Foldy-Wouthuysen transformation in strong magnetic fields and relativistic corrections for quantum cyclotron energy levels

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We carry out a direct iterative Foldy-Wouthuysen transformation of a general Dirac Hamiltonian coupled to an electromagnetic field, including the anomalous magnetic moment. The transformation is carried out through an iterative disentangling of the particle and antiparticle Hamiltonians in the expansion for higher orders of the momenta. The time-derivative term from the unitary transformation is found to be crucial in supplementing the transverse component of the electric field in higher orders. Final expressions are obtained for general combined electric and magnetic fields, including strong magnetic fields. The time derivative of the electric field is shown to enter only in the seventh order of the fine-structure constant if the transformation is carried out in the standard fashion. We put special emphasis on the case of strong fields, which are important for a number of applications, such as electrons bound in Penning traps.

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I. INTRODUCTION

The purpose of this paper is threefold: First, to discuss the role of nonstandard and standard Foldy-Wouthuysen transformations, up to seventh order in the momenta, second, to clarify the role of higher-order terms in the magnetic fields which become relevant for particles bound in strong magnetic fields (Penning traps), and third, to apply the results to the calculation of quantum cyclotron energy levels.

Let us start with the first purpose, which requires some background discussion. The Foldy-Wouthuysen transformation [1] is a cornerstone of the description of electronic bound states in simple atomic systems. The purpose of the transformation is to start from a (generalized) Dirac Hamiltonian and to disentangle the particle and antiparticle degrees of freedom. We recall that the Dirac Hamiltonian describes particles and antiparticles simultaneously, and the Foldy-Wouthuysen transformation is used to find separate effective Hamiltonians for the particle (positive-energy) and antiparticle (negative-energy) states. In simple cases, such as a free electron, one can disentangle the particle and antiparticle Hamiltonians to all orders in the coupling parameter [2], but this is, in general, not possible when the Dirac particle is bound in external fields because of difficulties in expressing infinite series of multicommutators in closed analytic form. One can do the exact transformation (to all orders in the momenta) only in rare cases. As a consequence, for atomic bound states, one resorts to a perturbative scheme, which involves an expansion in higher orders of the momenta or in powers of a suitably chosen coupling parameter. The coupling parameter can be the fine-structure constant $\alpha = \alpha_{\rm QED} \approx 1/137.036$ or a suitable generalization (see Ref. [3]).

For an electron bound to a nucleus, in the fourth order in the momenta, starting from the Dirac-Coulomb Hamiltonian, one obtains [2,4] the relativistic corrections to the hydrogen bound states, i.e., the relativistic p^4 correction, the zitterbewegung term (the Darwin term), and the spin-orbit coupling (Russell-Saunders coupling). The Foldy-Wouthuysen method was generalized to sixth order in the momenta in Ref. [5], using a nonstandard transformation given in Eq. (8) of Ref. [5], which makes the decoupling transformation computationally easier. It gives rise to a term (see Eq. (18) of Ref. [5]) which involves the time derivative of the electric field,

$$H \sim -\frac{e}{16m^3}\{\sigma \cdot \vec{\pi}, \sigma \cdot \dot{\vec{E}}\}, \tag{1}$$

where $\vec{\pi} = \vec{p} - e\vec{A}$ is the kinetic momentum (throughout this paper, $e = -|e|$ is the electron charge). Furthermore, $\vec{E}$ is the electric field, and $\{A, B\} = AB + BA$ denotes the anticommutator. One may eliminate the time derivative of the electric field by an additional unitary transformation given in Eq. (19) of Ref. [6].

Throughout this paper, we use the Coulomb gauge so that one can easily identify the longitudinal and transverse parts of the electric-field $\vec{E}$, which are related to the vector potential $\vec{A}$ as

$$\vec{A} = \vec{A}_\perp, \qquad \vec{E}_\parallel = -\vec{\nabla}A^0, \qquad \vec{E}_\perp = -\frac{\partial}{\partial t}\vec{A}, \tag{2}$$

where $\perp$ denotes the transverse (divergence-free) field and $\parallel$ denotes the longitudinal (curl-free) field component. Furthermore, we will use the convention,

$$V = eA^0 \tag{3}$$

for the binding potential (here, e is the electron charge). In the treatment of atomic bound states, the binding potential is often approximated by the Coulomb potential $V(r) = -Z\alpha/r$,

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where Z is the nuclear charge number, α is the fine-structure constant, and r is the distance of the orbiting particle and the nucleus. However, in the treatment of bound states in a Penning trap [7–9], the binding potential is given by the electric quadrupole field of the Penning trap, whereas an additional strong magnetic field provides the axial confinement. The binding Coulomb field is replaced by the binding field of the Penning trap.

The problem of the calculation of the higher-order corrections to the Foldy-Wouthuysen transformation has been considered, quite recently, in Ref. [10] where the general Hamiltonian for particles with arbitrary spin has been investigated. The special case of $s = 1/2$ has been treated in Eqs. (36)–(38) of Ref. [10]. Furthermore, in Eq. (7) of Ref. [11], a Hamiltonian has been indicated which has been obtained from the nonrelativistic quantum electrodynamics (NRQED) approach outlined in Ref. [12]. Indeed, in Ref. [12], the coefficients in the effective Hamiltonian were obtained by matching of the NRQED Hamiltonian, given in Eq. (1) of Ref. [12], with scattering amplitude calculations. It is an interesting question to compare the NRQED approach to the sixth-order generalization of the standard Foldy-Wouthuysen transformation, outlined in Refs. [1,2,4].

Thus, we here present an application of the *standard* Foldy-Wouthuysen transformation [1,2,4], which is based on the iterative elimination of "odd" operators in the Hamiltonian via unitary transformations, to sixth order in the momenta, for general electric and magnetic fields. Our approach is sufficiently general to be valid for strong magnetic fields and is, thus, applicable to electrons bound to Penning traps [7–9]. The bound states in Penning traps differ from atomic bound states in the sense that the primary binding fields are the static magnetic field, directed along the trap axis, and the electric quadrupole field of the trap. The standard Foldy-Wouthuysen approach, in higher orders, offers technical difficulties which are overcome in the current investigation.

In particular, we do not rely on any nonstandard transformations, which were otherwise used in Ref. [5]. As a consequence, we are able to compare the standard sixth-order Foldy-Wouthuysen approach to the generalized nonstandard Foldy-Wouthuysen transformations outlined in Ref. [5]. In the standard approach, one eliminates odd operators by a well-defined iterative procedure. Here, the odd operators are understood as the off-diagonal entries in the bispinor basis. Let us consider an example. For a Hermitian Hamiltonian H of the form

$$H = \begin{pmatrix} \mathcal{E} & O \\ O^\dagger & \mathcal{E}' \end{pmatrix}, \qquad H^\dagger = H, \tag{4}$$

where $\mathcal{E} = \mathcal{E}^\dagger$, $\mathcal{E}' = \mathcal{E}'^\dagger$ and O are 2×2 matrices, the odd operator is just O. The iterative elimination of O, through successive applications of the unitary transformations, is the aim of the Foldy-Wouthuysen method.

