Larmor diamagnetism and Van Vleck paramagnetism in relativistic quantum theory: The Gordon decomposition approach

Radosław Szmytkowski*
Atomic Physics Division, Department of Atomic Physics and Luminescence, Faculty of Applied Physics and Mathematics, Technical University of Gdańsk, Narutowicza 11/12, PL 80-952 Gdańsk, Poland
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We consider a charged Dirac particle bound in a scalar potential perturbed by a classical magnetic field derivable from a vector potential $\mathbf{A}(\mathbf{r})$. Using a procedure based on the Gordon decomposition of a field-induced current, we identify diamagnetic and paramagnetic contributions to the second-order perturbation-theory correction to the particle's energy. In contradiction to earlier findings, based on the sum-over-states approach, it is found that the resulting diamagnetic term is $\mathcal{E}_{\mathrm{d}}^{(2)}=(q^2/2m)\langle\Psi^{(0)}|\beta\mathbf{A}^2\Psi^{(0)}\rangle$, where $\Psi^{(0)}(\mathbf{r})$ is an unperturbed eigenstate and β is the matrix associated with the rest-energy term in the Dirac Hamiltonian.

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I. INTRODUCTION

A nonrelativistic quantum-mechanical problem of a spin-$\frac{1}{2}$ particle of electric charge q bound in a potential $V(\mathbf{r})$ perturbed by a classical static magnetic field derivable from a vector potential $\mathbf{A}(\mathbf{r})$ is frequently encountered in physics. It is well known [1–3] that if the perturbing magnetic field is weak and the potential $\mathbf{A}(\mathbf{r})$ has no singularities, the first-order perturbation-theory correction to an unperturbed energy level $E^{(0)}$ associated with an unperturbed wave function $\psi^{(0)}(\mathbf{r})$ may be expressed in the form

$$E^{(1)}=\langle\psi^{(0)}|\hat{H}^{(1)}\psi^{(0)}\rangle, \tag{1.1}$$

and the second-order one in the form

$$E^{(2)}=E_{\mathrm{d}}^{(2)}+E_{\mathrm{p}}^{(2)}, \tag{1.2}$$

with the contributions given by

$$E_{\mathrm{d}}^{(2)}=\langle\psi^{(0)}|\hat{H}^{(2)}\psi^{(0)}\rangle \tag{1.3}$$

and

$$E_{\mathrm{p}}^{(2)}=-\langle\psi^{(0)}|\hat{H}^{(1)}\hat{G}^{(0)}\hat{H}^{(1)}\psi^{(0)}\rangle. \tag{1.4}$$

Here $\hat{G}^{(0)}$ is the generalized Green operator of the unperturbed energy eigenproblem, associated with the energy level $E^{(0)}$, and the particle-field interaction operators $\hat{H}^{(1)}$ and $\hat{H}^{(2)}$ are

$$\hat{H}^{(1)}=\frac{iq\hbar}{2m}[\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{r})+\mathbf{A}(\mathbf{r})\cdot\boldsymbol{\nabla}]-\frac{q\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}(\mathbf{r}) \tag{1.5}$$

[with $\mathbf{B}(\mathbf{r})=\mathrm{curl}\,\mathbf{A}(\mathbf{r})$ and $\boldsymbol{\sigma}$ denoting the vector composed of the Pauli matrices] and

$$\hat{H}^{(2)}=\frac{q^2}{2m}\mathbf{A}^2(\mathbf{r}). \tag{1.6}$$

The contribution $E_{\mathrm{d}}^{(2)}$ is clearly positive and is called a *diamagnetic* (or Larmor) component of $E^{(2)}$. If $E^{(0)}$ is the ground-state energy of $\hat{H}^{(0)}$, the contribution $E_{\mathrm{p}}^{(2)}$ is negative; it is called a *paramagnetic* component of $E^{(2)}$ and is usually associated with the name of Van Vleck [1,3]. It is to be mentioned that since the vector potential $\mathbf{A}(\mathbf{r})$ is gauge dependent, the splitting of $E^{(2)}$ into $E_{\mathrm{d}}^{(2)}$ and $E_{\mathrm{p}}^{(2)}$ is not unique. Still, $E^{(2)}$ and $E^{(1)}$ are gauge invariant.

Feneuille [4] and, more recently, Aucar *et al.* [5] (cf. also Ref. [6]) attempted to explain the origin of diamagnetism within the framework of the Dirac relativistic quantum mechanics. Considerations based on the sum-over-states approach led these authors to the conclusion that diamagnetism had to be attributed to the "redressing" of a relativistic particle by a perturbing magnetic field. It was claimed that in the relativistic theory the diamagnetic contribution to the second-order energy expression was due to the negative-energy Dirac sea and was given by the following formula:

$$\mathcal{E}_{\mathrm{d}}^{(2)}=\frac{q^2}{2m}\langle\Psi^{(0)}|\mathbf{A}^2\Psi^{(0)}\rangle, \tag{1.7}$$

formally identical with its nonrelativistic counterpart (1.3) [7]. Here $\Psi^{(0)}(\mathbf{r})$ is a four-component eigenfunction of the zeroth-order (i.e., with the magnetic field switched off) Dirac Hamiltonian.

In the present paper, we reconsider the problem of determining diamagnetic and paramagnetic contributions to the second-order energy correction within the framework of the single-particle Dirac theory. Our approach is entirely different from that proposed in Refs. [4,5]. Instead of utilizing the sum-over-states scheme, we find a field-induced electric current in a linear-response approximation [8–12] and identify its diamagnetic and paramagnetic components. This is achieved using an ingenious (but, regrettably, not appreciated enough) procedure devised by Gordon [13–15] in the very early days of relativistic quantum mechanics. Subsequent use of the decomposed current in a formula linking the second-order energy correction $\mathcal{E}^{(2)}$ with a vector potential and the induced current allows us to identify diamagnetic and paramagnetic contributions to the former. Somewhat surprisingly,

*Electronic address: radek@mif.pg.gda.pl

our procedure leads us to the conclusion that $\mathcal{E}_{\mathrm{d}}^{(2)}$ is not given by Eq. (1.7) but rather has the form

$$\mathcal{E}_{\mathrm{d}}^{(2)}=\frac{q^2}{2m}\langle\Psi^{(0)}|\beta\mathbf{A}^2\Psi^{(0)}\rangle, \tag{1.8}$$

where β is the matrix associated with the rest-energy term in the Dirac Hamiltonian [notice that both expressions (1.7) and (1.8) have the same nonrelativistic limit].

