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

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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 reemphasized in the context of the non-Hermitian Dirac and Klein-Gordon Hamiltonians. Complex Coulombic potentials are considered.

In one of the first explicit studies of the non-Hermitian Schrödinger Hamiltonians, Caliceti et al [1] have considered the imaginary cubic oscillator problem in the context of perturbation theory. They have 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 reemerged and emphasized [3]. Initiating thereafter an extensive discussion which 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 prograning [10], pseudo-perturbation technique [11,12], ..etc (cf [13-15]). However such studies remain in the context of Schrödinger Hamiltonian and need to be complemented by the non-Hermitian setting of Dirac and Klein-Gordon Hamiltonians. Starting, say, with our forthcoming oversimplified generalized complex Coulombic examples.

A priori, a generalized Dirac - Coulomb equation for a mixed potential consists of a Lorentz-scalar Coulomb-like and a Lorentz-vector Coulomb potentials. 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 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 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 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 et al [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. \( m \to m - i A_2/r \) and \( V(r) = -i A_1/r \), the Dirac Hamiltonian reads (with the units \( \hbar = c = 1 \))

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

where the Dirac matrices \( \vec{\alpha} \) and \( \beta \) have their usual meanings. With the similarity transformation

\[
S = a + i b \beta \vec{\alpha} \cdot \hat{r}; \quad S^{-1} = \frac{a - i b \beta \vec{\alpha} \cdot \hat{r}}{a^2 - b^2}. \tag{2}
\]

applied to Dirac equation one gets

\[
H' \Psi' = E \Psi' \quad ; \quad H' = S H S^{-1}, \quad \Psi' = S \Psi, \tag{3}
\]
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 wave function is given by

\[
\Psi' = \begin{bmatrix}
    i R(r) \Phi_{jm}' \\
    Q(r) \vec{\sigma} \cdot \hat{r} \Phi_{jm}'
\end{bmatrix}.
\]  
(4)

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

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

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

with

\[
\xi_1(r) = m - \frac{i A_2}{r} + \frac{i A_1}{r} \cosh \theta + \frac{K}{r} \sinh \theta + E \cosh \theta,
\]  
(7)

\[
\xi_2(r) = m - \frac{i A_2}{r} - \frac{i A_1}{r} \cosh \theta - \frac{K}{r} \sinh \theta - E \cosh \theta.
\]  
(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

\[
\gamma = \sqrt{K^2 + A_2^2 - A_1^2}.
\]  
(9)
The negative sign of the square root has to be discarded to avoid divergence of the wave functions 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

$$ -i A_2 + i A_1 \cosh \theta + K \sinh \theta = 0, $$

(10)

$$ K \cosh \theta + i A_1 \sinh \theta = \bar{\omega} \gamma, $$

(11)

This requirement yields

$$ \sinh \theta = -i \bar{\omega} \left[ \frac{A_1 \gamma - |K| A_2}{|K|^2 + A_1^2} \right], \quad \cosh \theta = \left[ \frac{|K| \gamma + A_1 A_2}{|K|^2 + A_1^2} \right]. $$

(12)

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

$$ [E^2 - m^2] R(r) = \left[ -\partial_r^2 - \frac{2}{r} \partial_r + \frac{(\gamma^2 + \bar{\omega} \gamma)}{r^2} - \frac{2i (mA_2 + A_1 E)}{r} \right] R(r). $$

(13)

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

$$ [E^2 - m^2] U(r) = \left[ -\partial_r^2 + \frac{(\gamma^2 + \bar{\omega} \gamma)}{r^2} - \frac{2i (mA_2 + A_1 E)}{r} \right] U(r). $$

(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 $\ell' = -1/2 + \gamma + \bar{\omega}/2 > 0$. Its solution can therefore be inferred from the known non-relativistic $\mathcal{PT}$-symmetric Coulomb problem (c.f., e.g., Mustafa and Znojil [11] and
Znojil and Levai [15] for more details on this problem). That is

\[ \left[ E^2 - m^2 \right]^{1/2} \tilde{n} = [mA_2 + A_1 E] \ ; \ \tilde{n} = n_r + \ell' + 1 > 0. \]  

(15)

This in turn implies

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

(16)

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

In connection with the result in equation (16), several especial 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 \( V(r) = -i A_1/r = -i Z \alpha/r \) \((\alpha \approx 1/137)\) 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

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

(17)

where the negative sign is excluded because negative energies would not fulfill 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 hereby the energy gap. Nevertheless, for states with \( n = j + 1/2 \) one obtains
\[
\frac{E}{m} = + \sqrt{1 + \frac{(Z\alpha)^2}{n^2}},
\] (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
\[
\frac{E}{m} = \pm \left[ 1 + \frac{A_2^2}{(n - j - 1/2 + \gamma)^2} \right]^{1/2}, \quad (19)
\]

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 *flew away states* phenomenon reemerges 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., \( A_{2,\text{crit}} = |K| \)) where imaginary energies would be manifested.

