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Dirac and Klein–Gordon particles in complex Coulombic fields: a similarity transformation

Omar Mustafa

Department of Physics, Eastern Mediterranean University, G Magusa, North Cyprus, Mersin 10, Turkey

E-mail: omar.mustafa@emu.edu.tr

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Abstract
The observation that the existence of the amazing reality and discreteness of the spectrum need not necessarily be attributed to the Hermiticity of the Hamiltonian is re-emphasized in the context of the non-Hermitian Dirac and Klein–Gordon Hamiltonians. Complex Coulombic potentials are considered.

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1. Introduction

In one of the first explicit studies of the non-Hermitian Schrödinger Hamiltonians, Caliceti *et al* [1] considered the imaginary cubic oscillator problem in the context of perturbation theory. They offered the first rigorous explanation why the spectrum in such a model may be real and discrete. Only many years later, after being quoted as just a mathematical curiosity [2] in the literature, the possible physical relevance of this result re-emerged and was emphasized [3]. Initiating, thereafter, an extensive discussion resulted in the proposal of the so-called $\mathcal{PT}$-symmetric quantum mechanics by Bender and Boettcher [4].

The spiritual wisdom of the new formalism lies in the observation that the existence of the real spectrum need not necessarily be attributed to the Hermiticity of the Hamiltonian. This observation has offered a sufficiently strong motivation for the continued interest in the complex, non-Hermitian, cubic model which may be understood as a characteristic representation of a very broad class of the so-called pseudo-Hermitian models with real spectra.

In such non-Hermitian settings, new intensive studies employed, for example, the idea of the strong coupling expansion [5], the complex WKB [6], Hill determinants and Fourier transformation [7], functional analysis [8], variational and truncation techniques [9], linear programming [10], pseudo-perturbation technique [11, 12], etc (cf [13–15]). However, such studies remain in the context of the Schrödinger Hamiltonian and need to be complemented by the non-Hermitian setting of Dirac and Klein–Gordon Hamiltonians. Let us start, say, with our forthcoming *oversimplified* generalized complex Coulombic examples.

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2. Generalized complex Coulombic fields in Dirac equation

A priori, a generalized Dirac–Coulomb equation for a mixed potential consists of a Lorentz-scalar Coulomb-like potential and a Lorentz-vector Coulomb potential. Whilst the former is added to the mass term of the Dirac equation, the minimal coupling is used, as usual, for the latter. The ordinary (Hermitian) Dirac Hamiltonian is exactly solvable in this case (cf, e.g., [16, 17]). In fact the exact solution to the Dirac equation for an electron in a Coulomb field was first obtained by Darwin [18] and Gordon [19].

The key idea is that instead of solving the Dirac–Coulomb equation directly, one can solve the second-order Dirac equation [16–22] which is obtained by multiplying the original equation, from the left, by a differential operator. The second-order equation is similar to the Klein–Gordon equation in a Coulomb field. The latter reduces to a form nearly identical to that of the Schrödinger equation and its solution can thus be inferred from the known non-relativistic solution.

In what follows, we recycle the *modified similarity transformation* (used by Mustafa and Barakat [17]) and obtain exact solutions for the non-Hermitian generalized Dirac and Klein–Gordon Coulomb Hamiltonians. Although this problem might be seen as *oversimplified*, it offers a benchmark for the *yet to be adequately explored* non-Hermitian relativistic Hamiltonians.

For a mixed scalar and electrostatic complex Coulombic potentials, i.e. $m \to m - \mathrm{i}A_2/r$ and $V(r) = -\mathrm{i}A_1/r$, the Dirac Hamiltonian reads (with the units $\hbar = c = 1$)

$$H = \vec{\alpha}\cdot\vec{p} + \beta(m - \mathrm{i}A_2/r) - \mathrm{i}A_1/r \tag{1}$$

where the Dirac matrices $\vec{\alpha}$ and β have their usual meanings. With the *similarity transformation*

$$S = a + \mathrm{i}b\beta\vec{\alpha}\cdot\hat{r} \qquad S^{-1} = \frac{a - \mathrm{i}b\beta\vec{\alpha}\cdot\hat{r}}{a^2 - b^2} \tag{2}$$

applied to the Dirac equation, one gets

$$H'\Psi' = E\Psi' \qquad H' = SHS^{-1} \qquad \Psi' = S\Psi \tag{3}$$

where $\hat{r}$ is the unit vector $\vec{r}/r$ and a and b are constants to be determined below. For the above central problem, the transformed wavefunction is given by

$$\Psi' = \begin{bmatrix} \mathrm{i}R(r)\Phi^{l}_{jm} \\ Q(r)\vec{\sigma}\cdot\hat{r}\Phi^{l}_{jm} \end{bmatrix}. \tag{4}$$