Units with $\hbar = c = \epsilon_0 = 1$ are employed. This paper is organized as follows. In Sec. II, we consider the scaling of operators for an electron bound in a Penning trap. This scaling is different from that encountered in an atom because the binding fields (in particular, the magnetic field) have to be given more weight. In particular, the magnetic field enters at a lower order in a generalized coupling parameter (generalized fine-structure constant) than in atomic bound systems. In fact, in Sec. II, we define suitable generalized coupling parameters for the electron bound in the Penning trap. In Sec. III, we carry out the main part of the calculations for the sixth-order and seventh-order Foldy-Wouthuysen transformation pertaining to bound electrons. We obtain general results which allow us to carry out a detailed comparison between the different approaches previously pursued in Refs. [5,6,10–12]. We then specialize the general expressions to the case of a Penning trap (Sec. IV) and derive a few higher-order terms, supplementing previous investigations [7–9]. These are important for the determination of the fine-structure constant from measurements of the anomalous magnetic moment of the electron. Finally, in Sec. V, we draw some conclusions.

II. PREPARATORY CONSIDERATIONS

A. Penning trap

We will attempt to devise a formalism for the systematic analysis of higher-order corrections to the bound energy levels for electrons bound in field configurations where the wave functions are spatially confined by the field geometry, and a discrete spectrum of bound states results. Due to the spatial confinement, one obtains a discrete spectrum of bound states. Our investigations are motivated, to a large extent, by the necessity to extend the usual Foldy-Wouthuysen formalism to situations with strong confining magnetic fields. An example is given by an electron confined in a Penning trap (see Refs. [7–9]).

In a Penning trap, one has a strong constant uniform confining magnetic field along the trap axis (the z axis), given as $\vec{B}_{\rm T} = \hat{e}_z B_{\rm T}$. The corresponding vector potential is

$$\vec{A}_{\rm T} = \tfrac{1}{2}(\vec{B}_{\rm T} \times \vec{r}) = \tfrac{1}{2}(\vec{B}_{\rm T} \times \vec{\rho}), \tag{5}$$

where $\vec{\rho}$ is the position vector on the xy plane,

$$\vec{\rho} = \vec{r}_\parallel = x\hat{e}_x + y\hat{e}_y. \tag{6}$$

We decompose the momentum operator as $\vec{p} = \vec{p}_\parallel + \vec{p}_\perp$, where $\vec{p}_\parallel = p_x\hat{e}_x + p_y\hat{e}_y$ and $\vec{p}_\perp = p_z\hat{e}_z$. The kinetic trap momentum $\vec{\pi}_{\rm T}$ is

$$\vec{\pi}_{\rm T} = \vec{p} - e\vec{A}_{\rm T} = \vec{p}_\parallel - \frac{e}{2}(\vec{B}_{\rm T} \times \vec{r}) + \vec{p}_\perp = \vec{\pi}_\parallel + \vec{p}_\perp, \tag{7}$$

$$\vec{\pi}_\parallel = \vec{p}_\parallel - \frac{e}{2}(\vec{B}_{\rm T} \times \vec{r}). \tag{8}$$

The scalar potential is A^0. The quadrupole potential V of the Penning trap is

$$V = eA^0 = V_0 \frac{z^2 - \frac{1}{2}\rho^2}{2d^2} = V_z + V_\parallel, \tag{9a}$$

$$V_z = \frac{1}{2} m\omega_z^2 z^2, \qquad V_\parallel = -\frac{1}{4} m\omega_z^2 \rho^2, \tag{9b}$$

$$\omega_z^2 = \frac{V_0}{md^2}, \tag{9c}$$

where $V_0 > 0$ and $d > 0$ are constants. Note that $V_\parallel$ is repulsive, whereas V_z is an attractive harmonic potential. We also note that V_0 has physical dimension of energy, and d has a physical dimension of length. We found it convenient to absorb the elementary charge e in the definition of V_0, which leads to a slight change in the notation as compared to Ref. [9]. We write the spin g factor of the electron as $g = 2(1+\kappa)$, where $\kappa \approx \alpha/(2\pi)$ is the anomalous magnetic-moment term [13]. The nonrelativistic Hamiltonian, including the anomalous magnetic-moment term, can be written as

$$H_0 = \frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2}{2m} + V - \frac{e}{2m}\kappa\vec{\sigma}\cdot\vec{B}_{\rm T} = \frac{(\vec{\sigma}\cdot\vec{\pi}_{\parallel})^2}{2m} - \frac{e}{2m}\kappa\vec{\sigma}\cdot\vec{B}_{\rm T} + \frac{p_z^2}{2m} + V. \tag{10}$$

Using the result,

$$(\vec{\sigma}\cdot\vec{\pi}_{\parallel})^2 = \vec{p}_{\parallel}^{\,2} - e\vec{L}\cdot\vec{B}_{\rm T} + \frac{m^2\omega_c^2}{4}\rho^2 - e\vec{\sigma}\cdot\vec{B}_{\rm T}, \tag{11}$$

$$\omega_c = \frac{|e|B_{\rm T}}{m}, \tag{12}$$

where ω_c is the cyclotron frequency and $\vec{L}$ is the angular momentum operator, one can write $H_0 = H_{\parallel} + H_{\sigma} + H_z$ as the sum of an orbital Hamiltonian $H_{\parallel}$ which acts on the xy plane, of a magnetic Hamiltonian H_{σ} which couples to the spin, and of a Hamiltonian H_z which confines the particle along the z axis, in a harmonic potential due to the quadrupole field of the trap,

$$H_0 = H_{\parallel} + H_{\sigma} + H_z, \tag{13a}$$

$$H_{\parallel} = \frac{\vec{p}_{\parallel}^{\,2}}{2m} - \frac{e}{2m}\vec{L}\cdot\vec{B}_{\rm T} + \frac{m\omega_c^2}{8}\rho^2 + V_{\parallel}, \tag{13b}$$

$$H_{\sigma} = -\frac{e}{2m}(1+\kappa)\vec{\sigma}\cdot\vec{B}_{\rm T}, \tag{13c}$$

$$H_z = \frac{p_z^2}{2m} + V_z. \tag{13d}$$

Due to its harmonic-oscillator structure, H_z can be written as

$$H_z = \frac{p_z^2}{2m} + \frac{1}{2}m\omega_z^2 z^2 = \omega_z\left(a_z^{\dagger}a_z + \frac{1}{2}\right), \tag{14}$$

where the lowering and raising operators a_z and $a_z^{\dagger}$ are the usual ones for a quantum harmonic oscillator,

$$a_z = \sqrt{\frac{m\omega_z}{2}}z + i\left(\frac{1}{2m\omega_z}\right)^{1/2}p_z, \tag{15a}$$

$$a_z^{\dagger} = \sqrt{\frac{m\omega_z}{2}}z - i\left(\frac{1}{2m\omega_z}\right)^{1/2}p_z. \tag{15b}$$