Searching through the literature of the subject, we found that our idea of applying the Gordon decomposition to determine diamagnetic and paramagnetic contributions to magnetic properties was anticipated by a similar idea of Pyper who exploited it in the context of the theories of nuclear shielding [16–19] and hyperfine interaction [20]. There are, however, two main differences between Pyper's and our work. First, somewhat different physical problems are considered. Second, different procedures are used: while Pyper used the sum-over-states approach performing decompositions of *virtual transition currents* between unperturbed eigenstates of the zeroth-order Dirac Hamiltonian, we apply the linear-response approach decomposing the *field-induced current*.

II. RELATIVISTIC THEORY OF FIRST- AND SECOND-ORDER MAGNETIC CORRECTIONS TO ENERGY

A. Generalities

Consider a relativistic Dirac particle of electric charge q (for an electron $q=-e$) bound in a field of force derivable from a potential $V(\mathbf{r})$ (not necessarily of an electromagnetic origin) and perturbed by a classical static magnetic field characterized by a real nonsingular vector potential $\mathbf{A}(\mathbf{r})$. The time-independent wave equation for the particle has the form

$$[\hat{\mathcal{H}}-\mathcal{E}]\Psi(\mathbf{r})=0 \tag{2.1}$$

with the Hamiltonian

$$\hat{\mathcal{H}}=c\boldsymbol{\alpha}\cdot[-i\hbar\boldsymbol{\nabla}-q\mathbf{A}(\mathbf{r})]+\beta mc^2+V(\mathbf{r}). \tag{2.2}$$

Here $\boldsymbol{\alpha}$ and β are standard Dirac matrices. The Hamiltonian $\hat{\mathcal{H}}$ may be conveniently written as

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}^{(0)}+\hat{\mathcal{H}}^{(1)}, \tag{2.3}$$

where

$$\hat{\mathcal{H}}^{(0)}=-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2+V(\mathbf{r}), \tag{2.4}$$

$$\hat{\mathcal{H}}^{(1)}=-qc\boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{r}). \tag{2.5}$$

Henceforth, we shall assume that the magnetic field is weak, which implies that the operator $\hat{\mathcal{H}}^{(1)}$ may be treated as a small perturbation of $\hat{\mathcal{H}}^{(0)}$. Then, if $\Psi^{(0)}(\mathbf{r})$ and $\mathcal{E}^{(0)}$ are particular eigensolutions to the zeroth-order Dirac eigenproblem

$$[\hat{\mathcal{H}}^{(0)}-\mathcal{E}^{(0)}]\Psi^{(0)}(\mathbf{r})=0 \tag{2.6}$$

(for the sake of brevity, henceforth we shall assume that the eigenvalue $\mathcal{E}^{(0)}$ is nondegenerate), we may seek corresponding eigensolutions to the problem (2.1) in the form

$$\Psi(\mathbf{r})=\Psi^{(0)}(\mathbf{r})+\Psi^{(1)}(\mathbf{r})+\Psi^{(2)}(\mathbf{r})+\cdots, \tag{2.7}$$

$$\mathcal{E}=\mathcal{E}^{(0)}+\mathcal{E}^{(1)}+\mathcal{E}^{(2)}+\cdots. \tag{2.8}$$

From this, in the standard way we obtain equations

$$[\hat{\mathcal{H}}^{(0)}-\mathcal{E}^{(0)}]\Psi^{(1)}(\mathbf{r})=-[\hat{\mathcal{H}}^{(1)}-\mathcal{E}^{(1)}]\Psi^{(0)}(\mathbf{r}), \tag{2.9}$$

$$[\hat{\mathcal{H}}^{(0)}-\mathcal{E}^{(0)}]\Psi^{(2)}(\mathbf{r})=-[\hat{\mathcal{H}}^{(1)}-\mathcal{E}^{(1)}]\Psi^{(1)}(\mathbf{r})+\mathcal{E}^{(2)}\Psi^{(0)}(\mathbf{r}), \tag{2.10}$$

which are to be supplemented by pertinent boundary conditions. Imposing the constraints

$$\langle\Psi^{(0)}|\Psi^{(0)}\rangle=1,\quad\langle\Psi^{(0)}|\Psi^{(1)}\rangle=0, \tag{2.11}$$

from Eqs. (2.9) and (2.10) we infer

$$\mathcal{E}^{(1)}=\langle\Psi^{(0)}|\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle, \tag{2.12}$$

$$\mathcal{E}^{(2)}=\langle\Psi^{(0)}|\hat{\mathcal{H}}^{(1)}\Psi^{(1)}\rangle. \tag{2.13}$$

Formally, a solution to Eq. (2.9) is

$$\Psi^{(1)}(\mathbf{r})=-\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}^{(1)}\Psi^{(0)}(\mathbf{r}). \tag{2.14}$$

where $\hat{\mathcal{G}}^{(0)}$ [possessing the property $\hat{\mathcal{G}}^{(0)}\Psi^{(0)}(\mathbf{r})=0$] is the generalized Green operator for the zeroth-order Dirac Hamiltonian $\hat{\mathcal{H}}^{(0)}$, associated with the eigenvalue $\mathcal{E}^{(0)}$ of the latter. The operator $\hat{\mathcal{G}}^{(0)}$ has an integral kernel $\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')$ which is a solution to the equation

$$[\hat{\mathcal{H}}^{(0)}-\mathcal{E}^{(0)}]\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')=\mathcal{I}\,\delta(\mathbf{r}-\mathbf{r}')-\Psi^{(0)}(\mathbf{r})\Psi^{(0)\dagger}(\mathbf{r}') \tag{2.15}$$

