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Hydrogen Atom and Equivalent Form of the Lévy-Leblond Equation

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We discuss the equivalent form of the Lévy-Leblond equation such that the nilpotent matrices are two-dimensional. We show that this equation can be obtained in the non-relativistic limit of the (2+1)-dimensional Dirac equation. Furthermore, we analyze the case with four-dimensional matrices, propose a Hamiltonian for the equation in (3+1) dimensions, and solve it for a Coulomb potential. The quantized energy levels for the hydrogen atom are obtained, and the result is consistent with the non-relativistic quantum mechanics.

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An equivalent form of the Lévy-Leblond equation[1] proposed in Ref. [2] was shown to be consistent with the standard quantum mechanical results. The Lévy-Leblond equation is the analogue of the Dirac equation and describes spin-1/2 particles in the non-relativistic limit. In Refs. [2,3], it was shown that the equivalent form of the Lévy-Leblond equation can be employed to solve the step potential problem and the finite potential barrier problem. It was also shown that this equation is the non-relativistic limit of the Dirac equation and the Pauli Hamiltonian can be obtained from this equation by requiring it to be locally invariant.

In this work, we present this equation with two-dimensional nilpotent matrices and derive it from the (2+1)-dimensional Dirac equation. We further illustrate its applications by solving it for a Coulomb potential in (3+1) dimensions when the nilpotent matrices are 4-dimensional. We show that the known expression for the quantized energy levels of the hydrogen atom is obtained from this equation. The novelty of the approach employed herein is that the spectrum of the hydrogen atom is derived from the Lévy-Leblond equation which takes into account the spin of the particle in the non-relativistic limit.

In the following we introduce the equivalent form of the equivalent form of the Lévy-Leblond equation where the nilpotent matrices are 2-dimensional. It was shown in Refs. [1,2] that the Schrödinger equation can be derived from a first order equation similar to the manner in which the Klein–Gordon equation can be derived from the Dirac equation. The nilpotent matrices considered in Refs. [1,2] were 4-dimensional. Next, we consider the nilpotent matrices to be 2-dimensional. In (1+1) dimensions the equivalent form of the Lévy-Leblond equation is given by[2]

$$-i\partial_z\psi = (i\eta\partial_t + \eta^\dagger m)\psi, \tag{1}$$

where the matrix η is a 2×2 nilpotent matrix given by

$$\eta = \frac{\sigma_1 - i\sigma_2}{\sqrt{2}} = \sqrt{2}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

Following the procedure presented in Ref. [2], we can show that the probability current in this case as well is given by

$$J = \psi^\dagger(\eta + \eta^\dagger)\psi, \tag{3}$$
$$\rho = \psi^\dagger\eta^\dagger\eta\psi, \tag{4}$$

where $\eta + \eta^\dagger = \sqrt{2}\sigma_1$ and $\eta^\dagger\eta = I + \sigma_3$. In the momentum space, Eq. (1) is given by

$$p_z = (i\eta\partial_t + \eta^\dagger m)\psi. \tag{5}$$

The eigenvectors of the momentum operator are given by

$$e_{1,2} = \begin{pmatrix} \pm\sqrt{\frac{E}{m}} \\ 1 \end{pmatrix}, \tag{6}$$

which correspond to eigenvalues $\pm p_z = \pm\sqrt{2Em}$, respectively. Note that, in contrast to the equation with four-dimensional matrices,[2,3] the spin of the particle is not taken into account by Eq. (1). We have checked that the step potential problem and the finite step potential problems solved with Eq. (1) yield the results that are consistent with the standard quantum mechanical results as in the case of four-dimensional matrices.[2,3]

The (2+1)-dimensional version of the Lévy-Leblond equation for 2×2 matrices, in the momentum space, is given by

$$\mu_i p_i = (\eta E + \eta^\dagger m), \tag{7}$$

where $\mu_1 = I$ and $\mu_2 = i\sigma_3$. We can show that Eq. (7) is the non-relativistic limit of the Dirac equation in (2+1) dimensions. Consider the following form of the (2+1)-dimensional Dirac equation in momentum space,

$$\gamma_i p_i = (\sigma_1 E + i\sigma_2 m)\psi, \tag{8}$$

where $\gamma_1 = I$ and $\gamma_2 = i\sigma_3$. The above equation yields the dispersion relation of a massive relativistic

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particle in 2D. As shown in Ref. [3], we can substitute $\sigma_1 = (\eta + \eta^\dagger)/\sqrt{2}$ and $-i\sigma_2 = (\eta - \eta^\dagger)/\sqrt{2}$ and apply the non-relativistic limit $E - m \simeq E'$ and $E + m \simeq 2m$ to obtain Eq. (7) from Eq. (8).