With reference to Eq. (13b), we have the relations,

$$H_{\parallel} = \frac{\vec{p}_{\parallel}^{\,2}}{2m} + \frac{\omega_c}{2}L_z + \frac{m(\omega_c^2 - 2\omega_z^2)}{8}\rho^2 = \omega_{(+)}\left(a_{(+)}^{\dagger}a_{(+)} + \frac{1}{2}\right) - \omega_{(-)}\left(a_{(-)}^{\dagger}a_{(-)} + \frac{1}{2}\right), \tag{16a}$$

$$\omega_{(+)} = \frac{1}{2}\left(\omega_c + \sqrt{\omega_c^2 - 2\omega_z^2}\right), \tag{16b}$$

$$\omega_{(-)} = \frac{1}{2}\left(\omega_c - \sqrt{\omega_c^2 - 2\omega_z^2}\right) = \omega_{\rm m} \approx \frac{\omega_z^2}{2\omega_c}. \tag{16c}$$

The quantities $\omega_{(+)}$ and $\omega_{(-)}$ are corrected cyclotron (ω_c) and magnetron ($\omega_{\rm m}$) frequencies; they correspond to the conventions used in Eq. (2.14) of Ref. [9]. Physically, we can understand the minus sign in front of the $\omega_{(-)}$ term in Eq. (16a) in terms of the repulsive character of the potential $V_{\parallel}$ defined in Eq. (9b). The lowering and raising operators $a_{(+)}$, $a_{(-)}$, $a_{(+)}^{\dagger}$, and $a_{(-)}^{\dagger}$ are given in Eqs. (2.48a) and (2.48b) of Ref. [9]. The operators $a_{(+)}$ and $a_{(+)}^{\dagger}$ are associated with the cyclotron motion,

$$a_{(+)} = \left(\frac{m}{2(\omega_{(+)} - \omega_{(-)})}\right)^{1/2}(V_{(+)x} - iV_{(+)y}), \tag{17}$$

$$a_{(+)}^{\dagger} = \left(\frac{m}{2(\omega_{(+)} - \omega_{(-)})}\right)^{1/2}(V_{(+)x} + iV_{(+)y}), \tag{18}$$

and we will consider the operator $\vec{V}_{(+)}$, whose x and y components enter the definition of $a_{(+)}$ and $a_{(+)}^{\dagger}$ in the following, but first, let us consider the lowering and raising operators of the magnetron motion. One has the lowering operator $a_{(-)}$ and the raising operator $a_{(-)}^{\dagger}$,

$$a_{(-)} = \left(\frac{m}{2(\omega_{(+)} - \omega_{(-)})}\right)^{1/2}(V_{(-)x} + iV_{(-)y}), \tag{19}$$

$$a_{(-)}^{\dagger} = \left(\frac{m}{2(\omega_{(+)} - \omega_{(-)})}\right)^{1/2}(V_{(-)x} - iV_{(-)y}). \tag{20}$$

The quantum-mechanical formulation of the vector-valued operators $\vec{V}_{(+)}$ and $\vec{V}_{(-)}$ can, in principle, be inferred from the quantum-classical correspondence indicated in Eqs. (2.13) and (2.42) of Ref. [9]. The operators $\vec{V}_{(+)}$ and $\vec{V}_{(-)}$ are vector valued and act on the xy plane. It is instructive to indicate the explicit formulas,

$$\vec{V}_{(+)} = \frac{\vec{p}_{\parallel}}{m} + \frac{1}{2}\sqrt{\omega_c^2 - 2\omega_z^2}(\hat{\rm e}_z \times \vec{\rho}), \tag{21a}$$

$$\vec{V}_{(-)} = \frac{\vec{p}_{\parallel}}{m} - \frac{1}{2}\sqrt{\omega_c^2 - 2\omega_z^2}(\hat{e}_z \times \vec{\rho}). \tag{21b}$$

An interesting feature is that the algebra of the cyclotron and magnetron lowering and raising operators commute

$$[a_{(-)}, a_{(+)}] = [a_{(-)}, a_{(+)}^{\dagger}] = [a_{(-)}^{\dagger}, a_{(+)}^{\dagger}] = 0. \tag{22}$$

This means that we can raise cyclotron and magnetron quantum numbers independently by using the $a_{(+)}$ and $a_{(+)}^{\dagger}$, and $a_{(-)}$ and $a_{(-)}^{\dagger}$ operators.

B. Unperturbed eigenfunctions

Eigenfunctions of the unperturbed nonrelativistic Hamiltonian H_0 [see Eqs. (10) and (13)] are described by the spin projection quantum number s, the axial quantum number k, and the magnetron quantum number ℓ, illustrating the fact that an electron bound in a Penning trap merely constitutes an "artificial atom" with the trap fields replacing the binding Coulomb field. The quantum numbers take the following values:

$$k = 0, 1, 2, \ldots, \quad \text{(axial)}, \tag{23}$$

$$\ell = 0, 1, 2, \ldots, \quad \text{(magnetron)}, \tag{24}$$

$$n = 0, 1, 2, \ldots, \quad \text{(cyclotron)}, \tag{25}$$

$$s = \pm 1, \quad \text{(spin)}. \tag{26}$$

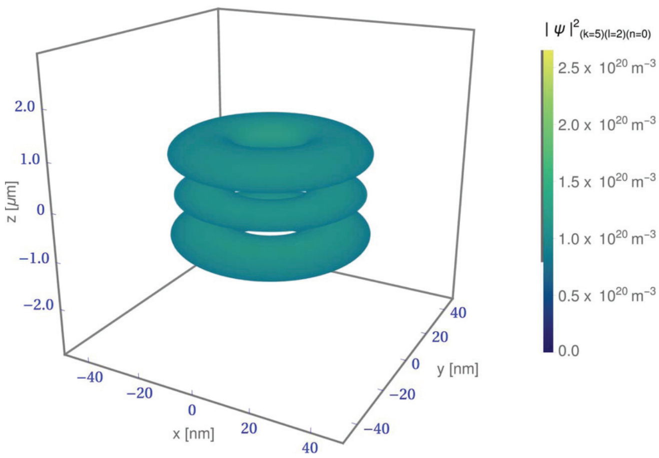

FIG. 1. We display the probability density $|\psi|^2 = |\psi_{k\ell ns}(\vec{r})|^2$ of the quantum cyclotron state with quantum numbers $k = 2$, $n = 0$, and $\ell = 2$ [see Eq. (28)]. This is the second axial excited-state ($k = 2$), the cyclotron ground-state ($n = 0$), and the second excited magnetron state ($\ell = 2$). The probability density is independent of the spin state ($s = \pm 1$). We use parameters from Ref. [9], i.e., $\omega_c = 2\pi \times 164.4$ GHz, $\omega_z = 2\pi \times 64.42$ MHz, which implies that the corrected magnetron frequency is $\omega_{(-)} = 2\pi \times 12.62$ kHz. Axial states with high average excitation form the basis of experiments [14,15]. One notes the large extent of the wave function in the axial direction, which is in the range of micrometers, whereas the confining magnetic field of the trap restricts the wave function in the x and y directions to range of about 50 nanometers.