(here $\mathcal{I}$ is the 4×4 unit matrix) supplemented by the same boundary conditions that have been imposed on $\Psi^{(0)}(\mathbf{r})$. On substituting the solution (2.14) into Eq. (2.13), we find

$$\mathcal{E}^{(2)}=-\langle\Psi^{(0)}|\hat{\mathcal{H}}^{(1)}\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle. \tag{2.16}$$

In principle, at this stage the problem of finding the first- and the second-order corrections to $\mathcal{E}^{(0)}$ may be considered as solved since Eq. (2.12) and, depending on the particular computational technique used, either Eq. (2.13) or Eq. (2.16) are suitable for computational purposes. Still, on a purely aesthetic ground, one may be slightly dissatisfied with the above results. First, Eqs. (1.1) and (2.12) are only seemingly similar since the operators $\hat{H}^{(1)}$ and $\hat{\mathcal{H}}^{(1)}$ have completely different structures [cf. Eqs. (1.5) and (2.5)]. Second, while in the nonrelativistic theory the second-order correction is the sum of the diamagnetic and paramagnetic parts [cf. Eqs. (1.2)–(1.4)], in the relativistic case the second-order correction has the compact form (2.16) which is, but only superficially [cf. again Eqs. (1.5) and (2.5)], similar to the nonrelativistic paramagnetic term (1.4). Thus, it is natural to ask the question: is it possible to transform the relativistic corrections (2.12) and (2.16) into expressions closely resembling their nonrelativistic counterparts? Below we shall show that the answer to this question is affirmative.

B. The Gordon decomposition approach

At first we focus on the first-order correction. The starting point is to rewrite Eq. (2.12) using the notion of the particle's current. According to the Dirac's theory, the current in the state $\Psi^{(0)}(\mathbf{r})$ is

$$\mathbf{J}^{(0)}(\mathbf{r})=qc\Psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi^{(0)}(\mathbf{r}). \tag{2.17}$$

It is then evident from Eqs. (2.5), (2.12), and (2.17) that

$$\mathcal{E}^{(1)}=-\int_{\mathbb{R}^3}d^3\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\mathbf{J}^{(0)}(\mathbf{r}). \tag{2.18}$$

In the next step, following Gordon [13–15], we rewrite Eq. (2.17) in the form

$$\mathbf{J}^{(0)}(\mathbf{r})=\tfrac{1}{2}qc\Psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi^{(0)}(\mathbf{r})+\tfrac{1}{2}qc\Psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi^{(0)}(\mathbf{r}), \tag{2.19}$$

the unperturbed Dirac equation (2.6) in the form

$$\Psi^{(0)}(\mathbf{r})=\frac{i\hbar}{mc}\beta\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\Psi^{(0)}(\mathbf{r})+\frac{\mathcal{E}^{(0)}-V(\mathbf{r})}{mc^2}\beta\Psi^{(0)}(\mathbf{r}), \tag{2.20}$$

and substitute Eq. (2.20) into the first term on the right-hand side of Eq. (2.19) and its Hermitian conjugate into the second term. After some elementary movements exploiting properties of the Dirac matrices $\boldsymbol{\alpha}$ and β, we arrive at

$$\mathbf{J}^{(0)}(\mathbf{r})=\frac{q\hbar}{m}\mathrm{Im}[\Psi^{(0)\dagger}(\mathbf{r})\beta\boldsymbol{\nabla}\Psi^{(0)}(\mathbf{r})]+\frac{q\hbar}{2m}\boldsymbol{\nabla}\times[\Psi^{(0)\dagger}(\mathbf{r})\beta\boldsymbol{\Sigma}\Psi^{(0)}(\mathbf{r})], \tag{2.21}$$

where $\boldsymbol{\Sigma}$ is the 4×4 matrix defined as

$$\boldsymbol{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{2.22}$$

Now, substitution of the decomposed current (2.21) into Eq. (2.18) leads, after elementary integration by parts, to the expression

$$\mathcal{E}^{(1)}=\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle, \tag{2.23}$$

where we have defined

$$\hat{\mathcal{H}}_{\beta}^{(1)}=\frac{iq\hbar}{2m}\beta[\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{r})+\mathbf{A}(\mathbf{r})\cdot\boldsymbol{\nabla}]-\frac{q\hbar}{2m}\beta\boldsymbol{\Sigma}\cdot\mathbf{B}(\mathbf{r}). \tag{2.24}$$

Comparison of Eqs. (1.1), (1.5), (2.23), and (2.24) shows their remarkable similarity. Thus, in the case of the first-order correction we have reached our goal.

Encouraged by the success achieved in the first-order case, we shall attempt to apply a similar procedure in the second-order case. On substituting the perturbation expansion (2.7) into the expression

$$\mathbf{J}(\mathbf{r})=qc\Psi^{\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi(\mathbf{r}), \tag{2.25}$$

defining the particle's current in the state $\Psi(\mathbf{r})$, and collecting terms of the same order in the perturbation, we obtain

$$\mathbf{J}(\mathbf{r})=\mathbf{J}^{(0)}(\mathbf{r})+\mathbf{J}^{(1)}(\mathbf{r})+\cdots, \tag{2.26}$$

where

$$\mathbf{J}^{(1)}(\mathbf{r})=2qc\,\mathrm{Re}[\Psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi^{(1)}(\mathbf{r})] \tag{2.27}$$

is the induced current linear in the perturbation. Then from Eqs. (2.5), (2.13), and (2.27) and from the reality of $\mathcal{E}^{(2)}$ [implied by Eq. (2.16)], it follows that

$$\mathcal{E}^{(2)}=-\tfrac{1}{2}\int_{\mathbb{R}^3}d^3\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\mathbf{J}^{(1)}(\mathbf{r}). \tag{2.28}$$

