On $v^2/c^2$ expansion of the Dirac equation with external potentials

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The $v^2/c^2$ expansion of the Dirac equation with external potentials is reexamined. A complete, gauge invariant form of the expansion to order $(1/c)^2$ is established which contains two additional terms, as compared to various versions existing in the literature. It is shown that the additional terms describe relativistic decrease of the electron spin magnetic moment with increasing electron energy.

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I. INTRODUCTION

A semirelativistic expansion of the Dirac equation ( up to $v^2/c^2$ terms ) is treated in almost all sources on quantum mechanics which include elements of the relativistic quantum theory. This expansion is of importance for problems involving electric and magnetic potentials for which exact solutions of the Dirac equation do not exist. The important examples include electron behavior in atoms, molecules and solids in the presence of a magnetic field. Surprisingly, various versions of the $v^2/c^2$ expansion quoted in the literature vary strongly from one source to the other [1, 2]. Almost all final forms are incomplete, quite a few are not gauge invariant.

The purpose of this contribution is to establish the complete and gauge invariant form of the $v^2/c^2$ expansion of the Dirac equation with electric and magnetic potentials and to interpret its physical content.

There exist two ways to carry the $v^2/c^2$ expansion. One is to consider large and small components of the wave function for electrons having positive ( or negative ) energies and to find the large component to the desired order of $1/c$ by iteration. In this method one has to take into account a changed normalization condition for the large components ( to the same order ). The other way is to use the Foldy-Wouthuysen unitary transformation in order to eliminate odd operators in the Dirac equation to the desired order. In this method the normalization condition is taken into account automatically since a unitary transformation is introduced.

Using this identity we obtain

$$H' = \exp(iS)H\exp(-iS) ,$$

where $S = (-i/2mc^2)\beta O$ . The exponentials in Eq. (2) are expanded into power series to the desired order of $1/c$, taking into account that $S \sim 1/c$. The choice of $S$ eliminates the odd term $O$ in Eq. (1), but introduces other odd terms of higher order in $1/c$. These are eliminated by two consecutive transformations $S'$ and $S''$ leading to the Hamiltonian $H_*$, which is free of odd operators to order $(1/c^2)$ . We do not quote this well known procedure [3, 4]. The final result is

$$H_* \approx U + \beta \left( mc^2 + \frac{1}{2mc^2}O^2 - \frac{1}{8m^2c^4}O^4 \right) - \frac{1}{8m^2c^4}O \left[ O, [O, O] \right] ,$$

where the brackets symbolize commutators.

Evaluating the above quantities we will use a 4x4 spin vector operator $\Sigma$.

$$\Sigma = \begin{vmatrix} \sigma & 0 \\ 0 & \sigma \end{vmatrix} .$$

It has the following property for any two vectors $C$ and $D$

$$(\alpha \cdot C)(\alpha \cdot D) = C \cdot D + i\Sigma \cdot (C \times D)$$

Using this identity we obtain

$$\frac{1}{2mc^2}O^2 = \frac{1}{2m}\Pi^2 + \mu \Sigma \cdot B ,$$

where $\mu = e\hbar/2m$ is the Bohr magneton and $B = \nabla \times A$ is a magnetic field. Clearly, the operator $O^4$ in Eq. (3) is just the square of $O^2$ given above.
The last term in Eq. (3) is calculated in two steps

\[ [O, U] = [\epsilon \alpha \cdot \Pi, U] = chie(\alpha \cdot E) , \tag{7} \]

where \( E = - \nabla V \) is an electric field. To evaluate the final commutator in Eq. (3) one needs two properties of the spin vector operator \( \Sigma \), which follow directly from the corresponding properties of \( \sigma \). We have

\[ \alpha_k \alpha_j = \delta_{kj} + i \epsilon_{kjl} \Sigma_l , \tag{8} \]

\[ [\alpha_k, \alpha_j] = - 2i \epsilon_{kjl} \Sigma_l , \tag{9} \]

