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COMMENT

Comment on 'New non-unitary representations in a Dirac hydrogen atom'

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Abstract. Nonunitary representations of a novel realization of the $su(2)$ algebra recently introduced for the Dirac relativistic hydrogen atom are found to be actually unitary representations of a related $su(1, 1)$ algebra.

Dynamical symmetry methods have been widely used in various fields of physics [1] and their power is especially demonstrated in the nonrelativistic and relativistic Coulomb problems. In recent work by R P Martínez-y-Romero, A L Salas-Brito and J Saldaña-Vega [2, 3], a novel realization of the classic $su(2)$ algebra was introduced for the Dirac hydrogen problem and non-unitary representations were used to explain the bound-state energy spectrum. Although non-unitary representations could be important in certain dynamical symmetry problems related to periodic potentials [4], a careful analysis shows that the representations in [2, 3] are actually unitary with respect to a $su(1, 1)$ realization.

Let us first write down the realization of the $su(2)$ algebra in [2, 3]:

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

$$\Omega_3 = -i\frac{\partial}{\partial \xi} \tag{2}$$

where x is the transformed radial variable and ξ is essentially an extra phase. For details on how this is related to the Dirac hydrogen Hamiltonian, please refer to [2, 3]. The operators satisfy the usual $su(2)$ commutation relations:

$$[\Omega_3, \Omega_\pm] = \pm\Omega_\pm,\ [\Omega_+, \Omega_-] = 2\Omega_3. \tag{3}$$

The authors of [2, 3] proved that, for a certain scalar product,

$$\Omega_3^\dagger = \Omega_3,\ \Omega_\pm^\dagger = -\Omega_\mp \tag{4}$$

so that the realization of the algebra is not Hermitian. That is why non-unitary representations of $su(2)$ were introduced.

However, we can change the realization a little bit to produce unitary representations of a $su(1,1)$ algebra. All we need to do is to change Ω_- to $-\Omega_-$, so that we have

$$\Omega_\pm = \mathrm{e}^{\pm \mathrm{i}\xi}\left(\pm\frac{\partial}{\partial x} - \mathrm{e}^x - \mathrm{i}\frac{\partial}{\partial \xi} \pm \frac{1}{2}\right) \tag{5}$$

$$\Omega_3 = -\mathrm{i}\frac{\partial}{\partial \xi} \tag{6}$$

with commutation relations

$$[\Omega_3, \Omega_\pm] = \pm\Omega_\pm,\ [\Omega_+, \Omega_-] = -2\Omega_3. \tag{7}$$

This is obviously a $su(1,1)$ algebra and it is similar to the $su(1,1)$ realization for the Morse potential in [5] except for a sign change in x. Besides, $\Omega_\pm^\dagger = \Omega_\mp$, so the realization is Hermitian and the representations should be unitary with respect to the $su(1,1)$ algebra.

Let us recall the classification of unitary irreducible representations of $su(1,1)$ [6],where $k(k+1)$ is the eigenvalue of the Casimir operator and m is the eigenvalue of the operator Ω_3:

- The principal series $k = -\frac{1}{2} + \mathrm{i}\rho,\ \rho > 0,\ m = 0, \pm 1, \ldots$ or $m = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$.
- The complementary series $-\frac{1}{2} < k < 0,\ m = 0, \pm 1, \ldots$.
- The discrete series D_k^+, where k is a negative integer or half-integer and $m = -k, -k+1, \ldots$.
- The discrete series D_k^-, where k is a negative integer or half-integer and $m = k, k-1, \ldots$.

For our realization of $su(1,1)$, the Casimir is

$$\begin{aligned}\Omega^2 =& -\Omega_+\Omega_- + \Omega_3^2 - \Omega_3 \\ =& \frac{\partial^2}{\partial x^2} - \mathrm{e}^{2x} - 2\mathrm{i}\mathrm{e}^x\frac{\partial}{\partial\xi} - \frac{1}{4}.\end{aligned} \tag{8}$$

According to [2, 3], the eigenvalue of the Casimir operator should be

$$\omega = j(j+1) - Z^2e^4 \tag{9}$$

where j is the total angular momentum and Z is the atomic number. ω is positive for at least $Z = 1, 2, \cdots$, up to 118, because $j \geqslant \frac{1}{2}$. The eigenvalue of Ω_3 should be related to the energy of a bound state by [2, 3]

$$\mu = \frac{Ze^2E}{\sqrt{m_\mathrm{e}^2 - E^2}} + \frac{1}{2} \tag{10}$$

which obviously need not to be restricted to integer values. (Note that the formula for μ is misprinted in [3], where the last term is 1 instead of $\frac{1}{2}$.) This observation reminds us to use projective unitary representations of $su(1,1)$ as in [5]. The classification is listed below [7]:

- The principal series $k = -\frac{1}{2} + \mathrm{i}\rho,\ \rho > 0,\ 0 \leqslant m_0 < 1,\ m = m_0 \pm n,\ n = 0, 1, 2, \ldots$.
- The complementary series $-\frac{1}{2} < k < 0,\ 0 \leqslant m_0 < 1,\ m_0(m_0-1) > k(k+1) \geqslant -\frac{1}{4},\ m = m_0 \pm n, n = 0, 1, \ldots$.
- The discrete series D_k^+, $k < 0$ and $m = -k, -k+1, \ldots$.
- The discrete series D_k^-, $k < 0$ and $m = k, k-1, \ldots$.

So we should use the projective discrete series D_k^+ with

$$k = -\sqrt{\omega + \tfrac{1}{4}} - \tfrac{1}{2} = -\sqrt{(j+\tfrac{1}{2})^2 - Z^2e^4} - \tfrac{1}{2} \tag{11}$$

and $\mu = -k + n,\ n = 0, 1, \ldots$. This will give us the correct energy spectrum:

$$E = \frac{m_\mathrm{e}}{\sqrt{1 + Z^2e^4/(\mu - \frac{1}{2})^2}}. \tag{12}$$

To conclude, we would like to remark that it is already known that the harmonic oscillator, Coulomb and Morse potentials are equivalent under certain transformations , and that they are supersymmetric shape-invariant potentials [8]. So it is not surprising that the Morse potential can be used in the Coulomb problem and that the system has hidden supersymmetric properties as remarked in [2, 3]. All these potentials are related to $su(1, 1)$ algebra [5, 9]. Since $su(1, 1)$ and $su(2)$ are both real forms of the complex Lie algebra $sl(2)$, unitary representations of $su(1, 1)$ will always be non-unitary representations of $su(2)$. However, we prefer to regard the representations as unitary with respect to $su(1, 1)$ because we believe unitarity is fundamental to quantum physics. The authors of [3] mentioned that the algebra of the Lorenz group is not necessarily unitary in physical applications. But underlying the non-unitary representations of the Lorenz group are actually the unitary representations of the encompassing Poincaré group in relativistic quantum physics [10]. As to the appearance of non-unitary representations of $su(1, 1)$ in the band structure problem [4], since the origin is unclear, it is still an open question deserving more research.

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