The decomposition of $\mathbf{J}^{(1)}(\mathbf{r})$ analogous to that in Eq. (2.21) is achieved by performing the Gordon decomposition of the current $\mathbf{J}(\mathbf{r})$ and making use of Eq. (2.26). After steps completely analogous to those which have led us to Eq. (2.21), we arrive at

$$\mathbf{J}(\mathbf{r})=\frac{q\hbar}{m}\mathrm{Im}[\Psi^{\dagger}(\mathbf{r})\beta\boldsymbol{\nabla}\Psi(\mathbf{r})]+\frac{q\hbar}{2m}\boldsymbol{\nabla}\times[\Psi^{\dagger}(\mathbf{r})\beta\boldsymbol{\Sigma}\Psi(\mathbf{r})]-\frac{q^2}{m}\mathbf{A}(\mathbf{r})\Psi^{\dagger}(\mathbf{r})\beta\Psi(\mathbf{r}). \tag{2.29}$$

Then the desired form of $\mathbf{J}^{(1)}(\mathbf{r})$ is obtained by substituting the expansion (2.7) into Eq. (2.29), subtracting Eq. (2.21) from the result, and retaining only first-order terms. This yields

$$\mathbf{J}^{(1)}(\mathbf{r})=\mathbf{J}_{\mathrm{d}}^{(1)}(\mathbf{r})+\mathbf{J}_{\mathrm{p}}^{(1)}(\mathbf{r}) \tag{2.30}$$

with

$$\mathbf{J}_{\mathrm{d}}^{(1)}(\mathbf{r})=-\frac{q^2}{m}\mathbf{A}(\mathbf{r})\Psi^{(0)\dagger}(\mathbf{r})\beta\Psi^{(0)}(\mathbf{r}) \tag{2.31}$$

and

$$\mathbf{J}_{\mathrm{p}}^{(1)}(\mathbf{r})=\frac{q\hbar}{m}\mathrm{Im}[\Psi^{(1)\dagger}(\mathbf{r})\beta\boldsymbol{\nabla}\Psi^{(0)}(\mathbf{r})+\Psi^{(0)\dagger}(\mathbf{r})\beta\boldsymbol{\nabla}\Psi^{(1)}(\mathbf{r})]+\frac{q\hbar}{m}\boldsymbol{\nabla}\times\mathrm{Re}[\Psi^{(0)\dagger}(\mathbf{r})\beta\boldsymbol{\Sigma}\Psi^{(1)}(\mathbf{r})]. \tag{2.32}$$

The above expressions for the induced currents $\mathbf{J}_{\mathrm{d}}^{(1)}(\mathbf{r})$ and $\mathbf{J}_{\mathrm{p}}^{(1)}(\mathbf{r})$ are strikingly similar to the following expressions:

$$\mathbf{j}_{\mathrm{d}}^{(1)}(\mathbf{r})=-\frac{q^2}{m}\mathbf{A}(\mathbf{r})\psi^{(0)\dagger}(\mathbf{r})\psi^{(0)}(\mathbf{r}), \tag{2.33}$$

$$\mathbf{j}_{\mathrm{p}}^{(1)}(\mathbf{r})=\frac{q\hbar}{m}\mathrm{Im}[\psi^{(1)\dagger}(\mathbf{r})\boldsymbol{\nabla}\psi^{(0)}(\mathbf{r})+\psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\nabla}\psi^{(1)}(\mathbf{r})]$$
$$+\frac{q\hbar}{m}\boldsymbol{\nabla}\times\mathrm{Re}[\psi^{(0)\dagger}(\mathbf{r})\boldsymbol{\sigma}\psi^{(1)}(\mathbf{r})] \tag{2.34}$$

for induced diamagnetic $[\mathbf{j}_{\mathrm{d}}^{(1)}(\mathbf{r})]$ and paramagnetic $[\mathbf{j}_{\mathrm{p}}^{(1)}(\mathbf{r})]$ currents derivable within the framework of the nonrelativistic Pauli theory [15]. Therefore, it seems judicious to identify $\mathbf{J}_{\mathrm{d}}^{(1)}(\mathbf{r})$ and $\mathbf{J}_{\mathrm{p}}^{(1)}(\mathbf{r})$ as induced relativistic diamagnetic and paramagnetic currents, respectively. Accordingly, from Eqs. (2.28) and (2.30) we have

$$\mathcal{E}^{(2)}=\mathcal{E}_{\mathrm{d}}^{(2)}+\mathcal{E}_{\mathrm{p}}^{(2)}, \tag{2.35}$$

where

$$\mathcal{E}_{\mathrm{d}}^{(2)}=-\tfrac{1}{2}\int_{\mathbb{R}^3}d^3\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\mathbf{J}_{\mathrm{d}}^{(1)}(\mathbf{r}) \tag{2.36}$$

and

$$\mathcal{E}_{\mathrm{p}}^{(2)}=-\tfrac{1}{2}\int_{\mathbb{R}^3}d^3\mathbf{r}\mathbf{A}(\mathbf{r})\cdot\mathbf{J}_{\mathrm{p}}^{(1)}(\mathbf{r}) \tag{2.37}$$

are the diamagnetic and paramagnetic contributions to $\mathcal{E}^{(2)}$, respectively. If we define

$$\hat{\mathcal{H}}_{\beta}^{(2)}=\frac{q^2}{2m}\beta\mathbf{A}^2(\mathbf{r}), \tag{2.38}$$

Eqs. (2.36) and (2.38) imply that $\mathcal{E}_{\mathrm{d}}^{(2)}$ may be rewritten as

$$\mathcal{E}_{\mathrm{d}}^{(2)}=\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(2)}\Psi^{(0)}\rangle \tag{2.39}$$

[cf. Eq. (1.8)]. Similarly, after elementary integrations by parts, Eqs. (2.37) and (2.32) yield

$$\mathcal{E}_{\mathrm{p}}^{(2)}=\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(1)}\rangle, \tag{2.40}$$

with $\hat{\mathcal{H}}_{\beta}^{(1)}$ defined in Eq. (2.24), or equivalently, after making use of Eq. (2.14),

$$\mathcal{E}_{\mathrm{p}}^{(2)}=-\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle. \tag{2.41}$$