where \( \delta_{kj} \) is the Kronecker delta and \( \epsilon_{kjl} \) is the anti-symmetric unit tensor. The summation convention over repeated subscripts is employed. Using Eqs (8) and (9) we calculate

\[ [\alpha \cdot \Pi, \alpha \cdot E] = \alpha_k \alpha_j [\Pi_k, E_j] + [\alpha_k, \alpha_j] E_j \Pi_k \]

\[ = (\delta_{kj} + i \epsilon_{kjl} \Sigma_l) \frac{\hbar \partial E_j}{i \partial x_k} - 2i \epsilon_{kjl} \Sigma_l E_j \Pi_k \]

\[ = - i \hbar (\nabla \cdot E) + i \Sigma \cdot (\nabla \times E) - 2i \Sigma \cdot (E \times \Pi) . \tag{10} \]

If the scalar potential \( V(r) \) has continuous first derivatives, then \( \nabla \times E = - \nabla \times \nabla V = 0 \), and the second term vanishes.

There exists an alternative way to evaluate the above commutator using directly Eq. (5)

\[ [\alpha \cdot \Pi, \alpha \cdot E] = - i \hbar (\nabla \cdot E) + i \Sigma \cdot (\nabla \times E) - 2i \Sigma \cdot (E \times \Pi) . \tag{11} \]

Both above forms are clearly equivalent. In agreement with the common practice we use the gradient sign \( \nabla \) to emphasize that the differentiation concerns the electric field alone and not the wave function.

The Hamiltonian (3) factorizes into two 2x2 blocks for upper and lower components of the wave function. For the upper block (positive energies) \( \beta \) is to be replaced by \(+1\) and \( \Sigma \) by \( \sigma \) [cf. Eq. (4)]. This finally gives for an electron with positive energies the following Hamiltonian

\[ H_0 = mc^2 - eV + \frac{1}{2m} \Pi^2 + \mu \sigma \cdot B + \frac{1}{2mc^2} (\frac{1}{2m} \Pi^2 + \mu \sigma \cdot B)^2 + \frac{e\hbar}{4mc^2} \sigma \cdot (E \times \Pi) + \frac{e\hbar^2}{8mc^2} (\nabla \cdot E) \]

\[ = \frac{1}{2mc^2} (\frac{1}{2m} \Pi^2 + \mu \sigma \cdot B)^2 + \frac{e\hbar}{4mc^2} \sigma \cdot (E \times \Pi) + \frac{e\hbar^2}{8mc^2} (\nabla \cdot E) . \tag{12} \]

This is the main result of our paper. Now we briefly discuss its physical content.

The fourth Pauli term is nonrelativistic although it results from the relativistic Dirac equation. As shown by Huang [21] and Feshbach and Villars [22], this term is related to electron’s Zitterbewegung.

The sixth term represents the spin-orbit interaction. It is written in the form calculated in Eq. (10) accounting for \( \nabla \times E = 0 \). The alternative form is [see Eq. (11)]

\[ H_{so} = \frac{e\hbar}{8mc^2} \sigma \cdot (E \times \Pi - \Pi \times E) . \tag{13} \]

In both forms the canonical momentum \( \Pi \) appears, assuring the gauge invariance of the Hamiltonian (12). Unfortunately, many well known references give noninvariant form with \( p \). As demonstrated by Feshbach and Villars [22], the spin-orbit term results from the linear contribution \( \Delta r \) to the electron displacement caused by the Zitterbewegung.

The seventh term proportional to \( \nabla \cdot E \) is the Darwin term. It is commonly interpreted as coming from the quadratic contribution \( (\nabla r)^2 \) to the electron displacement caused by the Zitterbewegung.