- **Case 3**: For \( A_1 = A_2 = A \), \( \gamma = |K| \) and
\[
\frac{E}{m} = \frac{A^2}{\tilde{n}^2 - A^2} \pm \frac{\tilde{n}^2}{\tilde{n}^2 - A^2},
\] (20)

Obviously, the negative sign must be discarded for it implies \( E = -m \) and thus contradicts equation (15). Hence, equation (20) reduces to
\[
\frac{E}{m} = 1 + \frac{2A^2}{\tilde{n}^2 - A^2}, \quad (21)
\]

Part of this spectrum (i.e. for the principle 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 $-m$ to $m$. 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, $S(r) = -i A_2/r$ and $V(r) = -i A_1/r$, respectively. That is

$$[E^2 - m^2] U(r) = \left[-\partial_r^2 + \frac{\tilde{\ell} (\tilde{\ell} + 1)}{r^2} - \frac{2i (mA_2 + A_1 E)}{r}\right] U(r). \quad (22)$$

Which when compared with the non-Hermitian $\mathcal{PT}$—symmetric Schrödinger-Coulomb equation implies that

$$\left[E^2 - m^2\right]^{1/2} \tilde{N} = [mA_2 + A_1 E]; \quad \tilde{N} = n_r + \tilde{\ell} + 1 > 0, \quad (23)$$

and

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

This in turn, following similar analysis as above, yields

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

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

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

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

$$\frac{E}{m} = + \left[1 + \frac{2 A_2^2}{n^2 - A_2^2}\right] ; \quad \tilde{N} = n; \quad (27)$$

for $A_1 = 0$. For $A_2 = 0$, the lower energy states are exactly recovered from the original case.
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.).

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

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

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

[1] Caliceti E, Graffi S and Maioli M 1980 Commun. Math. Phys. **75** 51

[2] Alvarez G 1995 J. Phys. A: Math. Gen. 27 4589

[3] Buslaev V and Grecchi V 1993 J. Phys. A: Math. Gen. **26** 5541

[4] Bender C M and Boettcher S 1998 Phys. Rev. Lett. **24** 5243

Bender C M, Boettcher S and Meisinger P N 1999 J. Math. Phys. **40** 2201

[5] Fernandez F, Guardiola R, Ros J and Znojil M 1998 J. Phys. A: Math. Gen. **31** 10105

[6] Voros A 1983 Ann. Inst. H. Poincaré, Phys. Théor. **39** 211;

Delabaere E and Pham F 1998 Phys. Lett. A **250** 25 and 29;

Delabaere E and Trinh D T 2000 J. Phys. A: Math. Gen. **33** 8771

[7] Znojil M 1999 J. Phys. A: Math. Gen. **32** 7419.

[8] Mezinescu G A 2000 J. Phys. A: Math. Gen. **33** 4911;

Shin K C 2001 J. Math. Phys. **42** 2513

Japaridze G S 2002, J. Phys. A **35** 1709

[9] Bender C M, Cooper F, Meisinger P N and Savage V M 1999 Phys. Lett. A **259** 224.

Bender C M, Milton K A and Savage V M 2000 Phys. Rev. D **62** 085001

[10] Handy C R 2001 J. Phys. A: Math. Gen. **34** 5065;

Handy C R, Khan D, Wang Xiao-Xian and Tomczak C J 2001 J. Phys. A: Math. Gen. **34** 5593

[11] Mustafa O and Znojil M 2002 J. Phys. A **35** 8929, with further references

[12] Znojil M, Gemperle F and Mustafa O 2002 J. Phys. A: Math. Gen. **35** 5781

[13] Mostafazadeh A 2002 J. Math. Phys. **43** 205 with further references
[14] Dorey P, Dunning C and Tateo R 2001 J. Phys. A: Math. Gen. 34 5679 and L291

[15] Znojil M and Lévai G 2000 Phys. Lett. A 271 327

Znojil M 1999 Phys. Lett. A. 259 220

[16] Tutik R S 1992 J. Phys. A 25 L413.

[17] Mustafa O and Barakat T 1998 Commun. Theor. Phys. 30 411

[18] Darwin C G 1928, Soc. London, Ser. A118, 654

[19] Gordon W 1928, Z Phys. 48, 11

[20] Biedenharn L C 1962, Phys Rev 126, 845

Hostler L 1964, J Math Phys 5, 591

[21] Su J Y 1985, Phys Rev A32, 3251 with further references

[22] Wong M K F 1990, J Math Phys 31, 1677

[23] Barakat T, Odeh M and Mustafa O 1998, J Phys A31, 3469
Figure 2