LETTER TO THE EDITOR

New non-unitary representations in a Dirac hydrogen atom

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Abstract. New non-unitary representations of the SU(2) algebra are introduced for the case of the Dirac equation with a Coulomb potential; an extra phase, needed to close the algebra, is also introduced. The new representations does not require integer or half-integer labels. The set of operators defined are used to span the complete space of bound-state eigenstates of the problem thus solving it in an essentially algebraic way.

Hydrogen-like atoms are some of the most important quantum systems solved. Even for describing stabilization properties and for testing QED and weak interaction theories a great deal can be done at the relativistic atomic physics level (Greiner 1991, Kylstra *et al* 1997, Quiney *et al* 1997). It is, therefore, very important to extend our insight into the properties of hydrogen-like systems. An important tool has been the algebraic properties of the set of operators defining the system; these are not only connected with the corresponding group and its symmetry algebra but often offer simplified methods for carrying out some calculations. It is the purpose of this letter to define a new set of operators for the Dirac relativistic hydrogen atom. This comprises a non-unitary representation of the SU(2) algebra and defines ladder operators for the problem. An extra phase is needed to close the algebra but this allows us to solve the Dirac hydrogen atom in a neat algebraic way.

The Dirac Hamiltonian for a hydrogen-like atom is

$$H = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m - \frac{Ze^2}{r} \tag{1}$$

where $\boldsymbol{\alpha}$ and β are Dirac matrices (Bjorken and Drell 1964), Z is the atomic number, r is the relative distance between the electron and the nucleus, $m = m_{\mathrm{e}} m_{\mathrm{p}}/(m_{\mathrm{e}} + m_{\mathrm{p}})$ is the reduced mass of an electron and a proton; we use units such that $\hbar = c = 1$.

Taking advantage of the obvious rotational symmetry of H, we can express the bound eigenstates of the hydrogen atom as

$$\psi(\boldsymbol{r}, t) = \frac{1}{r} \begin{pmatrix} F(r)\mathcal{Y}_{jm}(\theta, \phi) \\ \mathrm{i}G(r)\mathcal{Y}'_{jm}(\theta, \phi) \end{pmatrix} \tag{2}$$

where $\mathcal{Y}_{jm}$ and $\mathcal{Y}'_{jm}$ are spinor spherical harmonics of opposite parity and j is the total angular momentum (Greiner 1991). It is convenient to define the quantum number ϵ such that it equals $+1$ when $l = j + \frac{1}{2}$ and it equals -1 when $l = j - \frac{1}{2}$ and use it instead of

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parity. The 'big' and 'small' radial components of the bi-spinor (2) describing bound states of a hydrogen atom are solutions of the system

$$\left(-\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{\tau_j}{\rho}\right) G(\rho) = \left(-\nu + \frac{\zeta}{\rho}\right) F(\rho) \tag{3}$$

$$\left(+\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{\tau_j}{\rho}\right) F(\rho) = \left(\nu^{-1} + \frac{\zeta}{\rho}\right) G(\rho) \tag{4}$$

where we have defined the positive definite quantity $k := \sqrt{m^2 - E^2}$, where E is the energy of the bound state and we have expressed the equations in terms of the dimensionless variable $\rho := kr$. For the sake of simplicity we also used $\zeta := Ze^2$, $\tau_j := \epsilon(j + \frac{1}{2})$, and $\nu := \sqrt{(m - E)/(m + E)}$.

Let us now change to the new variable x defined by $\rho = e^x$ such that the range of x is the open interval $(-\infty, \infty)$ and redefine the radial functions as

$$F(\rho(x)) := \sqrt{m + E}[\psi_-(x) + \psi_+(x)]$$
$$G(\rho(x)) := \sqrt{m - E}[\psi_-(x) - \psi_+(x)]. \tag{5}$$

With the new functions $\psi_+(x)$ and $\psi_-(x)$, defining

$$\mu := \frac{\zeta E}{k} + 1 \tag{6}$$

and after some manipulations we obtain the following system of differential equations

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2\mu e^x - e^{2x} - \frac{1}{4}\right]\psi_+(x) = \left(\tau_j^2 - \zeta^2 - \frac{1}{4}\right)\psi_+(x) \tag{7}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2(\mu - 1)e^x - e^{2x} - \frac{1}{4}\right]\psi_-(x) = \left(\tau_j^2 - \zeta^2 - \frac{1}{4}\right)\psi_-(x) \tag{8}$$

for describing the radial part of a hydrogen atom. As should become clear in what follows, the inclusion of the term $\frac{1}{4}$ in the above equations is necessary to close the algebra we purport to construct. Note that equations (7) and (8) can be regarded as an eigensystem with the known eigenvalue

$$\omega := \tau_j^2 - \zeta - \frac{1}{4} = j(j+1) - \zeta^2 \tag{9}$$

as follows from the radial symmetry of the hydrogen atom.