Finally, we want to discuss the fifth term in the Hamiltonian (12). Of all the enumerated references [1-20], only Corinaldesi and Strocchi [6], Messiah [17] and Hecht [20] quote the term \( (\sigma \cdot \Pi)^4 \), but, since it is nowhere separated into the orbital and spin parts and interpreted, it merits attention. To facilitate the discussion, it is helpful to consider first a simple situation of an electron in a constant magnetic field \( B \). In this case the Dirac equation has exact solutions and the positive eigenenergies are \[23, 24\]

\[ \epsilon = [(mc^2)^2 + 2mc^2 D(n, p_z, \pm)]^{1/2} , \tag{14} \]

where

\[ D(n, p_z, \pm) = \hbar \omega_c (n + \frac{1}{2}) + \frac{p_z^2}{2m} \pm \mu B , \tag{15} \]

in which \( n = 0, 1, 2, \ldots \) is the Landau quantum number and \( \omega_c = eB/m \) is the cyclotron frequency. Expanding the square root for \( 2D \ll mc^2 \), one obtains

\[ \epsilon \approx mc^2 + D - \frac{1}{2mc^2} D^2 . \tag{16} \]

We can identify the above expression with the first, third, fourth and fifth terms of the Hamiltonian (12) because, for the free electron, the eigenvalue of the orbital term \( \Pi^2/2m \) is \( \hbar \omega_c (n + 1/2) + p_z^2/2m \). Thus the fifth term in Eq. (12) corresponds to \((1/c)^2\) order in expansion of relativistic energy (including the Pauli term \( \mu \sigma \cdot B \)).

If we keep \( V = 0 \) but have otherwise arbitrary time independent magnetic field \( B(r) \), one can transform the Dirac Hamiltonian for positive energies into the form (see Case [22], Eriksen and Kolsrud [24])

\[ H' = \beta mc^2 [1 + \frac{2}{mc^2} (\frac{1}{2m} \Pi^2 + \mu \sigma \cdot B)]^{1/2} . \tag{17} \]

Expanding the square root and retaining the first three terms we obtain exactly the corresponding terms in Eq. (12).

Equation (15) shows that the spin contribution to the fifth term is not negligible in comparison to the orbital.
contribution. In fact, for the $n = 0$ Landau level the two contributions are exactly equal. In other words, the spin splitting of electron energies is equal to the orbital splitting.

Turning to the physical meaning of the term in question, it is often stated that the $-(1/8m^3c^2)\Pi^4$ term in the $v^2/c^2$ expansion reflects relativistic increase of the electron mass with increasing energy. As to the spin term, it was demonstrated by Zawadzki [27] that in the limit of vanishing magnetic fields the spin magnetic moment of a free relativistic electron is

$$\mu(\epsilon) = \frac{e\hbar}{2m(\epsilon)}, \quad (18)$$

where $m(\epsilon) = \epsilon/c^2$ is the energy dependent relativistic mass. Thus, for the electron at rest, $\epsilon = mc^2$, the spin magnetic moment reduces to the Bohr magneton, but, as the energy and the mass increase, the moment $\mu(\epsilon)$ decreases tending to zero. In the presence of magnetic field the decrease of the magnetic moment means that the spin splitting of the energy decreases with increasing energy. This decrease of the spin splitting can be seen from Eqs (14) and (15): for a given value of $B$ both the orbital and the spin splittings diminish as $n$ grows. It is then clear that the appearance of the complete fifth term in Eq. (12) which, as shown above, corresponds to the expansion (16) or, more precisely, to the expansion of Eq. (17), expresses not only relativistic increase of the electron mass but also relativistic decrease of the spin magnetic moment.

Since the orbital and spin contributions to the fifth term commute, one can perform the indicated squaring directly. In this form the $v^2/c^2$ expansion of the Dirac equation, as given by Eq. (12), contains two additional terms compared to the expressions given in the literature.

In summary, we have critically examined the semirelativistic expansion of the Dirac equation with scalar and vector potentials. The complete, gauge invariant form of the expansion to order $(1/c)^2$ is established. This form contains two additional terms, as compared to different expressions given in original papers and textbooks. It is demonstrated that the additional terms describe relativistic decrease of the electron spin magnetic moment with increasing electron energy.

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