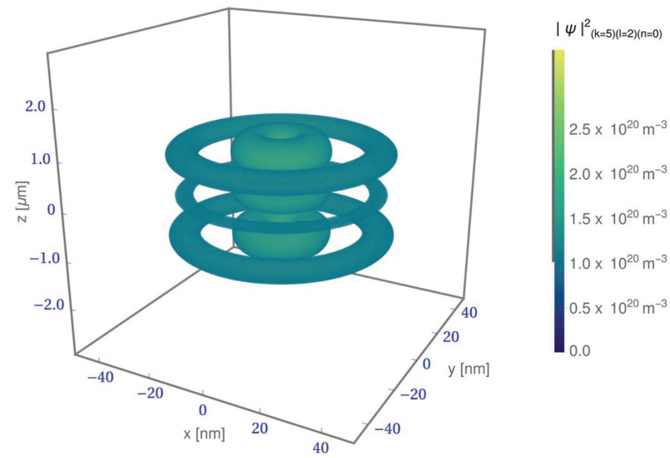

FIG. 2. We present the analog of Fig. 1 for the quantum cyclotron state with quantum numbers $k = 2$, $n = 1$, and $\ell = 2$. In contrast to Fig. 1, this is the first excited cyclotron state ($n = 1$). Again, we use parameters from Ref. [9], i.e., $\omega_c = 2\pi \times 164.4$ GHz, and $\omega_z = 2\pi \times 64.42$ MHz. One notes the large extent of the wave function in the axial direction, whereas the wave function is much more confined in the x and y directions.

The energy eigenvalues of H_0 are not bounded from below in view of the repulsive character of the radial quadrupole potential,

$$E_{k\ell ns} = \omega_c(1+\kappa)\frac{s}{2} + \omega_{(+)}\left(n + \frac{1}{2}\right) + \omega_z\left(k + \frac{1}{2}\right) - \omega_{(-)}\left(\ell + \frac{1}{2}\right). \tag{27}$$

One takes note of the negative sign in front of the last term. The eigenfunctions of the unperturbed Hamiltonian can be constructed as (see Figs. 1 and 2)

$$\psi_{k\ell ns}(\vec{r}) = \frac{(a_z^\dagger)^k}{\sqrt{k!}} \frac{(a_{(-)}^\dagger)^\ell}{\sqrt{\ell!}} \frac{(a_{(+)}^\dagger)^n}{\sqrt{n!}} \psi_0(\vec{r}) \chi_{s/2}, \tag{28}$$

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{29}$$

where the $\chi_{s/2}$'s denote fundamental spinors. The orbital part of the ground-state wave function is

$$\psi_0(\vec{r}) = \sqrt{\frac{m\sqrt{\omega_c^2 - 2\omega_z^2}}{2\pi}} \exp\left(-\frac{m}{4}\sqrt{\omega_c^2 - 2\omega_z^2}\rho^2\right) \times \left(\frac{m\omega_z}{\pi}\right)^{1/4} \exp\left(-\frac{1}{2}m\omega_z z^2\right), \tag{30}$$

where

$$\omega_{(+)} - \omega_{(-)} = \sqrt{\omega_c^2 - 2\omega_z^2}. \tag{31}$$

The spin-up sublevel of the cyclotron ground state and the spin-down sublevel of the first excited cyclotron state are of interest for spectroscopy and determination of the anomalous magnetic moment of the electron (see also Fig. 3). The

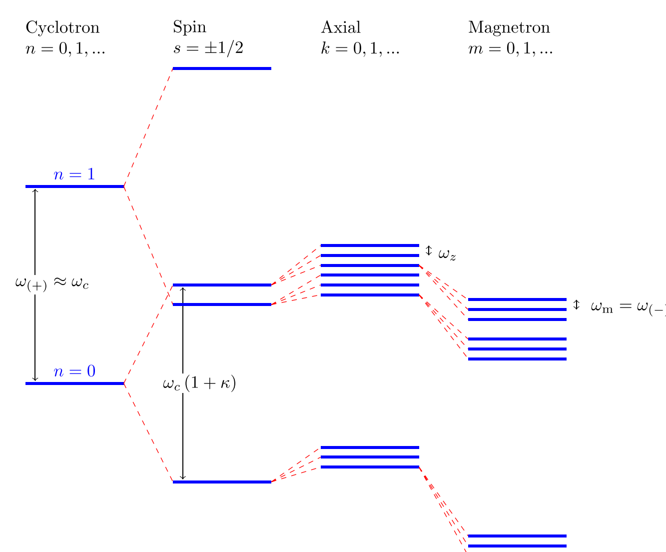

FIG. 3. The figure provides an illustration of the bound-state spectrum of an electron in a Penning trap. The cyclotron levels are separated by the frequency $\omega_{(+)} \approx \omega_c$, whereas the dominant contribution comes from the spin projection $s = \pm 1/2$, because the spin-flip frequency is $\omega_c(1+\kappa)$, where $\kappa \approx \alpha/(2\pi)$. Two important quasidegenerate levels have the quantum numbers $s = +1/2$, $n = 0$ (spin-up cyclotron ground state), $s = -1/2$, and $n = 1$ (spin-down first excited cyclotron state). They are energetically degenerate were it not for the effect of the anomalous magnetic moment of the electron.

spin-up sublevel of the cyclotron ground state fulfills the relations

$$H_0\psi_{0001}(\vec{r}) = E_{0001}\psi_{0001}(\vec{r}), \tag{32a}$$

$$E_{0001} = \frac{\omega_c}{2}(1+\kappa) + \frac{\omega_{(+)}}{2} + \frac{\omega_z}{2} - \frac{\omega_{(-)}}{2}. \tag{32b}$$

The spin-down sublevel of the first excited cyclotron state fulfills the relations

$$H_0\psi_{001-1}(\vec{r}) = E_{001-1}\psi_{001-1}(\vec{r}), \tag{33a}$$

$$E_{001-1} = -\frac{\omega_c}{2}(1+\kappa) + \frac{3\omega_{(+)}}{2} + \frac{\omega_z}{2} - \frac{\omega_{(-)}}{2}. \tag{33b}$$

Here we consider, for simplicity, the sublevels with $k = \ell = 0$, i.e., without axial or magnetron excitations. This approximation will be lifted in Sec. IV. Due to the anomalous magnetic moment, E_{0001} is a little higher than E_{001-1}, and the energy difference is

$$\Delta E = E_{0001} - E_{001-1} = \omega_c(1+\kappa) - \omega_{(+)} = \omega_c(1+\kappa) - \frac{1}{2}\left(\omega_c + \sqrt{\omega_c^2 - 2\omega_z^2}\right). \tag{34}$$

In the limit $\omega_z \to 0$, one has $\Delta E \to \kappa\,\omega_c$, which relates energy levels inside the trap to the anomalous magnetic moment of the electron. The energy difference ΔE serves to determine the anomalous magnetic moment of the electron [7,14–18].