In order to rewrite the system (7) and (8) making clear the relation with a SU(2) algebra let us define the two operators

$$\Omega_\pm := e^{\pm i\xi}\left(\frac{\partial}{\partial x} \mp e^x \mp i\frac{\partial}{\partial \xi} + \frac{1}{2}\right) \tag{10}$$

where we introduced the extra phase ξ besides the 'radial' variable x, and a third operator

$$\Omega_3 := -i\frac{\partial}{\partial \xi} \tag{11}$$

which depends exclusively on ξ; we can alternatively define the two operators Ω_1 and Ω_2 as

$$\Omega_1 = \tfrac{1}{2}(\Omega_+ + \Omega_-) \qquad \Omega_2 = \frac{1}{2i}(\Omega_+ - \Omega_-). \tag{12}$$

The previously defined operators are easily seen to satisfy all the relationships of the SU(2) algebra

$$[\Omega_i, \Omega_j] = i\epsilon_{ijk}\Omega_k \qquad i, j, k = 1, 2, 3 \tag{13}$$

where Einstein summation convention is implied; the algebra can be also expressed in terms of the operators $\Omega_\pm$

$$[\Omega_3, \Omega_\pm] = \pm\Omega_\pm \qquad \text{and} \qquad [\Omega_+, \Omega_-] = 2\Omega_3 \tag{14}$$

which thus play the role of raising and lowering operators. The operator

$$\Omega^2 := \mathbf{\Omega} \cdot \mathbf{\Omega} = \Omega_1^2 + \Omega_2^2 + \Omega_3^2 = \frac{\partial^2}{\partial x^2} - e^{2x} - 2ie^x\frac{\partial}{\partial\xi} - \frac{1}{4} \tag{15}$$

where $\mathbf{\Omega} := \Omega_1\boldsymbol{i} + \Omega_2\boldsymbol{j} + \Omega_3\boldsymbol{k}$, is the Casimir operator since $[\Omega^2, \Omega_i] = 0$ for all $i = 1, 2, 3$.

Given these properties, we can choose the operators Ω^2 and Ω_3 and define the simultaneous eigenstates $V_\omega^\mu(x, \xi)$ where ω and μ are, repectively, the eigenvalues of Ω^2 and Ω_3—the notation is chosen in analogy with the spherical harmonic $Y_l^m(\theta, \phi)$ case. It must be kept in mind though that we are not here restricted to a compact set of parameters given the infinite range of x. Our choice of eigenstates allows us to write

$$\Omega_3 V_\omega^\mu(x, \xi) = \mu V_\omega^\mu(x, \xi) \qquad \Omega^2 V_\omega^\mu(x, \xi) = \omega V_\omega^\mu(x, \xi) \tag{16}$$

and thus

$$V_\omega^\mu(x, \xi) = e^{i\mu\xi}\mathcal{P}_\omega^\mu(x) \tag{17}$$

where we have tried to use a notation for the x-function reminiscent of the associated Legendre polynomials.

Now, using equations (7) and (8) we can immediately obtain $\psi_+(x) = V_\omega^\mu(x, \xi)$ and $\psi_-(x) = V_\omega^{\mu-1}(x, \xi)$; besides, we can easily show that the operators $\Omega_\pm$ change the eigenvalue μ to the eigenvalue $\mu \pm 1$, i.e.

$$\Omega_\pm V_\omega^\mu(x, \xi) = C_\mu^\pm V_\omega^{\mu\pm1}(x, \xi) \tag{18}$$

where the numbers $C_\mu^\pm$ can be determined from $\langle\omega\mu|\Omega_+\Omega_-|\omega\mu\rangle = C_\mu^- C_{\mu-1}^+$ and, with an appropriate selection of phase, they become $C_\mu^\pm = \pm\sqrt{\mu(\mu \pm 1) - \lambda(\lambda - 1)}$. These definitions also establish the conection of our operators with the hydrogen-atom problem since applying Ω^2 to $V_\omega^\mu(x, \xi)$ or to $V_\omega^{\mu-1}(x, \xi)$ essentially reproduces equations (7) and (8)—as the second of equations (16) clearly exhibits.