In a straightforward manner one obtains, through $E\Psi' = SHS^{-1}\Psi'$, two coupled equations for $R(r)$ (the upper component) and $Q(r)$ (the lower component):

$$\left[\partial_r + \frac{1}{r} + \frac{K}{r}\cosh\theta + \frac{\mathrm{i}A_1}{r}\sinh\theta + E\sinh\theta\right]R(r) = \xi_1(r)Q(r) \tag{5}$$

$$\left[\partial_r + \frac{1}{r} - \frac{K}{r}\cosh\theta - \frac{\mathrm{i}A_1}{r}\sinh\theta - E\sinh\theta\right]Q(r) = \xi_2(r)R(r) \tag{6}$$

with

$$\xi_1(r) = m - \frac{\mathrm{i}A_2}{r} + \frac{\mathrm{i}A_1}{r}\cosh\theta + \frac{K}{r}\sinh\theta + E\cosh\theta \tag{7}$$

$$\xi_2(r) = m - \frac{\mathrm{i}A_2}{r} - \frac{\mathrm{i}A_1}{r}\cosh\theta - \frac{K}{r}\sinh\theta - E\cosh\theta \tag{8}$$

where $K = \tilde{\omega}(j + 1/2), \tilde{\omega} = \mp 1$ for $l = j + \tilde{\omega}/2, \cosh\theta = (a^2 + b^2)/(a^2 - b^2)$ and $\sinh\theta = 2ab/(a^2 - b^2)$.

Incorporating the regular asymptotic behaviour of the radial functions near the origin, i.e. $R(r) \to a_1 r^{\gamma-1}$ and $Q(r) \to a_2 r^{\gamma-1}$ as $r \to 0$, and neglecting all constant terms proportional to mass and energy, one obtains

$$\gamma = \sqrt{K^2 + A_1^2 - A_2^2}. \tag{9}$$

The negative sign of the square root has to be discarded to avoid divergence of the wavefunctions at the origin.

It is obvious that one has the freedom to proceed either with the upper radial component $R(r)$ or with the lower component $Q(r)$. We shall, hereinafter, work with the upper component and determine $\sinh\theta$ and $\cosh\theta$ (hence the constants a and b) by requiring

$$-\mathrm{i}A_2 + \mathrm{i}A_1\cosh\theta + K\sinh\theta = 0 \tag{10}$$

$$K\cosh\theta + \mathrm{i}A_1\sinh\theta = \tilde{\omega}\gamma. \tag{11}$$

This requirement yields

$$\sinh\theta = -\mathrm{i}\tilde{\omega}\frac{[A_1\gamma - |K|A_2]}{\left[K^2 + A_1^2\right]} \qquad \cosh\theta = \frac{[|K|\gamma + A_1A_2]}{\left[K^2 + A_1^2\right]}. \tag{12}$$

Equations (5) and (6) would, as a result, imply

$$[E^2 - m^2]R(r) = \left[-\partial_r^2 - \frac{2}{r}\partial_r + \frac{(\gamma^2 + \tilde{\omega}\gamma)}{r^2} - \frac{2\mathrm{i}(mA_2 + A_1E)}{r}\right]R(r). \tag{13}$$

With the substitution $R(r) = r^{-1}U(r)$, it reads

$$[E^2 - m^2]U(r) = \left[-\partial_r^2 + \frac{(\gamma^2 + \tilde{\omega}\gamma)}{r^2} - \frac{2\mathrm{i}(mA_2 + A_1E)}{r}\right]U(r). \tag{14}$$

Evidently this equation is nearly identical to that of the non-Hermitian and $\mathcal{PT}$-*symmetric* radial Schrödinger–Coulombic one, of course with the irrational angular momentum quantum number $\ell' = -1/2 + \gamma + \tilde{\omega}/2 > 0$. Its solution can therefore be inferred from the known non-relativistic $\mathcal{PT}$-*symmetric* Coulomb problem (cf, e.g., Mustafa and Znojil [11] and Znojil and Levai [15] for more details on this problem). That is

$$[E^2 - m^2]^{1/2}\tilde{n} = [mA_2 + A_1E] \qquad \tilde{n} = n_r + \ell' + 1 > 0. \tag{15}$$

This in turn implies

$$\frac{E}{m} = \frac{A_1A_2}{\tilde{n}^2 - A_1^2} \pm \left[\left(\frac{A_1A_2}{\tilde{n}^2 - A_1^2}\right)^2 + \frac{\left(\tilde{n}^2 + A_2^2\right)}{\tilde{n}^2 - A_1^2}\right]^{1/2} \tag{16}$$

with $\tilde{n} = n - j - 1/2 + \gamma$, where $n_r = n - \ell + 1$ is the radial quantum number, n the principal quantum number and $\ell = j + \tilde{\omega}/2$ is the angular momentum quantum number.