C. Scaling for strong fields and Penning trap

In order to illustrate the analogy of the bound spectrum inside a Penning trap and an electron bound in an atom, we introduce coupling parameters. With reference to the QED coupling $\alpha_{\rm QED} = e^2/(4\pi) \approx 1/137.036$, we refer to these as the cyclotron coupling parameter α_c (which could, otherwise, be referred to as the cyclotron fine-structure constant), and the axial coupling parameter α_z,

$$\alpha_c = \sqrt{\frac{\omega_c}{m}}, \qquad \alpha_z = \sqrt{\frac{\omega_z}{m}}. \tag{35}$$

A third coupling parameter, pertaining to the magnetron frequency, is defined in Eq. (39). Because of the hierarchy of typical frequencies in a trap [9], one has

$$\alpha_z \ll \alpha_c. \tag{36}$$

Once the cyclotron and the axial frequencies are defined, we can calculate the magnetron frequency based on Eq. (16c). One can define a trap fine-structure constant $\alpha_{\rm T}$ in terms of the maximum of the coupling parameters α_c and α_z,

$$\alpha_{\rm T} = \max(\alpha_z, \alpha_c), \qquad \omega_{\rm T} = \max(\omega_z, \omega_c). \tag{37}$$

Then, we can define scaling parameters ξ_c and ξ_z by

$$\alpha_c = \xi_c\alpha_{\rm T}, \qquad \alpha_z = \xi_z\alpha_{\rm T}, \qquad \max(\xi_c, \xi_z) = 1. \tag{38}$$

For the magnetron coupling parameter $\alpha_{\rm m}$, it follows that:

$$\alpha_{\rm m} = \sqrt{\frac{\omega_{(-)}}{m}} = \xi_{\rm m}\alpha_{\rm T}, \tag{39a}$$

$$\xi_{\rm m} = \frac{1}{\sqrt{2}}\left(\xi_c^2 - \sqrt{\xi_c^4 - 2\xi_z^4}\right)^{1/2} \approx \frac{\xi_z^2}{\sqrt{2}\xi_c}, \tag{39b}$$

where $\xi_{\rm m}$ is smaller than either ξ_c or ξ_z. Electron momenta in the trap can be shown to be of order,

$$p_{\rm T} \sim \alpha_{\rm T} m, \tag{40}$$

in analogy to an atom, where $\alpha_{\rm T}$ would be replaced by $\alpha_{\rm QED}$. (By $\sim$ we indicate that the quantities on the right and left are of the same order of magnitude, whereas $\approx$ is reserved to indicate approximate equality.) In atoms, the wave function is spread over a length scale commensurate with the Bohr radius $a_0 = \hbar/p$, where p is a characteristic momentum. We conclude that the "trapped Bohr radius" $a_{0\rm T}$ is

$$a_{0\rm T} = \sqrt{\frac{\hbar}{m\omega_{\rm T}}} = \frac{1}{\alpha_{\rm T} m} \sim \frac{\hbar}{p_{\rm T}}. \tag{41}$$

With these definitions, we can establish the scaling of frequencies, momenta and position operators inside a trap. In view of Eqs. (12) and (35), we have

$$\omega_c = \frac{|e|B_{\rm T}}{m} = \alpha_c^2 m \sim \alpha_{\rm T}^2 m. \tag{42}$$

It is clear that the position vector $\vec{r}$ scales as

$$|\vec{r}| \sim a_{0\rm T} = \frac{1}{\alpha_{\rm T} m}. \tag{43}$$

The scaling of the quadrupole potential follows as:

$$V \sim \omega_z^2(z^2 - \rho^2) \sim \alpha_{\rm T}^4\alpha_{\rm T}^{-2} m = \alpha_{\rm T}^2 m, \tag{44}$$

and

$$e\vec{A}_T \sim eB_{\rm T}|\vec{r}| \sim \alpha_{\rm T}^2\alpha_{\rm T}^{-1} m = \alpha_{\rm T} m. \tag{45}$$

Finally, the kinetic momentum in the trap, defined in Eq. (7), is of the order of

$$\vec{\pi}_{\rm T} = \underbrace{\vec{p}}_{\sim\alpha_{\rm T} m} - \underbrace{e\vec{A}_{\rm T}}_{\sim\alpha_{\rm T} m} \sim \alpha_{\rm T} m. \tag{46}$$

So, the appropriate scaling for the trap implies the following relations, which we summarize for convenience,

$$\vec{\pi} \sim \alpha_{\rm T}, \qquad e\vec{A}_{\rm T} \sim \alpha_{\rm T}, \qquad e\,\vec{B}_{\rm T} \sim \alpha_{\rm T}^2, \tag{47a}$$

$$e\vec{E}_{\rm T} = -\vec{\nabla}V \sim \alpha_{\rm T}^3, \qquad e\partial_t\vec{E} \sim \alpha_{\rm T}^5. \tag{47b}$$

The second of these implies that, if we wish to calculate Penning trap energy levels to order $\alpha_{\rm T}^2$, then we need to keep all terms quadratic in the magnetic trap field, and if we wish to calculate them to order $\alpha_{\rm T}^6$, then we need to keep all terms cubic in the magnetic fields. The scaling with the coupling parameters is notably different from atomic systems [19]. An expansion to third order in the magnetic fields is not necessary for atoms where terms of higher than the second order in the magnetic fields can be safely discarded [5,6,10–12]. This necessity, in addition to the other aspects described in Sec. I, motivates revisiting the Foldy-Wouthuysen transformation for general fields. The scaling of the magnetic field in a Penning trap is completely different from that in an atom. In typical atoms, the only important magnetic field is the dipole magnetic field generated by the atomic nucleus, which leads to the hyperfine splitting. In the Penning trap, by contrast, the magnetic field provides for the binding of the electron, which is why it needs to be taken out in higher orders.