For the sake of completeness, we observe that it is evident from Eq. (2.41) and from the reality of $\mathcal{E}_{\mathrm{p}}^{(2)}$ that the latter quantity may be rewritten in the form

$$\mathcal{E}_{\mathrm{p}}^{(2)}=\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}^{(1)}\Psi_{\beta}^{(1)}\rangle, \tag{2.42}$$

where

$$\Psi_{\beta}^{(1)}(\mathbf{r})=-\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}(\mathbf{r}), \tag{2.43}$$

obeying

$$\langle\Psi^{(0)}|\Psi_{\beta}^{(1)}\rangle=0, \tag{2.44}$$

is a solution to the inhomogeneous equation

$$[\hat{\mathcal{H}}^{(0)}-\mathcal{E}^{(0)}]\Psi_{\beta}^{(1)}(\mathbf{r})=-[\hat{\mathcal{H}}_{\beta}^{(1)}-\mathcal{E}^{(1)}]\Psi^{(0)}(\mathbf{r}) \tag{2.45}$$

subject to the same boundary conditions that have been imposed on $\Psi^{(1)}(\mathbf{r})$.

The expression (2.39) differs from Eq. (1.7) obtained in earlier works [4,5] based on the sum-over-states procedure. However, we believe that the physical character of our argumentation, based on the natural notion of the induced current, testifies in favor of our identification of the expression (2.39) as the relativistic analog of the nonrelativistic Larmor diamagnetic term (1.3).

With such an interpretation of $\mathcal{E}_{\mathrm{d}}^{(2)}$, it seems judicious to identify the paramagnetic correction (2.41) as the relativistic analog of the nonrelativistic Van Vleck term (1.4). This point of view is supported by the fact that since in the nonrelativistic limit $\mathcal{E}^{(2)}$ and $\mathcal{E}_{\mathrm{d}}^{(2)}$ tend to $E^{(2)}$ and $E_{\mathrm{d}}^{(2)}$, respectively, $\mathcal{E}_{\mathrm{p}}^{(2)}$ tends to $E_{\mathrm{p}}^{(2)}$. On the other hand, one might raise an objection pointing out the evident asymmetry between the right-hand sides of Eqs. (2.41) and (1.4). Continuing, one might argue that $\mathcal{E}_{\mathrm{p}}^{(2)}$ should be still decomposed in the following way:

$$\mathcal{E}_{\mathrm{p}}^{(2)}=\mathcal{E}_{\mathrm{p1}}^{(2)}+\mathcal{E}_{\mathrm{p2}}^{(2)}, \tag{2.46}$$

where

$$\mathcal{E}_{\mathrm{p1}}^{(2)}=-\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle, \tag{2.47}$$

$$\mathcal{E}_{\mathrm{p2}}^{(2)}=-\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\hat{\mathcal{G}}^{(0)}[\hat{\mathcal{H}}^{(1)}-\hat{\mathcal{H}}_{\beta}^{(1)}]\Psi^{(0)}\rangle, \tag{2.48}$$

and that $\mathcal{E}_{\mathrm{p1}}^{(2)}$ rather than $\mathcal{E}_{\mathrm{p}}^{(2)}$ is a right counterpart of the nonrelativistic Van Vleck term $E_{\mathrm{p}}^{(2)}$. With such an interpretation of $\mathcal{E}_{\mathrm{p1}}^{(2)}$, which may be also rewritten in the form

$$\mathcal{E}_{\mathrm{p1}}^{(2)}=\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi_{\beta}^{(1)}\rangle, \tag{2.49}$$

the term $\mathcal{E}_{\mathrm{p2}}^{(2)}$ is a separate correction to $\mathcal{E}^{(2)}$ of a purely relativistic origin, vanishing in the nonrelativistic limit.

It seems to us that the discussion whether $\mathcal{E}_{\mathrm{p}}^{(2)}$ or $\mathcal{E}_{\mathrm{p1}}^{(2)}$ is the relativistic counterpart of the Van Vleck term is of an academic character. Still, leaving aside interpretative questions, we observe that the decomposition (2.46) may be useful in actual calculations. Therefore, below we shall show that $\mathcal{E}_{\mathrm{p2}}^{(2)}$ may be written in a simpler form, which does not involve the generalized Green operator $\hat{\mathcal{G}}^{(0)}$. To this end, we observe that Eq. (2.15) may be rewritten as

$$\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')=\frac{i\hbar}{mc}\beta\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')+\frac{\mathcal{E}^{(0)}-V(\mathbf{r})}{mc^2}\beta\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')$$
$$+\frac{1}{mc^2}\beta\delta(\mathbf{r}-\mathbf{r}')-\frac{1}{mc^2}\beta\Psi^{(0)}(\mathbf{r})\Psi^{(0)\dagger}(\mathbf{r}'). \tag{2.50}$$

Interchanging the variables $\mathbf{r}\leftrightarrow\mathbf{r}'$ and making use of the property

$$\mathcal{G}^{(0)\dagger}(\mathbf{r}',\mathbf{r})=\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}'), \tag{2.51}$$

we transform Eq. (2.50) into

$$\begin{aligned}\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')=&-\frac{i\hbar}{mc}\boldsymbol{\nabla}'\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')\cdot\boldsymbol{\alpha}\beta\\&+\frac{\mathcal{E}^{(0)}-V(\mathbf{r}')}{mc^2}\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')\beta+\frac{1}{mc^2}\beta\delta(\mathbf{r}-\mathbf{r}')\\&-\frac{1}{mc^2}\Psi^{(0)}(\mathbf{r})\Psi^{(0)\dagger}(\mathbf{r}')\beta.\end{aligned} \tag{2.52}$$