In connection with the result in equation (16), several special cases should be interesting for they reveal the consequences of the above complexified non-Hermitian Dirac Hamiltonian:

- *Case 1*. For $A_2 = 0$, the complexified Coulomb energy $V(r) = -\mathrm{i}A_1/r = -\mathrm{i}Z\alpha/r$ ($\alpha \approx 1/137$) represents, say, the interaction energy of a point nucleus with an imaginary charge iZe and a particle of charge $-e$. In this case, $\gamma = \sqrt{(j + 1/2)^2 + (Z\alpha)^2}$ and

$$\frac{E}{m} = +\left[1 - \frac{(Z\alpha)^2}{(n - j - 1/2 + \gamma)^2}\right]^{-1/2} \tag{17}$$

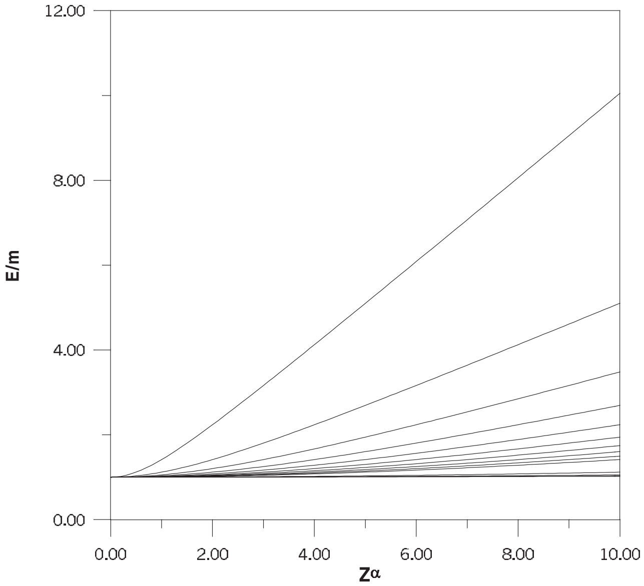

Figure 1. The ratio E/m of (18) at different vales of $Z\alpha$ for the states (from top to bottom) with the principal quantum number $n = 1, 2, 3, \ldots, 10, 20, 30, 40$ and 50.

where the negative sign is excluded because negative energies would not fulfil equation (15). For a vanishing potential ($Z = 0$) the energy eigenvalue is m. Obviously, unlike the ordinary (Hermitian) *Sommerfeld* fine structure formula, equation (17) suggests that a continuous increase of the coupling strength $Z\alpha$ from zero *pushes up* the electron states into the positive energy continuum, avoiding thereby the energy gap. Nevertheless, for states with $n = j + 1/2$ one obtains

$$\frac{E}{m} = +\sqrt{1 + \frac{(Z\alpha)^2}{n^2}}. \tag{18}$$

The ratio E/m in (18) is plotted in figure 1 for $n = 1, 2, 3, \ldots, 10, 20, \ldots, 50$. It is evident that as $n \to \infty$ the ratio $E/m \to 1$.

- *Case 2*. For $A_1 = 0$, $\gamma = \sqrt{K^2 - {A_2}^2}$ and equation (16) reads

$$\frac{E}{m} = \pm\left[1 + \frac{{A_2}^2}{(n - j - 1/2 + \gamma)^2}\right]^{1/2}. \tag{19}$$

In this case both signs are admissible and thus two branches of solutions exist, but not in the energy gap. The solutions of positive and negative energies exhibit identical behaviour, which reflects the fact that scalar interactions do not distinguish between positive and negative charges. Moreover, states with negative energies are *pulled down* to dive into the negative energy continuum, while states with positive energies are *pushed up* to dive into the positive energy continuum. Yet the *flown away states* phenomenon re-emerges and for $A_2 = |K|$ states with $n = j + 1/2$ *fly away* and disappear from the spectrum. Of course, one should worry about the critical values of the coupling (i.e., $A_{2,\mathrm{crit}} = |K|$), where imaginary energies would be manifested.