D. Time derivative and Foldy-Wouthuysen

Let us briefly review the formalism of the Foldy-Wouthuysen transformation with a particular emphasis on the time-derivative term. The Foldy-Wouthuysen method [1] is based on a unitary transformation,

$$U = \exp(iS). \tag{48}$$

In order to consistently derive the formalism, it is necessary to realize that the time derivative of an operator does not necessarily commute with the operator itself. The transformation is constructed so that, iteratively, the Foldy-Wouthuysen transformed Dirac Hamiltonian is given as follows:

$$\begin{aligned}\mathcal{H}_{\rm FW} &= \exp(iS)[\mathcal{H} - i\partial_t]\exp(-iS)\\ &= \mathcal{H} + [iS, \mathcal{H} - i\partial_t] + \frac{1}{2!}[iS, [iS, \mathcal{H} - i\partial_t]]\\ &\quad + \frac{1}{3!}[iS, [iS, [iS, \mathcal{H} - i\partial_t]]] + \cdots\\ &= \mathcal{H} + \delta\mathcal{H}^{(1)} + \delta\mathcal{H}^{(2)} + \delta\mathcal{H}^{(3)} + \cdots .\end{aligned} \tag{49}$$

Here, the differential operator $i\partial_t$ is understood to exclusively act on the unitary operator $\exp(-iS)$ but not on the wave function. The time derivatives add additional terms, which, in first order, read as follows:

$$\delta\mathcal{H}^{(1)} = [iS, \mathcal{H} - i\partial_t] = i[S, \mathcal{H}] - \partial_t S. \tag{50}$$

Note that one can iteratively calculate the multicommutators in Eq. (49),

$$\delta\mathcal{H}^{(n+1)} = \frac{1}{n+1}[iS, \delta\mathcal{H}^{(n)}]. \tag{51}$$

For a typical generalized Dirac Hamiltonian, the Foldy-Wouthuysen transformation operator S is proportional to

$$S \sim \vec{\alpha}\cdot\vec{\pi} \sim \alpha_{\rm T}, \qquad \partial_t S \sim \vec{\alpha}\cdot\partial_t\vec{\pi} \sim \alpha_{\rm T}^3. \tag{52}$$

Here, the $\vec{\alpha}$ and β matrices are used in the Dirac representation,

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{1}_{2\times 2} & 0\\ 0 & -\mathbb{1}_{2\times 2}\end{pmatrix}, \tag{53}$$

where $\vec{\sigma}$ denotes the vector of 2×2 Pauli matrices. It becomes clear that the higher-order terms in the multicommutator expansion (49) represent higher orders in the momenta.

In the Coulomb gauge, one can separate the electric field into its longitudinal and transverse components,

$$e\vec{E}_\parallel = -\vec{\nabla}V, \qquad \vec{E}_\perp = -\partial_t\vec{A}. \tag{54}$$

The longitudinal component is obtained as the commutator of kinetic momentum and potential V,

$$[\vec{\pi}, V] = -i\vec{\nabla}V = -ie\vec{\nabla}A^0 = ie\vec{E}_\parallel, \tag{55}$$

whereas the transverse component is obtained via the time derivative of the vector potential,

$$\partial_t\vec{\pi} = -e\partial_t\vec{A} = e\vec{E}_\perp. \tag{56}$$

The time-derivative term in Eq. (50) is decisive in ensuring that the Foldy-Wouthuysen-transformed Dirac Hamiltonian contains the complete electric field.

III. HIGHER-ORDER FOLDY-WOUTHUYSEN TRANSFORMATION

A. Higher-order corrections for strong fields

We start from the generalized Dirac Hamiltonian (see Chap. 7 of Ref. [4] and Chap. 1 of Ref. [20]), including the anomalous-magnetic-moment terms. The g factor of the electron is expressed as $g = 2(1+\kappa)$. The Hamiltonian is (see Chap. 7 of Ref. [4])

$$\mathcal{H} = \vec{\alpha}\cdot\vec{\pi} + \beta m + V + \frac{\kappa e}{2m}(i\vec{\gamma}\cdot\vec{E} - \beta\vec{\Sigma}\cdot\vec{B}). \tag{57}$$

The vector of Dirac γ matrices is used as $\vec{\gamma} = \beta\,\vec{\alpha}$ with reference to Eq. (53). The γ matrices and the 4×4 spin matrices $\vec{\Sigma}$, which we will need in the following, read as:

$$\vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma}\\ -\vec{\sigma} & 0\end{pmatrix}, \qquad \vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}. \tag{58}$$

As anticipated in Sec. I, the iterated Foldy-Wouthuysen method aims to eliminate the odd operators (in bispinor space) from the Dirac Hamiltonian, in successive higher orders of the momenta. If O is the odd operator in the Dirac Hamiltonian, then the unitary transformation is $U = \exp(iS)$ where $S = -i\beta O/(2m)$. For the general Hamiltonian given in Eq. (57), one needs to employ three transformations, $S = S^{(1)}$, $S = S^{(2)}$, and $S = S^{(3)}$, respectively, which are given as follows. For the first transformation, one can easily derive the expression for $S^{(1)}$ from Eq. (57),

$$S^{(1)} = -i\frac{\vec{\gamma}\cdot\vec{\pi}}{2m} + \frac{e\,\kappa}{4m^2}\vec{\alpha}\cdot\vec{E}. \tag{59}$$

One calculates the multicommutators given in Eq. (49) up to seventh order. The second transformation is used to eliminate further remaining odd operators in the first transformed Hamiltonian [21–23]. It is more complicated,

$$\begin{aligned} S^{(2)} &= \frac{i}{6m^3}(\vec{\gamma}\cdot\vec{\pi})^3 + \frac{e}{4m^2}(\vec{\alpha}\cdot\vec{E})\\ &\quad - \frac{ie\kappa}{8m^3}[\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}] - \frac{i}{60m^5}(\vec{\gamma}\cdot\vec{\pi})^5\\ &\quad + \frac{e}{96m^4}\beta[[\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}], \vec{\Sigma}\cdot\vec{\pi}]\\ &\quad + \frac{e\kappa}{12m^4}\beta[[\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}], \vec{\Sigma}\cdot\vec{\pi}]\\ &\quad - \frac{e\kappa}{4m^4}\beta(\vec{\gamma}\cdot\vec{\pi})(\vec{\Sigma}\cdot\vec{E})(\vec{\Sigma}\cdot\vec{\pi})\\ &\quad + \frac{ie\kappa}{192m^5}[\vec{\gamma}\cdot\vec{\pi}, [\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}]]\\ &\quad + \frac{ie\kappa}{48m^5}\vec{\gamma}\cdot\vec{\pi}\{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}\vec{\Sigma}\cdot\vec{\pi}\\ &\quad + \frac{ie\kappa}{8m^3}\vec{\gamma}\cdot\partial_t\vec{E}. \end{aligned} \tag{60}$$

Finally, the third transformation, which eliminates all odd operators up to seventh order, is given as follows:

$$\begin{aligned} S^{(3)} &= -\frac{i}{12m^5}(\vec{\gamma}\cdot\vec{\pi})^5 + \frac{ie}{8m^3}(\vec{\gamma}\cdot\partial_t\vec{E})\\ &\quad + \frac{5e\beta}{96m^4}[[\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}], \vec{\Sigma}\cdot\vec{\pi}] \end{aligned}$$

$$
\begin{aligned}
&- \frac{3e\beta}{32m^4}\{\{\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}\}, \vec{\Sigma}\cdot\vec{\pi}\} \\
&+ \frac{e^2\kappa}{8m^4}\beta\{\vec{\gamma}\cdot\vec{B}, \vec{\Sigma}\cdot\vec{E}\} \\
&+ \frac{e\kappa}{16m^4}\beta\{\vec{\Sigma}\cdot\partial_t\vec{B}, \vec{\Sigma}\cdot\vec{\pi}\} \\
&+ \frac{5ie\kappa}{96m^5}\{\{\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}, (\vec{\Sigma}\cdot\vec{\pi})^2\} \\
&- \frac{ie\kappa}{48m^5}[[\vec{\gamma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}], (\vec{\Sigma}\cdot\vec{\pi})^2]. \qquad (61)
\end{aligned}
$$

