define the operators $A_1 \equiv i\Xi_1, A_2 \equiv i\Xi_2, A_3 \equiv \Xi_3$, and construct with them the operators $K_i \equiv i(A_i - J_i)$ and $M_i \equiv A_i + J_i$; we then obtain

$$[K_i, K_j] = -i\epsilon_{ijk} M_k, \quad [M_i, M_j] = i\epsilon_{ijk} M_k, \quad [M_i, K_j] = i\epsilon_{ijk} K_k. \tag{40}$$

Thus, we have constructed the $so(3, 1)$ algebra, the same algebraic structure of the Lorentz group. As expected from the properties of such group, the representations are not, in general, unitary. In fact, A_1 and A_2 are not Hermitian, but since Ξ_3 is Hermitian, the ‘boost’ K_3 is anti-Hermitian, and the ‘rotation’ M_3 is Hermitian. We note in passing that the $so(3, 1)$ algebra is also the symmetry algebra of the unbounded ($E > 0$) states of the non-relativistic

hydrogen atom. We should also mention that the whole bound-state symmetry algebra of the non-extended problem can always be cast in the form of a $so(4, 1)$ algebra, as has been shown in [7].

4. The three-dimensional and Morse oscillators

The method developed here can be applied to other systems as well. In particular, it can be applied to the s -wave Morse problem and to the three-dimensional oscillator. This property is a manifestation of the shape invariance symmetry associated with the Natanzon class of potentials, which includes the Coulomb, the harmonic oscillator and the s -wave Morse problems [45, 46]. In this section, we shall briefly outline the case of the Morse and of the three-dimensional harmonic oscillator problems.

4.1. The Morse potential

The Morse potential is

$$V(r) = D(e^{-2r/a} - 2e^{-r/a}), \quad (41)$$

where a is a parameter with units of length. We give a quick proof that the method developed here also applies to it. In the generalized s -wave Morse problem ($\lambda = 1$ corresponds to the original undeformed problem) defining $x = r/a$ we obtain an equation very similar to (5). To prove this assertion, we define $K = \sqrt{2Da}$, $\rho = K e^{-r/a}$, $\mu = 2a^2 E$ and $R_M(\rho) = \rho F_M(\rho)$, where $R_M(\rho)$ is the radial part of the Morse wavefunction and E is the energy of the problem. When we write the Morse equation ($l = 0$), in terms of the above quantities, we obtain the same equation as in (4). So if both the equations are the same, we can follow the same path we followed for the hydrogen atom and construct the same $su(1, 1)$ algebra to solve the generalized s -wave Morse problem. The map relating the Coulomb to the Morse problem is [47]

$$R(\rho) \rightarrow \rho F_M(\rho), \quad Z\sqrt{2/(-E)} \rightarrow 2K, \quad l(l+1) \rightarrow \mu + 1/4. \quad (42)$$

4.2. The 3D harmonic oscillator

For the 3D oscillator case, with potential energy term $V(r) = \omega^2 r^2/2$, we define, in atomic units, $a^2 = 1/\omega$, $\rho = r/a$ and $\epsilon = E/\omega$, where ω is the frequency of the oscillator, r the radial variable and E the energy to obtain the Schrödinger equation of the problem as [48]

$$\left[-\frac{d^2}{d\rho^2} + \rho^2 + \frac{l(l+1)}{\rho^2} \right] R(\rho) = 2\epsilon R(\rho). \quad (43)$$

We now define $F(\rho) = R/\sqrt{\rho}$ and change the radial variable to $u = 1/2\rho^2$ to obtain

$$\left[u^2 \frac{d^2}{du^2} + u \frac{d}{du} + \left(\epsilon u - u^2 - \frac{1}{4} \right) \right] F(u) = \frac{1}{4} \left[l(l+1) - \frac{3}{4} \right] F(u). \quad (44)$$

In this equation, we change $u = e^x$ and $\lambda = \epsilon/2$ to obtain precisely equation (5), with eigenvalue $\xi = (1/4)[l(l+1) - 3/4]$; we may then follow step by step the same path we followed in the hydrogen problem. In particular, we found that $|\lambda|$ must be bounded by below. The only relevant representation, the lowest weight one, is when $\lambda > 0$. Let us call $\lambda_{\min} = s + 1/4$. From equation (28) we have that $\lambda_{\min}(\lambda_{\min} - 1) = \xi$, which implies, following the same reasoning as in the hydrogen problem, that $s = (1/2)(l+1)$. As before, $\lambda = \lambda_{\min}, \lambda_{\min} + 1, \dots$. So, we put $\lambda = s + 1/4 + n$, where $n = 1, 2, \dots$. Since $\lambda = \epsilon/2$, we

get $\epsilon = 2[s + 1/4 + n]$, or

$$E = \omega(2n + l + \frac{3}{2}), \quad (45)$$

which is precisely the expression for the energy of this problem [48]. The eigenfunctions of the problem follow from the same procedure as before.

5. Concluding remarks

In summary, we have constructed an $su(1, 1)$ Lie algebra for the non-relativistic hydrogen atom by introducing the Hermitian operators Ξ_i , $i = 1, 2, 3$. This formulation requires extending the radial configuration space of the system with the extra phase φ . The algebra predicts the correct energy spectrum and eigenfunctions of the system. We can calculate any radial eigenfunction by applying an operator with only a first-order derivative, namely Ξ_+ or Ξ_- . From the point of view of the algebra described here, the L^2 angular momentum eigenvalue plays a more important role than the principal quantum number N since we need to fix it first and then proceed to construct the wavefunctions. The angular momentum symmetry is then playing a central role in the behaviour of the system; this feature is related to the contribution of the centrifugal potential $l(l + 1)/r^2$ to the properties of the system. The representation spanned by the problem has been called the minimal M representation [34].

We emphasize that the extra variable φ is required in order to close the algebra. In terms of the solutions, φ plays the role of a phase. Also, when we perform an $SU(1, 1)$ rotation, the energy spectrum remains unchanged because the radial equation (5) commutes with any of the three generators of the algebra. This is a consequence of the fact that both the radial equation and the Casimir operator Ξ_c , are identical when $\lambda = N$.

In a certain way, it is remarkable that our method could be applied to the more complicated relativistic hydrogen atom. But this is due to the fact the hydrogen atom is a system with symmetry properties larger than the obvious geometrical symmetry of its Hamiltonian in both the relativistic and the non-relativistic descriptions [10, 29], and to the existence of the simple mapping (42) relating the parameters in both descriptions. The algebra needed in the relativistic description is exactly the same as the one described here though the eigenvalues and the relation with the energy is, of course, different [4].

The importance of symmetry methods for dealing with the dynamical Stark and Zeeman effects indicates that our method might be extended to deal with such and other related problems [30, 49]. The algebraic method of solution and the expression of the bound state eigenfunctions in terms of the ladder operators Ξ_{\pm} presented here may offer some simplifications in atomic physics calculations [31, 41], can be useful in diverse applications in quantum optics [35, 37] and it may be applied to the study of ionization states [42] by using non-discrete representations of $su(1, 1)$. But apart from the above considerations, the theory of one-electron atoms and ions has found uses in many different fields of modern physics including molecular, condensed and plasma physics, quantum optics and quantum information theory [33, 38, 50–52].

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