- *Case 3*. For $A_1 = A_2 = A$, $\gamma = |K|$ and

$$\frac{E}{m} = \frac{A^2}{\tilde{n}^2 - A^2} \pm \frac{\tilde{n}^2}{\tilde{n}^2 - A^2}. \tag{20}$$

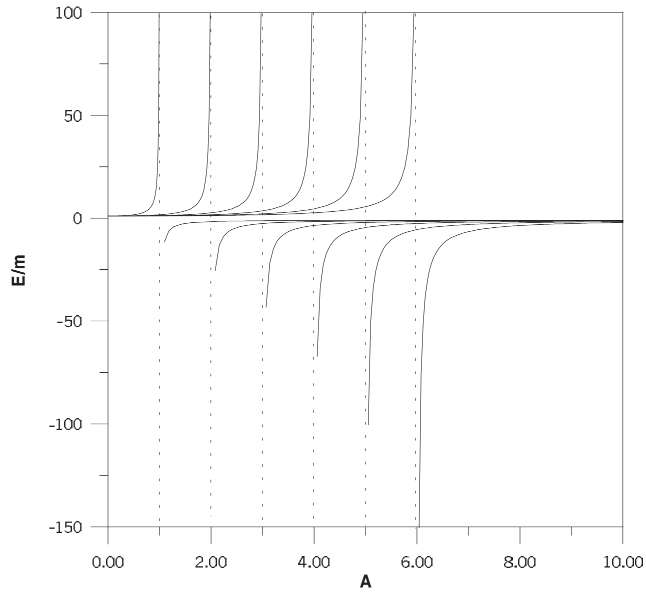

Figure 2. Part of the spectrum E/m of (21) at different values of the coupling A and for states with $n = 1, 2, 3, \ldots, 6$.

Obviously, the negative sign must be discarded for it implies $E = -m$ and thus contradicts equation (15). Hence, equation (20) reduces to

$$\frac{E}{m} = 1 + \frac{2A^2}{n^2 - A^2}. \tag{21}$$

Part of this spectrum (i.e., for the principal quantum number $n = 1, 2, 3, \ldots, 6$) is plotted in figure 2. As the coupling strength A increases from zero to n, the electron states are *pushed up* from $E = m$ into the positive energy continuum avoiding the energy gap between $-m$ and m. However, all states with $n = A$ *fly away* and disappear from the spectrum. Nevertheless, as A increases from n and at $A \to \infty$ all energy states *cluster* just below $E = -m$.

- *Case 4*. If we replace $(\gamma^2 + \tilde{\omega}\gamma)$ with $\tilde{\ell}(\tilde{\ell}+1)$, where $\tilde{\ell} = -1/2 + \sqrt{(\ell + 1/2)^2 + A_1^2 - A_2^2}$, equation (14) reduces to Klein–Gordon [23] with complex Coulomb-like Lorentz scalar and Lorentz vector potentials, $S(r) = -\mathrm{i}A_2/r$ and $V(r) = -\mathrm{i}A_1/r$, respectively. That is

$$[E^2 - m^2]U(r) = \left[-\partial_r^2 + \frac{\tilde{\ell}(\tilde{\ell}+1)}{r^2} - \frac{2\mathrm{i}(mA_2 + A_1E)}{r}\right]U(r) \tag{22}$$

which when compared with the non-Hermitian $\mathcal{PT}$-*symmetric*, the Schrödinger–Coulomb equation implies that

$$[E^2 - m^2]^{1/2}\tilde{N} = [mA_2 + A_1E] \qquad \tilde{N} = n_r + \tilde{\ell} + 1 > 0 \tag{23}$$

and

$$\frac{E}{m} = \frac{A_1A_2}{\tilde{N}^2 - A_1^2} \pm \left[\left(\frac{A_1A_2}{\tilde{N}^2 - A_1^2}\right)^2 + \frac{\left(\tilde{N}^2 + A_2^2\right)}{\tilde{N}^2 - A_1^2}\right]^{1/2}. \tag{24}$$

This, in turn, following similar analysis as above, yields

$$\frac{E}{m} = +\left[1 - \frac{A_1^2}{\tilde{N}^2}\right]^{-1/2} \qquad \tilde{N} = n - \ell - 1/2 + \sqrt{(\ell + 1/2)^2 + A_1^2} \tag{25}$$

for $A_2 = 0$ and $A_1 \neq 0$,

$$\frac{E}{m} = \pm\left[1 + \frac{A_2^2}{\tilde{N}^2}\right]^{1/2} \qquad \tilde{N} = n - \ell - 1/2 + \sqrt{(\ell + 1/2)^2 - A_2^2} \tag{26}$$

for $A_1 = 0$ and $A_2 \neq 0$, and

$$\frac{E}{m} = +\left[1 + \frac{2A^2}{n^2 - A^2}\right] \qquad \tilde{N} = n \tag{27}$$

for $A_1 = A_2 = A$. Clearly, spin-0 states follow similar scenarios as those for spin-1/2 states (i.e., e.g., *flown away states, pushed up into the positive continuum and/or pulled down into the negative continuum* etc).

3. Summary

To summarize, we have used a similarity transformation to extract exact energies for the Dirac particle in the generalized complex Coulomb potential. Within such non-Hermitian settings we have also obtained exact energies for the Klein–Gordon particle.

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