The result of the iterative seventh-order standard Foldy-Wouthuysen transformation [23] can be written as

$$\mathcal{H}_{\text{FW}} = \mathcal{H}^{[0]} + \mathcal{H}^{[2]} + \mathcal{H}^{[3]} + \mathcal{H}^{[4]} + \mathcal{H}^{[5]} + \mathcal{H}^{[6]} + \mathcal{H}^{[7]}. \qquad (62)$$

The superscript denotes the power of the coupling parameter at which the term becomes relevant. The coupling parameter can either be α_{T} (for the Penning trap) or $\alpha = \alpha_{\text{QED}} \approx 1/137.036$ (for an atom). In zeroth order in α, we only have the rest mass term,

$$\mathcal{H}^{[0]} = \beta m. \qquad (63)$$

In the second order in α, we have the nonrelativistic term,

$$\mathcal{H}^{[2]} = \beta\frac{1}{2m}(\vec{\Sigma}\cdot\vec{\pi})^2 + V. \qquad (64)$$

In the third order in α, we only have a single term,

$$\mathcal{H}^{[3]} = -\frac{e\kappa}{2m}\beta\vec{\Sigma}\cdot\vec{B}, \qquad (65)$$

where the one-loop (Schwinger) correction [13] to the anomalous magnetic moment of the electron is $\kappa = \alpha/(2\pi)$. The α^4 terms can be expressed very succinctly,

$$\mathcal{H}^{[4]} = -\beta\frac{1}{8m^3}(\vec{\Sigma}\cdot\vec{\pi})^4 - \frac{ie}{8m^2}[\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]. \qquad (66)$$

The α^5 anomalous magnetic-moment terms are also expressed in quite a compact form

$$\mathcal{H}^{[5]} = -\frac{ie\kappa}{4m^2}[\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}] + \beta\frac{e\kappa}{16m^3}\{\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}\}. \qquad (67)$$

From the direct iterative application of the multicommutator expansion (49), one obtains the α^6 terms,

$$
\begin{aligned}
\mathcal{H}^{[6]} = {}& \beta\frac{1}{16m^5}(\vec{\Sigma}\cdot\vec{\pi})^6 \\
&- \frac{5ie}{128m^4}\underbrace{[\vec{\Sigma}\cdot\vec{\pi}, [\vec{\Sigma}\cdot\vec{\pi}, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]]]}_{\equiv X} \\
&+ \frac{ie}{8m^4}\{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\} + \beta\frac{e^2\vec{E}^2}{8m^3}, \qquad (68)
\end{aligned}
$$

where we implicitly define the X term. It is computationally advantageous in the consideration of the α^6 terms to map the algebra of the commutators of the operators onto a computer symbolic program [22]. It is also instructive to present an alternative expression for the sixth-order terms $\mathcal{H}^{[6]}$. One derives the identity,

$$
\begin{aligned}
X = {}& \{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\} \\
&- 2\underbrace{(\vec{\Sigma}\cdot\vec{\pi})[\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}](\vec{\Sigma}\cdot\vec{\pi})}_{\equiv Y}. \qquad (69)
\end{aligned}
$$

The second term in the above expression can be reformulated as follows:

$$
\begin{aligned}
Y = {}& \tfrac{1}{2}[(\vec{\Sigma}\cdot\vec{\pi})^2, \{\vec{\Sigma}\cdot\vec{E}, \vec{\Sigma}\cdot\vec{\pi}\}] \\
&- \tfrac{1}{2}\{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\}. \qquad (70)
\end{aligned}
$$

Using Eqs. (69) and (70), we can establish that

$$
\begin{aligned}
X = {}& 2\{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\} \\
&- [(\vec{\Sigma}\cdot\vec{\pi})^2, \{\vec{\Sigma}\cdot\vec{E}, \vec{\Sigma}\cdot\vec{\pi}\}]. \qquad (71)
\end{aligned}
$$

The result for the sixth-order terms can, thus, alternatively be written as

$$
\begin{aligned}
\mathcal{H}^{[6]} = {}& \beta\frac{(\vec{\Sigma}\cdot\vec{\pi})^6}{16m^5} + \frac{5ie}{128m^4}[(\vec{\Sigma}\cdot\vec{\pi})^2, \{\vec{\Sigma}\cdot\vec{E}, \vec{\Sigma}\cdot\vec{\pi}\}] \\
&+ \frac{3ie}{64m^4}\{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\} + \beta\frac{e^2\vec{E}^2}{8m^3}. \qquad (72)
\end{aligned}
$$

The α^7 terms contain the anomalous magnetic moment,

$$
\begin{aligned}
\mathcal{H}^{[7]} = {}& \beta\frac{e^2\kappa}{8m^3}\vec{E}^2 - \frac{e\kappa}{16m^3}\beta\{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\partial_t\vec{E}\} \\
&+ \frac{ie\kappa}{16m^4}\{(\vec{\Sigma}\cdot\vec{\pi})^2, [\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{E}]\} \\
&- \beta\frac{e\kappa}{32m^5}[\vec{\Sigma}\cdot\vec{\pi}, [\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}\}]] \\
&- \beta\frac{3e\kappa}{256m^5}\{\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}\}\}\} \\
&+ \frac{ie^2\kappa}{16m^4}[\vec{\Sigma}\cdot\vec{E}, \{\vec{\Sigma}\cdot\vec{\pi}, \vec{\Sigma}\cdot\vec{B}\}]. \qquad (73)
\end{aligned}
$$

We here include all terms relevant for strong magnetic fields.

B. Particles and antiparticles

Let us concentrate on the upper left 2×2 submatrix of $\mathcal{H}_{\text{FW}}$, which is the particle (as opposed to the antiparticle) Hamiltonian. It is well known that the Dirac Hamiltonian describes particle and antiparticle states simultaneously [21], and that the lower right 2×2 submatrix of $\mathcal{H}_{\text{FW}}$ describes the antiparticle. In principle, the particle Hamiltonian can be obtained from the results given in Eqs. (64)–(73) by simply replacing $\vec{\Sigma} \to \vec{\sigma}$ and $\beta \to \mathbb{1}_{2\times 2}$, but it is still instructive to give the results separately.