After these preparatory steps, we rewrite Eq. (2.14) as

$$\begin{aligned}\Psi^{(1)}(\mathbf{r})=&\tfrac{1}{2}qc\int_{\mathbb{R}^3}d^3\mathbf{r}'\,\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')\boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{r}')\Psi^{(0)}(\mathbf{r}')\\&+\tfrac{1}{2}qc\int_{\mathbb{R}^3}d^3\mathbf{r}'\,\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')\boldsymbol{\alpha}\cdot\mathbf{A}(\mathbf{r}')\Psi^{(0)}(\mathbf{r}')\end{aligned} \tag{2.53}$$

and substitute Eqs. (2.52) and (2.20) into the first and second integrals, respectively, on the right-hand side of Eq. (2.53). Further integration by parts of the term containing $\boldsymbol{\nabla}'\mathcal{G}^{(0)}(\mathbf{r},\mathbf{r}')$ yields

$$\begin{aligned}\Psi^{(1)}(\mathbf{r})=&-\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}(\mathbf{r})-\frac{1}{2mc^2}\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}(\mathbf{r})\\&+\frac{1}{2mc^2}\langle\Psi^{(0)}|\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle\Psi^{(0)}(\mathbf{r}).\end{aligned} \tag{2.54}$$

Inserting the above result into Eq. (2.40), we arrive at

$$\begin{aligned}\mathcal{E}_{\mathrm{p}}^{(2)}=&-\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\hat{\mathcal{G}}^{(0)}\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle\\&-\frac{1}{2mc^2}\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle\\&+\frac{1}{2mc^2}\mathrm{Re}[\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle\langle\Psi^{(0)}|\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle].\end{aligned} \tag{2.55}$$

The first term on the right-hand side of Eq. (2.55) is seen to be identical with $\mathcal{E}_{\mathrm{p1}}^{(2)}$ given by Eq. (2.47), hence, we infer

$$\begin{aligned}\mathcal{E}_{\mathrm{p2}}^{(2)}=&-\frac{1}{2mc^2}\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle\\&+\frac{1}{2mc^2}\mathrm{Re}[\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle\langle\Psi^{(0)}|\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle].\end{aligned} \tag{2.56}$$

Equation (2.56) may be still simplified. Indeed, since the matrix element $\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\Psi^{(0)}\rangle$ is evidently real while, because of the easily proved relation

$$\beta\hat{\mathcal{H}}^{(1)}+(\beta\hat{\mathcal{H}}^{(1)})^{\dagger}=0, \tag{2.57}$$

the matrix element $\langle\Psi^{(0)}|\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle$ is purely imaginary, Eq. (2.56) becomes

$$\mathcal{E}_{\mathrm{p2}}^{(2)}=-\frac{1}{2mc^2}\mathrm{Re}\langle\Psi^{(0)}|\hat{\mathcal{H}}_{\beta}^{(1)}\beta\hat{\mathcal{H}}^{(1)}\Psi^{(0)}\rangle. \tag{2.58}$$

This is the sought suitable expression for the correction $\mathcal{E}_{\mathrm{p2}}^{(2)}$, which does not contain the generalized Green operator $\hat{\mathcal{G}}^{(0)}$.

Concluding this section, we mention that while the corrections $\mathcal{E}^{(1)}$ and $\mathcal{E}^{(2)}$ are gauge invariant, the decompositions (2.35) and (2.46) are not [cf. the remarks following Eq. (1.6)].

III. AN EXAMPLE: CHARGED PARTICLE IN A CENTRAL FIELD PERTURBED BY A UNIFORM MAGNETIC FIELD

As an example illustrating the above general discussion, we shall consider a Dirac particle bound in a central field of potential $V(r)$ perturbed by a static *uniform* magnetic field of induction $\mathbf{B}$ directed along the z axis of a coordinate system. In the symmetric gauge, which we adopt here, the vector potential of the magnetic field is

$$\mathbf{A}(\mathbf{r})=\tfrac{1}{2}\mathbf{B}\times\mathbf{r}. \tag{3.1}$$

We shall be interested in those solutions to the zeroth-order (i.e., magnetic-field-free) problem, associated with the *ground-state* energy $\mathcal{E}^{(0)}$, which are eigenfunctions of the projection of the total angular momentum on the field direction. Such solutions are of the form

$$\Psi_{M}^{(0)}(\mathbf{r})=\frac{1}{r}\begin{pmatrix}P^{(0)}(r)\Omega_{-1M}(\mathbf{n}_r)\\ iQ^{(0)}(r)\Omega_{+1M}(\mathbf{n}_r)\end{pmatrix}. \tag{3.2}$$

Here $M=\pm1/2$ is the magnetic quantum number, $\Omega_{\kappa M}(\mathbf{n}_r)$, with $\mathbf{n}_r=\mathbf{r}/r$, are spherical spinors while the real radial functions $P^{(0)}(r)$ and $Q^{(0)}(r)$, normalized according to

$$\int_0^{\infty}dr[P^{(0)2}(r)+Q^{(0)2}(r)]=1, \tag{3.3}$$

obey

$$\begin{pmatrix}mc^2+V(r)-\mathcal{E}^{(0)} & c\hbar(-d/dr-1/r)\\ c\hbar(d/dr-1/r) & -mc^2+V(r)-\mathcal{E}^{(0)}\end{pmatrix}\begin{pmatrix}P^{(0)}(r)\\ Q^{(0)}(r)\end{pmatrix}=0 \tag{3.4}$$

subject to the vanishing boundary conditions for $r\to0$ and $r\to\infty$.

Although the energy level $\mathcal{E}^{(0)}$ is twofold degenerate with respect to the magnetic quantum number M, we observe that the perturbation (2.5) does not mix states with different M. Therefore we may directly apply the results of Sec. II to determine the first and the second-order corrections to $\mathcal{E}^{(0)}$.