Note also that in the limit $m = 0$, Eq. (8) reduces to the Dirac equation for massless fermions,

$$E = \sigma_i p_i, \tag{9}$$

which, as an example, is employed to describe massless fermions in condensed matter systems, such as graphene.

Here we present the Hamiltonian corresponding to the equivalent form of the Lévy-Leblond equation with four-dimensional matrices and discuss the constants of motion. The (3+1)-dimensional version of equation is given by[2,3]

$$-i\gamma_i \partial_i \psi = (i\eta\partial_t + \eta^\dagger m)\psi, \tag{10}$$

where γ_i are the Dirac gamma matrices, and $\eta = (\gamma_0 + i\gamma_5)/\sqrt{2}$. One of the issues in obtaining the Hamiltonian of Eq. (10) is that the matrix η is singular. Recently, a Hamiltonian was proposed[4] and we adopt a different approach herein. To obtain the Hamiltonian, we replace $\eta \to \eta' = \eta - \epsilon\eta^\dagger$ and analyze the limit $\epsilon \to 0$. We thereby obtain the following Hamiltonian for Eq. (10),

$$H = \eta'^{-1}(-i\gamma_i\partial_i - m\eta'^\dagger), \tag{11}$$

where $\eta' = \eta - \epsilon\eta^\dagger$ and we choose $\hbar = c = 1$. In the limit $\epsilon \to 0$, two of the eigenvalues of the Hamiltonian in Eq. (11) are finite as two approach infinities,

$$E_{1,2} = \frac{\boldsymbol{p}^2}{2m}, \tag{12}$$

$$E_{3,4} = -\frac{\boldsymbol{p}^2}{2m} + \frac{m}{\epsilon}. \tag{13}$$

The Hamiltonian yields the two finite energy states in addition to the negative energy states with an infinite part. The infinity associated with the negative energy states can be interpreted as the 'sea' of the filled negative energy states. For the negative energy states we can define the renormalized energy as

$$E'_{3,4} = E_{3,4} - \frac{m}{\epsilon} = -\frac{\boldsymbol{p}^2}{2m}.$$

The Hamiltonian (11) is not Hermitian, while the eigenvalues of the operator are real. Interestingly, the Hamiltonian (11) commutes with the total angular momentum operator $\boldsymbol{J} = \boldsymbol{L} + 1/2\boldsymbol{\Sigma}$ and the operators J^2, J_z and K, i.e.,

$$[H, J^2] = 0,$$
$$[H, J_z] = 0,$$
$$[H, K] = 0,$$

and the operator K also commutes with the total angular momentum operators J^2 and J_z. The operator K is given by

$$K = i\gamma_5\gamma_0(\boldsymbol{\Sigma}\cdot\boldsymbol{J} - \frac{1}{2}I), \tag{14}$$

$$= i\gamma_5\gamma_0(\boldsymbol{\Sigma}\cdot\boldsymbol{L} + I)$$
$$= i\begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot\boldsymbol{L} + I \\ -\boldsymbol{\sigma}\cdot\boldsymbol{L} - I & 0 \end{pmatrix}, \tag{15}$$

where $\boldsymbol{J} = \boldsymbol{L} + 1/2\boldsymbol{\Sigma}$. We can construct simultaneous eigenfunctions of the mutually commuting operators H, J^2, J_z and K. The corresponding eigenvalues of these operators are denoted by E, $j(j+1)$, m_j and $-\kappa$. We consider the following four component wave function as the simultaneous eigenfunction of these operators,

$$\psi = \begin{pmatrix} \psi_{\rm A} \\ \psi_{\rm B} \end{pmatrix} = \begin{pmatrix} g(r) Y_{l_{\rm A}}^{j,m_j}(\theta,\phi) \\ i f(r) Y_{l_{\rm B}}^{j,m_j}(\theta,\phi) \end{pmatrix} \equiv \begin{pmatrix} g(r) Y_{\rm A} \\ i f(r) Y_{\rm B} \end{pmatrix}, \tag{16}$$

and for the angular part $Y_{l_{\rm A},l_{\rm B}}^{j,m_j}(\theta,\phi)$ we consider the case of $\theta = 0$,[5]

$$Y_{l=j\mp 1/2}^{j,m_j}(\theta = 0, \phi) = \sqrt{\frac{j+1/2}{4\pi}} \begin{pmatrix} \pm\delta_{m,1/2} \\ \delta_{m,-12} \end{pmatrix}, \tag{17}$$