For establishing the Hermiticity (or lack thereof) of the operators introduced, we need a scalar product; to this end it suffices to use the following product

$$\langle\phi, \psi\rangle = \int_0^{2\pi} \frac{d\xi}{2\pi} \int_{-\infty}^{\infty} \phi^*(\xi, x)\psi(\xi, x)\,dx. \tag{19}$$

With this interior product, the eigenstates $V_\omega^\mu(x, \xi) := |\omega, \mu\rangle$ form a complete orthogonal basis $\langle\omega', \mu'|\omega, \mu\rangle = \delta_{\mu\mu'}\delta_{\omega\omega'}$. Definition (19) also implies that Ω_3 is an Hermitian operator, but that $\Omega_1 = -\Omega_1^\dagger$ and $\Omega_2 = -\Omega_2^\dagger$, that is they are anti-Hermitian (Martínez-y-Romero *et al* 1997). Therefore Ω^2 is not necessarily positive definite; a positive definite operator can be anyway defined as

$$\mathbf{\Omega}^\dagger \cdot \mathbf{\Omega} = \Omega_3^2 - \Omega_1^2 - \Omega_2^2 = 2\Omega_3^2 - \Omega^2. \tag{20}$$

The action of this operator can be shown to imply that $2\mu^2 \geqslant \omega$, meaning that $|\mu|$ is bounded below; let us call λ this minimum value, i.e. $\lambda := |\mu|_{\min}$. With this we easily find that $\omega = \lambda(\lambda - 1)$ and so, since $\omega = \tau_j^2 - \zeta^2 - \frac{1}{4}$ and we are looking for positive λ,

$$|\mu|_{\min} = \lambda = s + \tfrac{1}{2} \tag{21}$$

where $s := +(\tau_j^2 - \zeta^2)^{1/2}$. The most important conclusion we can draw from our discussion is that λ no longer has to be restricted to integer or half-integer values as happens necessarily in the standard angular momentum or SU(2) (Hermitian) case.

This curious and interesting result means that looking for solutions to the Dirac hydrogen atom can also be regarded as looking for non-unitary representations of a SU(2) algebra labelled by real numbers λ—that is, no longer restricted to integer or half-integer numbers. In fact, according to equation (21) we have two series of eigenvalues depending on whether μ is a positive number or not. In the first case, λ is the minimum number of an infinite set of positive eigenvalues: $\mu = -\lambda - k$, in the second case, $-\lambda$ is the maximum value of the infinite set of negative eigenvalues: $\mu = -\lambda - k$; in both cases $k = 0, 1, 2, \ldots$ is a non-integer. Note that from the physical point of view the existence of infinite representations of the SU(2) algebra makes sense since it is associated with the denumerably infinite set of energy eigenvalues of the hydrogen atom. In fact, the energy spectrum of the system is easily obtained from (6) and is found to be

$$E = m \left[1 + \frac{\zeta^2}{(\mu - \frac{1}{2})^2} \right]^{-1/2} \tag{22}$$

in the case of positive eigenvalues we have $\mu = \lambda + k = s + k + \frac{1}{2}$, $k = 0, 1, 2, \ldots$, this is precisely the energy spectrum for a Dirac hydrogen atom (Bjorken and Drell 1964, Greiner 1991). The negative eigenvalues do not lead to physically admissible eigenstates as we shall see in what follows.

The ground state of the system follows from the equation $\Omega_- |\lambda\lambda\rangle = 0$ for the positive eigenvalues. The solution of this differential equation can be found to be

$$\mathcal{P}_\lambda^\lambda(x) = \frac{2^{(\lambda - 1/2)}}{\sqrt{\Gamma(2\lambda - 1)}} e^{(\lambda - 1/2)x} \exp(-e^x) \tag{23}$$

where $\Gamma(y)$ stands for the Euler-gamma function. As λ is the lowest eigenvalue, we trivially obtain

$$\psi_+(x) = \mathcal{P}_\lambda^\lambda(x) \qquad \text{and} \qquad \psi_-(x) = 0 \tag{24}$$

