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COMMENT

Comment on 'Kepler problem in Dirac theory for a particle with position-dependent mass'

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Abstract

This comment strongly disputes the recently published approach of Vakarchuk for a relativist problem with position-dependent mass.

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Back in 1973 Soff *et al* [1] found the analytic solution of the Dirac equation with an arbitrary mixing of vector and scalar potentials. The solution for the spin and angular variables was expressed in terms of spinor spherical harmonics, also called spherical spinors, resulting from the coupling among two-component spinors and spherical harmonic functions. The radial equations for the upper and lower components of the Dirac spinor were treated by the brute force power series expansion method. Recently the solution of this problem was used to speculate about the breaking of pseudospin symmetry in heavy nuclei [2]. It is also worthwhile to mention that a pedagogical approach to the Dirac equation coupled to a mixed vector–scalar Coulomb potential is already crystallized in a textbook [3].

In a recent paper published in this journal, Vakarchuk [4] approached the Dirac equation coupled to a vector Coulomb potential for a particle with an effective mass dependent on the position vector. He assumed that the effective mass has a form of a multipole expansion and took only the first three lowest terms into account. In effect, he considered a fermion in the background of a mixed vector–scalar Coulomb potential. Vakarchuk presented a more elegant method to find the analytic solution. Although it may seem strange, the author mapped the Dirac equation into an effective Schrödinger equation for all the components of the Dirac spinor. Nevertheless, I am afraid that something might be seriously wrong.

In order to clarify my criticisms, let me begin writing the Dirac equation with the effective mass and the Coulomb interaction as given in [4]:

$$[(\hat{\alpha}\hat{\mathbf{p}})c + m^* c^2\hat{\beta} + U]\psi = E\psi, \qquad m^* = m[1 + a/r + (\hat{\boldsymbol{\sigma}}\mathbf{n})\varphi], \qquad U = -e^2/r \tag{1}$$

where $\varphi = \varphi(r)$, a and e are constants. With $\bar{\psi}$ and $\hat{W}$ defined as

$$\psi = [(\hat{\alpha}\hat{\mathbf{p}})c + m^* c^2\hat{\beta} + (E - U)]\bar{\psi} \tag{2}$$

$$\hat{W} = \frac{mc^2}{2}\varphi^2 + mc^2\varphi\left(1+\frac{a}{r}\right)(\boldsymbol{\sigma}\mathbf{n}) - \frac{\mathrm{i}\hbar c}{2r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\varphi)\hat{\beta}'' \tag{3}$$

where $\mathbf{n} = \mathbf{r}/r$, $\hat{\boldsymbol{\sigma}}$ stands for a 4×4 matrix whose block diagonal elements are Pauli matrices and whose off-diagonal block elements are zero (I assume that $\boldsymbol{\sigma}$ does too), and with the 4×4 matrices $\hat{\beta}'$ and $\hat{\beta}''$ are defined as

$$\hat{\beta}' = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad \hat{\beta}'' = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \tag{4}$$

the author of [4] obtains

$$\left\{\frac{\hat{\mathbf{p}}^2}{2m} - \left(\frac{E}{mc^2}e^2 - mc^2a\right)\frac{1}{r} + \frac{1}{2mr^2}\left[\frac{\mathrm{i}\hbar}{c}(\boldsymbol{\sigma}\mathbf{n})(mc^2a\hat{\beta}'' + e^2\hat{\beta}') + m^2c^2a^2 - \frac{e^4}{c^2} + \hat{W}\right]\right\}\bar{\psi} = \left(\frac{E^2-m^2c^4}{2mc^2}\right)\bar{\psi}. \tag{5}$$

At this point the author of [4] states: *we note that our equation has the form of the Schrödinger equation for a particle moving in the Coulomb potential with an addition to the centrifugal barrier. Operator* $\hat{W}$ *is considered as a perturbation*. In addition he states: *as the operator in square brackets depends solely on the angles*... and introducing the operator

$$\hat{\Lambda} = -[(\boldsymbol{\sigma}\hat{\mathbf{L}}) + \hbar] + \frac{\mathrm{i}}{c}(\boldsymbol{\sigma}\mathbf{n})(mc^2a\hat{\beta}'' + e^2\hat{\beta}') \tag{6}$$

where $\hat{\mathbf{L}}$ is the angular momentum operator, equation (5) for $\hat{W} = 0$ is supposed to reduce to [4]:

$$\left\{-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + \frac{\hbar^2 l^*(l^*+1)}{2mr^2} - \left(\frac{E}{mc^2}e^2 - mc^2a\right)\frac{1}{r}\right\}R = \frac{E^2-m^2c^4}{2mc^2}R \tag{7}$$

where R is the radial part of $\bar{\psi}$, $\hbar^2 l^*(l^*+1)$ is the eigenvalue of the operator $\hat{\Lambda}(\hat{\Lambda}+\hbar)$ and

$$l^* = \sqrt{(j+1/2)^2 + (mca/\hbar)^2 - (e^2/\hbar c)^2} - 1/2 \mp 1/2 \tag{8}$$

with the upper sign for $j = l + 1/2$ and the lower sign for $j = l - 1/2$. Equation (7) is equation (3.5) in [4]. Now, the author of [4] states: *formally, equation (3.5) coincides with the non-relativistic Schrödinger equation for the Kepler problem*...

Now I am in the position to make the criticisms

(1) The presence of $\hat{\boldsymbol{\sigma}}$ in the third term in the effective mass is invalid since m^* and m are scalar quantities (1×1) and the term $\hat{\boldsymbol{\sigma}}\mathbf{n}$ is a 4×4 matrix.

(2) Equation (5) (equation (2.9) in [4]) does not have the form of a Schrödinger equation at all. This criticism is endorsed by observing that the 'centrifugal barrier' as well as the operator $\hat{W}$ contain off-diagonal matrix elements which mix the upper and lower components of the quadrispinor $\bar{\psi}$.

(3) It is not true that the operator in the square brackets of equation (5) depends solely on the angles. The presence of the term $\boldsymbol{\sigma}\mathbf{n}$ indicates a dependence on both angles and spin, even if $\hat{W} = 0$.

(4) Equation (7) (equation (3.5) in [4]) does not coincide with the non-relativistic Schrödinger equation for the Kepler problem. This would be true if l^* could only assume non-negative integer values but it does not in general. Therefore, one can neither identify R with the usual radial functions of the non-relativistic hydrogen problem R_{nl}, with $n = 0, 1, 2, \ldots$ and $l = 0, 1, 2, \ldots, (n-1)$ nor identify $(E^2 - m^2c^4)/(2mc^2)$ with the 'Bohr formula' for the energy levels.

The author of [4] introduces the term $(\hat{\boldsymbol{\sigma}}\mathbf{n})\varphi$ in the effective mass as a mechanism to stop the multipole expansion. That term only effects the term $\hat{W}$ which is discarded in later calculations (supposedly $\varphi = 0$). If he had just considered the approximation to the effective mass until the first-order term that misleading term would not appear in the latter calculations.

Even if $\hat{W} = 0$, the off-diagonal matrix elements in the 'centrifugal barrier' ruin the interpretation of a Schrödinger equation for $\bar{\psi}$. Unfortunately, equation (6) is a compact expression for two coupled equations involving the upper and lower components of the Dirac spinor.

Note that the presence of the terms $\boldsymbol{\sigma}\hat{\mathbf{L}}$ and $\boldsymbol{\sigma}\mathbf{n}$ makes $\hat{\Lambda}$ operate on the spin and angular variables. As a matter of fact, it is a generalization of the spin–orbit coupling operator $\hat{K}$, part of the toolkit for studying the Dirac equation with spherically symmetric potentials (see, e.g., [1–3]) and has the spinor spherical harmonic as eigenfunction. The eigenfunction of the operator $\hat{\Lambda}$ is not specified in [4]. In that case, what is the generalized spinor spherical harmonic?

If one insists that (7) is the non-relativistic Schrödinger equation for the Kepler problem then the Dirac eigenenergy solution (equation (4.4) in [4]) should have two branches of solutions, corresponding to positive and negative energies in a general circumstance. Furthermore, the condition for the existence of bounded solutions should be written as $a < e^2E/(m^2c^4)$ and not $a < e^2/(mc^2)$ (see equation (4.1)). Note, though, that the identification is believed to be true when $e^2 = mc^2|a|$, i.e., when the scalar potential, if it is either attractive or repulsive, is as strong as the vector potential.

Based on the above considerations, it is not difficult to strongly dispute not only the solutions found in [4], but also the conclusions manifested there.

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