where $l_{\rm A} = j + 1/2$ and $l_{\rm B} = j - 1/2$. We choose $\theta = 0$ because the effect of the pseudo-scalar operator $\boldsymbol{\sigma}\cdot\boldsymbol{r}/r$ on Y_l^{j,m_j} is independent of θ.[5] The eigenvalues of the operator K are given by

$$K\psi = -\kappa\psi. \tag{18}$$

Since $J^2 = K^2 - 1/4I$, the eigenvalues of the two operators are related by $\kappa = \pm(j + 1/2)$. Plugging in for K yields the following equations

$$\boldsymbol{\sigma}\cdot\boldsymbol{L}\psi_{\rm A} = -i\kappa\psi_{\rm B} - \psi_{\rm A}, \tag{19}$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{L}\psi_{\rm B} = i\kappa\psi_{\rm A} - \psi_{\rm B}. \tag{20}$$

In addition, we have the following eigenvalue equations

$$\boldsymbol{J}^2\psi_{\rm A,B} = j(j+1)\psi_{\rm A,B}, \tag{21}$$

$$J_z\psi_{\rm A,B} = j_z\psi_{\rm A,B}. \tag{22}$$

Here we study the problem of an electron bound to a nucleus by a Coulomb potential for a hydrogen-like atom (for the analysis of the Dirac equation and further details can be found in Refs. [5–7]). For the case of a Coulomb potential, the Hamiltonian is given by

$$H = \eta'^{-1}(-i\gamma_i\partial_i - m\eta'^\dagger) + V(r), \tag{23}$$

where $V(r) = -Z\alpha/r$, $\alpha \approx 1/137$ is the fine structure constant, and Z is the atomic number of the atom. Since ψ is an eigenstate of the Hamiltonian,

$$H\psi = E\psi,$$
$$\eta'^{-1}(-i\gamma_i\partial_i - m\eta'^\dagger)\psi + V(r)\psi = E\psi,$$
$$(\gamma_i p_i - m\eta'^\dagger)\psi = (E - V(r))\eta'\psi,$$

where $p_i = -i\partial_i$. We obtain

$$\gamma_i p_i \psi = (\eta'(E - V(r)) + \eta'^{\dagger} m)\psi, \tag{24}$$

$$\begin{aligned}&\boldsymbol{\sigma}\cdot\boldsymbol{p}\begin{pmatrix}\psi_{\rm B}\\ -\psi_{\rm A}\end{pmatrix}\\ &=\frac{1}{\sqrt{2}}\begin{pmatrix}a'(E-V+m) & ia(E-V-m)\\ ia(E-V-m) & -a'(E-V+m)\end{pmatrix}\\ &\cdot\begin{pmatrix}\psi_{\rm A}\\ \psi_{\rm B}\end{pmatrix},\end{aligned} \tag{25}$$

where $a' = 1 - \epsilon$ and $a = 1 + \epsilon$. For brevity, we write

$$\boldsymbol{\sigma}\cdot\boldsymbol{p}\begin{pmatrix}\psi_{\rm B}\\ -\psi_{\rm A}\end{pmatrix} = \begin{pmatrix}h_1 & ih_2\\ ih_2 & -h_1\end{pmatrix}\begin{pmatrix}\psi_{\rm A}\\ \psi_{\rm B}\end{pmatrix}, \tag{26}$$

where

$$h_1(r) = a'/\sqrt{2}(E - V(r) + m), \tag{27}$$

$$h_2(r) = a/\sqrt{2}(E - V(r) - m). \tag{28}$$

The operator $\boldsymbol{\sigma}\cdot\boldsymbol{p}$ can be written in terms of the radial and angular operators as

$$\boldsymbol{\sigma}\cdot\boldsymbol{p} = \frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\Big(-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\Big). \tag{29}$$

The operator $\boldsymbol{\sigma}\cdot\boldsymbol{r}/r$ is a pseudo scalar and changes the parity of the state, i.e.,

$$\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}Y_{\rm A} = -Y_{\rm B}, \tag{30}$$

with $(\boldsymbol{\sigma}\cdot\boldsymbol{r}/r)^2 = 1$. We are interested in the effect of the operator $\boldsymbol{\sigma}\cdot\boldsymbol{r}/r$ on Y_l^{j,m_j}, and due to its pseudo-scalar nature its effect on Y_l^{j,m_j} is independent of θ.[5] Thus we choose $\theta = 0$ for the angular part and employ the expression given in Eq. (17) for the analysis. Plugging Eq. (29) in Eq. (26) we obtain the following two equations

$$\frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\Big(-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\Big)\psi_{\rm B} = h_1\psi_{\rm A} + ih_2\psi_{\rm B}, \tag{31}$$

$$-\frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r}\Big(-ir\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}\Big)\psi_{\rm A} = ih_2\psi_{\rm A} - h_1\psi_{\rm B}. \tag{32}$$