thus the base state is given by $|\lambda\lambda\rangle = e^{i\lambda\zeta} \mathcal{P}_\lambda^\lambda$. Using the original variable ρ, the big and the small components for the ground state can be shown to behave as $F(\rho) \propto \sqrt{m + E} \rho^s e^{-\rho}$ and $G(\rho) \propto \sqrt{m - E} \rho^s e^{-\rho}$ and, in the negative eigenvalue case, the solution behaves as $\sim \rho^s e^\rho$ resulting in a divergent behaviour as $\rho \to \infty$ making it unsuitable as an eigenfunction of the hydrogen atom; it is obvious that every other negative eigenvalue function is also unsuitable.

The excited states are obtained applying Ω_+ succesively to $|\lambda\lambda\rangle$; they end up being polynomials multiplied by the weight factor $\rho^{\lambda - 1/2} e^{-\rho}$ which assures the appropriate behaviour of the eigenstates both as $\rho \to 0$ as well as $\rho \to \infty$. A more detailed discussion of these new polynomials and graphical representations of them are given in a more detailed paper (Martínez-y-Romero *et al* 1997).

The main conclusion of this letter has to do with the infinite-dimensional non-unitary representation of SU(2) where each of the basic operators, except Ω_3, are also non-Hermitian. For example, the matrix elements of Ω_3 are

$$\langle \omega\mu | \Omega_3 | \omega\mu' \rangle = \mu \delta_{\mu\mu'} \tag{25}$$

where $\mu = \pm(\lambda + k)$, $k = 0, 1, 2, \ldots$, so its trace vanishes and the determinant of an element of the group of the form $\exp(i\Omega_3)\xi$ is always 1. The other two operators have as their only non-zero matrix elements

$$\langle \omega\mu | \Omega_1 | \omega\mu \pm 1 \rangle = \mp \frac{1}{2} \sqrt{\mu(\mu \pm 1) - \lambda(\lambda - 1)} \tag{26}$$

and

$$\langle\omega\mu|\Omega_2|\omega\mu \pm 1\rangle = -\frac{\mathrm{i}}{2}\sqrt{\mu(\mu \pm 1) - \lambda(\lambda - 1)}. \tag{27}$$

This means that the trace of both Ω_1 and Ω_2 vanish and that the determinant of group elements is 1 only when the parameter takes imaginary values. Note also that Ω_3 can be given the physical interpretation of producing infinitesimal changes in the phase of the state $|\lambda\omega\rangle = \mathrm{e}^{\mathrm{i}\mu\xi}\mathcal{P}_\omega^\lambda(x)$; that is, it can be associated with the unitary operator $U = \mathrm{e}^{\mathrm{i}\Omega_3\xi}$ which changes the phase of any state.

In summary, we have constructed an SU(2) algebra for the relativistic hydrogen in the Dirac formulation where the corresponding group is not necessarily compact. We must point out that in order to close the algebra we were forced to introduce an extra parameter ξ which plays the role of a phase. One of the most noteworthy features of the representations reported here is the mixing of a spinorial angular momentum character (implying an equally spaced spectrum) with the energy requirements of the problem (requiring a differently spaced spectrum); the interplay of these two spectral requirements is basically reflected in equations (15), (20), (21) and (22), and in the fact that the eigenvalues of the system (7), (8) follows from both the generic radial symmetry and the specific features of the interaction. From equation (6) we may also notice that in the limit of vanishing interaction, $\zeta \to 0$, the representation collapses and, in this case, $\mu = 1$ always. This behaviour is precisely as expected because there is no longer any restriction over the eigenvalues and thus the spectrum becomes continuous—corresponding to a free Dirac particle.

The representations of the algebra are labelled by numbers which are neither integers nor half-integers as they ought to be in the case of ordinary unitary representations. Nevertheless, the operator algebra introduced allows an essentially algebraic solution of the Dirac hydrogen atom which may have various applications (De Lange and Raab 1991). The similarity of our transformed equations with the corresponding ones for the case of the Morse potential (Núñez-Yépez *et al* 1995, 1997) should also be noted and the connections that all our formulation has with systems with hidden supersymmetric properties (Benítez *et al* 1990a, b, Martínez-y-Romero *et al* 1991, Martínez-y-Romero and Salas-Brito 1992, Haag *et al* 1976) as we shall discuss at length in a forthcoming paper.

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