We begin with the first-order correction. In the particular case considered in this section, the "non-Gordon" Eq. (2.12) takes the form

$$\mathcal{E}_M^{(1)}=-\tfrac{1}{2}qcB\langle\Psi_M^{(0)}|(\mathbf{r}\times\boldsymbol{\alpha})_z\Psi_M^{(0)}\rangle \tag{3.5}$$

or, after utilizing the explicit form (3.2) of the unperturbed eigenfunction and after some angular momentum algebra,

$$\mathcal{E}_M^{(1)}=\frac{4M}{3}qcB\int_0^\infty dr\, rP^{(0)}(r)Q^{(0)}(r). \tag{3.6}$$

Alternatively, we might compute the correction $\mathcal{E}_M^{(1)}$ from the Gordon formula (2.23), which in the present case becomes

$$\mathcal{E}_M^{(1)}=-\frac{q\hbar B}{2m}\langle\Psi_M^{(0)}|\beta(\hat{\Lambda}_z+\Sigma_z)\Psi_M^{(0)}\rangle, \tag{3.7}$$

where $\hat{\Lambda}_z$ is the zth component of the orbital angular momentum operator

$$\hat{\boldsymbol{\Lambda}}=-i\mathbf{r}\times\boldsymbol{\nabla}. \tag{3.8}$$

After utilizing Eq. (3.2), Eq. (3.7) yields

$$\mathcal{E}_M^{(1)}=-\frac{2M}{3}\frac{q\hbar B}{m}\left(\int_0^\infty dr[P^{(0)2}(r)-Q^{(0)2}(r)]+\frac{1}{2}\right), \tag{3.9}$$

or equivalently, in virtue of the normalization condition (3.3),

$$\mathcal{E}_M^{(1)}=-\frac{4M}{3}\frac{q\hbar B}{m}\left(\int_0^\infty dr\, P^{(0)2}(r)-\frac{1}{4}\right). \tag{3.10}$$

Equations (3.6) and (3.9) [or Eq. (3.10)] provide two alternative methods for evaluating $\mathcal{E}_M^{(1)}$. In the nonrelativistic limit either from Eq. (3.9) or from Eq. (3.10), one infers the well-known result

$$\mathcal{E}_M^{(1)}\overset{c\to\infty}{\longrightarrow}-M\frac{q\hbar B}{m}. \tag{3.11}$$

Having computed the first-order correction, we turn to the problem of evaluating the second-order one. We wish to avoid utilizing the generalized Green function. In the non-Gordon approach this means we have to use

$$\mathcal{E}^{(2)}=-\tfrac{1}{2}qcB\langle\Psi_M^{(0)}|(\mathbf{r}\times\boldsymbol{\alpha})_z\Psi_M^{(1)}\rangle, \tag{3.12}$$

which is the specialized form of Eq. (2.13) and requires solving directly the inhomogeneous equation (2.9) for $\Psi_M^{(1)}(\mathbf{r})$. (Here and below we do not put the subscript M in second-order energy corrections since, as we shall see, they are independent of M.) To this end, we decompose

$$\Psi_M^{(1)}(\mathbf{r})=\tfrac{1}{2}qcB\sum_\kappa a_{\kappa M}\frac{1}{r}\begin{pmatrix}P_\kappa^{(1)}(r)\Omega_{\kappa M}(\mathbf{n}_r)\\ iQ_\kappa^{(1)}(r)\Omega_{-\kappa M}(\mathbf{n}_r)\end{pmatrix}, \tag{3.13}$$

where

$$a_{\kappa M}=i\oint_{4\pi}d^2\mathbf{n}_r\Omega_{\kappa M}^\dagger(\mathbf{n}_r)(\mathbf{n}_r\times\boldsymbol{\sigma})_z\Omega_{+1M}(\mathbf{n}_r). \tag{3.14}$$

The coefficients $a_{\kappa M}$ do not vanish only for $\kappa=-1$ or $\kappa=+2$. In these two cases their values are

$$a_{\kappa M}=\begin{cases}-\dfrac{4M}{3} & \text{for}\quad \kappa=-1,\\[2ex] -\dfrac{\sqrt{2}}{3} & \text{for}\quad \kappa=+2,\end{cases} \tag{3.15}$$

(notice that $a_{\kappa M}^2$ is independent of M). To enforce the orthogonality constraint in Eq. (2.11), we require

$$\int_0^\infty dr[P^{(0)}(r)P_{-1}^{(1)}(r)+Q^{(0)}(r)Q_{-1}^{(1)}(r)]=0. \tag{3.16}$$

On substituting the expansion (3.13) into Eq. (2.9), after employing the angular momentum algebra, we arrive at the inhomogeneous radial system

$$\begin{pmatrix}mc^2+V(r)-\mathcal{E}^{(0)} & c\hbar(-d/dr+\kappa/r)\\ c\hbar(d/dr+\kappa/r) & -mc^2+V(r)-\mathcal{E}^{(0)}\end{pmatrix}\begin{pmatrix}P_\kappa^{(1)}(r)\\ Q_\kappa^{(1)}(r)\end{pmatrix}=r\begin{pmatrix}Q^{(0)}(r)\\ P^{(0)}(r)\end{pmatrix}+\epsilon^{(1)}\begin{pmatrix}P^{(0)}(r)\\ Q^{(0)}(r)\end{pmatrix}\delta_{\kappa,-1}, \tag{3.17}$$

with $\epsilon^{(1)}=-3\mathcal{E}_M^{(1)}/2MqcB$, which is to be solved subject to the vanishing boundary conditions for $r\to0$ and $r\to\infty$. With the knowledge of the radial functions $P_\kappa^{(1)}(r)$ and $Q_\kappa^{(1)}(r)$, Eq. (3.12) becomes

$$\mathcal{E}^{(2)}=-\tfrac{1}{4}q^2c^2B^2\sum_{\kappa=-1,+2}a_{\kappa M}^2\int_0^\infty dr\, r[P^{(0)}(r)Q_\kappa^{(1)}(r)+Q^{(0)}(r)P_\kappa^{(1)}(r)]. \tag{3.18}$$

To find $\mathcal{E}^{(2)}$, we may use the Gordon approach as well. In the particular case considered here, the diamagnetic contribution (2.39) is

$$\mathcal{E}_{\rm d}^{(2)}=\frac{q^2B^2}{8m}\langle\Psi_M^{(0)}|\beta(r^2-z^2)\Psi_M^{(0)}\rangle \tag{3.19}$$

and is easily evaluated to be

$$\mathcal{E}_{\rm d}^{(2)}=\frac{q^2B^2}{12m}\int_0^\infty dr\, r^2[P^{(0)2}(r)-Q^{(0)2}(r)], \tag{3.20}$$

which in the nonrelativistic limit yields the well-known result

$$\mathcal{E}_{\mathrm{d}}^{(2)} \stackrel{c\to\infty}{\to} \frac{q^2B^2}{12m}\int_0^\infty dr\, r^2 P^{(0)2}(r). \tag{3.21}$$