Plugging in $\psi_{\rm A} = g(r)Y_{\rm A}$ and $\psi_{\rm B} = if(r)Y_{\rm B}$ and using Eqs. (17), (19), (20), and (30) results in the following equations

$$\frac{\partial f}{\partial r} + \frac{1}{r}f + h_2 f + h_1 g + \frac{\kappa}{r}g = 0, \tag{33}$$

$$\frac{\partial g}{\partial r} + \frac{1}{r}g - h_2 g - h_1 f + \frac{\kappa}{r}f = 0. \tag{34}$$

The above equations are obtained for the $m = +1/2$ case. The analysis in the following also holds for the $m = -1/2$ case which yields similar results. Plugging in $f(r) = F(r)/r$ and $g(r) = G(r)/r$ and using Eqs. (27) and (28) we obtain

$$\frac{\partial F}{\partial r} + \Big(q_1 + \frac{q_2}{r}\Big)F + \Big(p_1 + \frac{p_2}{r} + \frac{\kappa}{r}\Big)G = 0, \tag{35}$$

$$\frac{\partial G}{\partial r} - \Big(q_1 + \frac{q_2}{r}\Big)G + \Big(-p_1 - \frac{p_2}{r} + \frac{\kappa}{r}\Big)F = 0. \tag{36}$$

Here we have defined the following constants

$$p_1 = \frac{a}{\sqrt{2}}(E + m),\ \ p_2 = \frac{a}{\sqrt{2}}Z\alpha, \tag{37}$$

$$q_1 = \frac{a'}{\sqrt{2}}(E - m),\ \ q_2 = \frac{a'}{\sqrt{2}}Z\alpha. \tag{38}$$

We postulate series solutions to Eqs. (35) and (36) in the form of

$$F(r) = e^{-\lambda r}\sum_{n=0}^{\infty} a_n r^{s+n}, \tag{39}$$

$$G(r) = e^{-\lambda r}\sum_{n=0}^{\infty} b_n r^{s+n}. \tag{40}$$

Plugging Eqs. (39) and (40) in Eqs. (35) and (36), we obtain the following equations for the coefficients of the two series

$$\begin{aligned}&q_2 a_{n+1} + (n+1)a_{n+1} + q_1 a_n + s a_{n+1}\\ &- \lambda a_n + p_2 b_{n+1} + \kappa b_{n+1} + p_1 b_n = 0,\end{aligned} \tag{41}$$

$$\begin{aligned}&- p_2 a_{n+1} + \kappa a_{n+1} - p_1 a_n - q_2 b_{n+1}\\ &+ (n+1)b_{n+1} - q_1 b_n + s b_{n+1} - \lambda b_n = 0.\end{aligned} \tag{42}$$

For $n = -1$, the above equations are given as follows:

$$q_1 a_{-1} + (q_2 + s)a_0 + p_1 b_{-1} + (p_2 + \kappa)b_0 = \lambda a_{-1}, \tag{43}$$

$$p_1 a_{-1} + p_2 a_0 + (q_1 + \lambda)b_{-1} + q_2 b_0 = \kappa a_0 + s b_0. \tag{44}$$

Setting $a_{-1} = b_{-1} = 0$ yields

$$(q_2 + s)a_0 + (p_2 + k)b_0 = 0, \tag{45}$$

$$p_2 a_0 + q_2 b_0 = \kappa a_0 + s b_0. \tag{46}$$

The solution to the above equations is

$$s = \pm\sqrt{\kappa^2 + q_2^2 - p_2^2}. \tag{47}$$

For the wave function to be normalizable we choose the positive sign of the square root. Furthermore, the series of $F(r)$ and $G(r)$ must terminate at some $n = n'$ for the state to be normalizable. This implies that the coefficients $a_i = b_i = 0$ for $i = n' + 1$ and we obtain the following relation

$$b_{n'} = \frac{\sqrt{q_1^2 - p_1^2} - q_1}{p_1}a_{n'}, \tag{48}$$

where we have chosen $\lambda = \sqrt{q_1^2 - p_1^2}$. Next we solve the recursion relations (41) and (42) for $n = n' - 1$,

$$\begin{aligned}&(q_1 - \lambda)a_{n'-1} + (q_2 + n' + s)a_{n'}\\ &+ p_1 b_{n'-1} + (p_2 + k)b_{n'} = 0,\end{aligned} \tag{49}$$

$$\begin{aligned}&- p_1 a_{n'-1} + (-p_2 + k)a_{n'} - (q_1 + \lambda)b_{n'-1}\\ &+ (-q_2 + n' + s)b_{n'} = 0.\end{aligned} \tag{50}$$

Multiplying Eq. (49) by $1/(\lambda - q_1)$ and Eq. (50) by $1/p_1$ and subtracting, we obtain the following equation

$$p_1((q_2 + n' + s)a_{n'} + (p_2 + k)b_{n'})) + (q_1 - \lambda)((-p_2 + k)a_{n'} + (-q_2 + n' + s)b_{n'}) = 0. \tag{51}$$

Taking the limit $\epsilon \to 0$ ($a = a' = 1$, $s = \kappa = j + 1/2$) and using Eq. (48) and $\lambda = \sqrt{-2Em}$ we obtain the relation for the energy level

$$E = -\frac{mZ^2\alpha^2}{2n^2}, \tag{52}$$

where $n = n' + s = n' + j + 1/2 = n' + l + 1$ is the principal quantum number. The above equation is the known expression for the energy level of a hydrogen-like atom. For the hydrogen atom $Z = 1$. Note that the parameter s has to be positive and since $s = \kappa$, only $\kappa = +(j + 1/2)$ is relevant. The functions $f(r)$ and $g(r)$ are therefore given by

$$\begin{aligned} f(r) &= e^{-\sqrt{-2Em}r} r^{\kappa-1} \sum_{m=0}^{\infty} a_m r^m \\ &= e^{-\frac{mZ\alpha}{n}r}\, r^l \sum_{m=0}^{\infty} a_m r^m, \end{aligned} \tag{53}$$

$$\begin{aligned} g(r) &= e^{-\sqrt{-2Em}r} r^{\kappa-1} \sum_{m=0}^{\infty} b_m r^{s+m} \\ &= e^{-\frac{mZ\alpha}{n}r}\, r^l \sum_{m=0}^{\infty} b_m r^m. \end{aligned} \tag{54}$$

The ground state wave function ($n' = 0$, $\kappa = 1$ and $j = 1/2$) of the Hydrogen atom can be written as

$$\psi_{\rm gd} = N\frac{1}{\sqrt{4\pi}}e^{-Zr/a_{\rm B}}\begin{pmatrix} g(r)\chi_{\rm s} \\ -if(r)\boldsymbol{\sigma}\cdot\hat{r}\chi_{\rm s}\end{pmatrix}, \tag{55}$$

where $a_{\rm B} = 1/\alpha m$ is Bohr's radius and

$$\boldsymbol{\sigma}\cdot\hat{r} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}, \tag{56}$$

$$\chi_{\rm s} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{57}$$

for the spin quantum number $m_{\rm s} = +1/2$ and $m_{\rm s} = -1/2$. For $m_{\rm s} = +1/2$ the wave function is given by

$$\psi_{\rm gd} = N\frac{1}{\sqrt{4\pi}}e^{-Zr/a_{\rm B}}\begin{pmatrix} 1 \\ 0 \\ -id_0\cos\theta \\ -id_0\sin\theta e^{i\phi}\end{pmatrix}. \tag{58}$$

For $m_{\rm s} = -1/2$

$$\psi_{\rm gd} = N\frac{1}{\sqrt{4\pi}}e^{-Zr/a_{\rm B}}\begin{pmatrix} 0 \\ 1 \\ -id_0\sin\theta e^{-i\phi} \\ id_0\cos\theta\end{pmatrix}, \tag{59}$$

where $d_0 = a_0/b_0 = \frac{2-\sqrt{2}Z\alpha}{2+\sqrt{2}Z\alpha}$. The normalization constant is given by

$$N = 2\sqrt{\pi}\Big(\frac{Z}{a_{\rm B}}\Big)^{3/2}\frac{2+\sqrt{2}Z\alpha}{\sqrt{2+Z^2\alpha^2}}. \tag{60}$$

In summary, we have presented an equivalent form of the Lévy-Leblond equation with two-dimensional nilpotent matrices and have shown that in (2+1) dimensions it can be obtained from the Dirac equation in the non-relativistic limit. In (3+1) dimensions we also proposed a Hamiltonian for this equation with four-dimensional nilpotent matrices and showed that the quantized energy levels of the hydrogen atom are obtained when the equation is solved for a Coulomb potential. We also derived the ground state wave function for spin up and down electrons for a hydrogen-like atom. The novelty of this approach is that the spin of the electron is taken into account in the non-relativistic limit to obtain the spectrum of the hydrogen atom. This analysis further illustrates the application of this equation which allows for additional insights into a problem corresponding to the spin of the particle.

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