In turn, the paramagnetic components, according to Eqs. (2.49) and (2.58), are

$$\mathcal{E}_{\mathrm{p1}}^{(2)} = -\frac{q\hbar B}{2m}\langle \Psi_M^{(0)}|\beta(\hat{\Lambda}_z+\Sigma_z)\Psi_{\beta M}^{(1)}\rangle, \tag{3.22}$$

$$\mathcal{E}_{\mathrm{p2}}^{(2)} = -\frac{q^2\hbar B^2}{8m^2c}\mathrm{Re}\langle \Psi_M^{(0)}|(\hat{\Lambda}_z+\Sigma_z)(\mathbf{r}\times\boldsymbol{\alpha})_z\Psi_M^{(0)}\rangle. \tag{3.23}$$

The contribution $\mathcal{E}_{\mathrm{p2}}^{(2)}$ is readily found to be

$$\mathcal{E}_{\mathrm{p2}}^{(2)} = \frac{q^2\hbar B^2}{12m^2c}\int_0^\infty dr\, rP^{(0)}(r)Q^{(0)}(r), \tag{3.24}$$

which obviously vanishes in the nonrelativistic limit. To find $\mathcal{E}_{\mathrm{p1}}^{(2)}$, we decompose

$$\Psi_{\beta M}^{(1)}(\mathbf{r}) = \frac{q\hbar B}{2m}\sum_{\kappa=-1,+2} a_{\kappa M}\frac{1}{r}\begin{pmatrix} P_{\beta\kappa}^{(1)}(r)\Omega_{\kappa M}(\mathbf{n}_r) \\ iQ_{\beta\kappa}^{(1)}(r)\Omega_{-\kappa M}(\mathbf{n}_r)\end{pmatrix} \tag{3.25}$$

with the coefficients $a_{\kappa M}$ given by Eq. (3.15) and with the constraint

$$\int_0^\infty dr[P_{\beta,-1}^{(1)}(r)P^{(0)}(r)+Q_{\beta,-1}^{(1)}(r)Q^{(0)}(r)]=0 \tag{3.26}$$

enforcing the orthogonality condition (2.44). Substitution of this expansion into the inhomogeneous equation (2.45) followed by application of Eq. (3.9) gives the following differential systems obeyed by the radial functions $P_{\beta\kappa}^{(1)}(r)$ and $Q_{\beta\kappa}^{(1)}(r)$:

$$\begin{pmatrix} mc^2+V(r)-\mathcal{E}^{(0)} & c\hbar(-d/dr-1/r) \\ c\hbar(d/dr-1/r) & -mc^2+V(r)-\mathcal{E}^{(0)}\end{pmatrix}\begin{pmatrix} P_{\beta,-1}^{(1)}(r) \\ Q_{\beta,-1}^{(1)}(r)\end{pmatrix} = \begin{pmatrix} (I_\beta^{(0)}-1)P^{(0)}(r) \\ (I_\beta^{(0)}+1)Q^{(0)}(r)\end{pmatrix}, \tag{3.27}$$

$$\begin{pmatrix} mc^2+V(r)-\mathcal{E}^{(0)} & c\hbar(-d/dr+2/r) \\ c\hbar(d/dr+2/r) & -mc^2+V(r)-\mathcal{E}^{(0)}\end{pmatrix}\begin{pmatrix} P_{\beta,+2}^{(1)}(r) \\ Q_{\beta,+2}^{(1)}(r)\end{pmatrix} = -\begin{pmatrix} 0 \\ Q^{(0)}(r)\end{pmatrix}, \tag{3.28}$$

where for brevity we have denoted

$$I_\beta^{(0)} = \int_0^\infty dr[P^{(0)2}(r)-Q^{(0)2}(r)] = 2\int_0^\infty dr\, P^{(0)2}(r)-1. \tag{3.29}$$

Equations (3.27) and (3.28) are to be solved subject to the vanishing boundary conditions for $r\to 0$ and $r\to\infty$. Once the solutions $P_{\beta\kappa}^{(1)}(r)$ and $Q_{\beta\kappa}^{(1)}(r)$ have been found, from Eqs. (3.22), (3.25), (3.15), and (3.26) we obtain

$$\mathcal{E}_{\mathrm{p1}}^{(2)} = \frac{2q^2\hbar^2B^2}{9m^2}\int_0^\infty dr[P^{(0)}(r)P_{\beta,-1}^{(1)}(r) + \tfrac{1}{4}Q^{(0)}(r)Q_{\beta,+2}^{(1)}(r)]. \tag{3.30}$$

In the nonrelativistic limit the right-hand sides of Eqs. (3.27) and (3.28) vanish. In conjunction with the constraint (3.26) this implies that in this limit both equations have only trivial solutions. From this we infer that $\mathcal{E}_{\mathrm{p1}}^{(2)} \to_{c\to\infty} 0$ (notice that this result is specific for the example considered here).

IV. CONCLUSIONS

We have presented the method, based on the Gordon decomposition of the field-induced current, for determination of diamagnetic and paramagnetic contributions to the second-order energy correction within the framework of the relativistic quantum theory based on the Dirac equation. Our results contradict earlier findings that the diamagnetic (Larmor) contribution is given by Eq. (1.7). Instead, we have found that this contribution is given by Eq. (1.8). We have also analyzed the paramagnetic (Van Vleck) contribution and found that it may be naturally split into two parts, one of which has a purely relativistic origin and vanishes in the nonrelativistic limit while the second one tends in the same limit to the nonrelativistic Van Vleck term. These inferences are in a qualitative agreement with those obtained by Pyper [16–19] in the context of the nuclear-shielding theory. The results presented by the latter author in Ref. [16] justify the supposition that a procedure analogous to that described in the present work should be applicable to many-electron systems within the framework of the Dirac-Hartree-Fock formalism, at least at the single-determinantal level.

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