Because the rest mass term βm given in Eq. (63) is a physically irrelevant constant, we write the general particle Hamiltonian H under the presence of the external electric and magnetic fields as

$$H = H^{[2]} + H^{[3]} + H^{[4]} + H^{[5]} + H^{[6]} + H^{[7]}, \qquad (74)$$

where we take into account up to seventh-order terms. One finds

$$H^{[2]} + H^{[3]} = \frac{\vec{\pi}^{\,2}}{2m} + V - \frac{e(1+\kappa)}{2m}\vec{\sigma}\cdot\vec{B}, \qquad (75)$$

where we have used the identity $(\vec{\sigma}\cdot\vec{\pi})^2 = \vec{\pi}^2 - e\vec{\sigma}\cdot\vec{B}$. The fourth-order terms find the compact representation

$$H^{[4]} = -\frac{1}{8m^3}(\vec{\sigma}\cdot\vec{\pi})^4 - \frac{ie}{8m^2}[\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}], \tag{76}$$

whereas the fifth-order terms contain the anomalous magnetic-moment,

$$H^{[5]} = -\frac{ie\kappa}{4m^2}[\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}] + \frac{e\kappa}{16m^3}\{\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{B}\}\}. \tag{77}$$

The general α^6 terms are given as

$$H^{[6]} = \frac{(\vec{\sigma}\cdot\vec{\pi})^6}{16m^3} + \frac{5ie}{128m^4}[(\vec{\sigma}\cdot\vec{\pi})^2, \{\vec{\sigma}\cdot\vec{E}, \vec{\sigma}\cdot\vec{\pi}\}] + \frac{3ie}{64m^3}\{(\vec{\sigma}\cdot\vec{\pi})^2, [\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}]\} + \frac{e^2\vec{E}^2}{8m^2}. \tag{78}$$

In the above form, the sixth-order terms in the Hamiltonian are compatible with those used in Eqs. (36)–(38) of Ref. [10] for spin-$1/2$ particles. The α^6 terms listed in Eq. (72) are also equal to those obtained by applying the unitary transformation outlined in Eq. (19) of Ref. [6] to the Hamiltonian given in Eq. (15) of Ref. [6], i.e., to the Hamiltonian obtained by adding the terms given in Eqs. (15) and (20) of Ref. [6]. Also, the result in Eq. (72) is equal to the Hamiltonian considered in Eq. (7) of Ref. [11], which, in turn, has been derived from the NRQED approach outlined in Ref. [12]. The α^7 terms attain the following structure:

$$\begin{aligned} H^{[7]} = {} & \frac{e^2\kappa}{8m^3}\vec{E}^2 - \frac{e\kappa}{16m^3}\{\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\partial_t\vec{E}\} \\ & + \frac{ie\kappa}{16m^4}\{(\vec{\sigma}\cdot\vec{\pi})^2, [\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{E}]\} \\ & - \frac{e\kappa}{32m^5}[\vec{\sigma}\cdot\vec{\pi}, [\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{B}\}\}]] \\ & - \frac{3e\kappa}{256m^5}\{\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \{\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{B}\}\}\}\} \\ & + \frac{ie^2\kappa}{16m^4}[\vec{\sigma}\cdot\vec{E}, \{\vec{\sigma}\cdot\vec{\pi}, \vec{\sigma}\cdot\vec{B}\}]. \end{aligned} \tag{79}$$

In general, we have not found ways to simplify the α^7 terms further than the expression given by Eq. (79).

IV. QUANTUM CYCLOTRON ENERGY LEVELS

A. Leading term

Now, we return to the problem considered in Sec. II A and perform simplifications for a Penning trap configuration. The trap field $\vec{B}_{\rm T}$ is assumed to be directed along the z axis as a constant uniform field so that

$$\vec{\pi} = \vec{\pi}_{\rm T} = \vec{p} - \frac{e}{2}(\vec{B}_{\rm T}\times\vec{r}), \qquad \vec{\pi}_{\rm T}^2 = \vec{p}^2 - e\vec{L}\cdot\vec{B}_{\rm T} + \frac{1}{4}m^2\omega_c^2\rho^2, \tag{80}$$

where we note the identity $(\vec{B}_{\rm T}\times\vec{r})^2 = B_{\rm T}^2\rho^2$. Furthermore, we ignore the radiative (transverse) electric field and set

$$e\vec{E} = e\vec{E}_\parallel = -\vec{\nabla}V. \tag{81}$$

Let us specialize the terms $H^{[k]}$ with $k = 2, \ldots, 6$, discussed in Sec. III B, to the case of a Penning trap. The sum of the terms $H^{[2]}$ and $H^{[3]}$ is just the Hamiltonian H_0 given in Eqs. (10) and (13),

$$\begin{aligned} H_0 &= H^{[2]} + H^{[3]} \\ &= \frac{\vec{p}^2}{2m} - \frac{e}{2m}\vec{L}\cdot\vec{B}_{\rm T} + \frac{m\omega_c^2}{8}\rho^2 + V - \frac{e(1+\kappa)}{2m}\vec{\sigma}\cdot\vec{B}_{\rm T}. \end{aligned} \tag{82}$$

We recall, from Eq. (27), the unperturbed energy $E^{[2+3]}$ of the unperturbed level eigenket $|k\ell ns\rangle$ as

$$\begin{aligned} E^{[2+3]} &= E_{k\ell ns} = \langle k\ell ns|H_0|k\ell ns\rangle = \langle H^{[2]} + H^{[3]}\rangle \\ &= \omega_c(1+\kappa)\frac{s}{2} + \omega_{(+)}\left(n + \frac{1}{2}\right) \\ &\quad + \omega_z\left(k + \frac{1}{2}\right) - \omega_{(-)}\left(\ell + \frac{1}{2}\right). \end{aligned} \tag{83}$$

The energy $E^{[2+3]} = E_0$ is the unperturbed (nonrelativistic) energy.

B. Relativistic corrections

In a Penning trap, the expression for $H^{[4]}$ simplifies as follows:

$$H^{[4]} = -\frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^4}{8m^3} + \frac{\vec{\nabla}^2V}{8m^2} + \frac{\vec{\sigma}\cdot(\vec{\nabla}V\times\vec{\pi}_{\rm T})}{4m^2}. \tag{84}$$

It is adequate to treat $H^{[4]}$ and $H^{[5]}$ together. For the fifth-order Hamiltonian $H^{[5]}$, we need the following relation, which is valid for a constant, uniform magnetic field:

$$\{\vec{\sigma}\cdot\vec{\pi}_{\rm T}, \{\vec{\sigma}\cdot\vec{\pi}_{\rm T}, \vec{\sigma}\cdot\vec{B}_{\rm T}\}\} = 4(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2(\vec{\pi}_{\rm T}\cdot\vec{B}_{\rm T}). \tag{85}$$

For the Penning trap, this implies that

$$H^{[5]} = \frac{\kappa\vec{\nabla}^2V}{4m^2} + \frac{\kappa\vec{\sigma}\cdot(\vec{\nabla}V\times\vec{\pi}_{\rm T})}{2m^2} + \frac{e\kappa\vec{\sigma}\cdot\vec{\pi}_{\rm T}\vec{B}_{\rm T}\cdot\vec{\pi}_{\rm T}}{4m^3}. \tag{86}$$

It is convenient to express the sum of $H^{[4]}$ and $H^{[5]}$ as follows:

$$\begin{aligned} H^{[4]} + H^{[5]} = {} & -\frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^4}{8m^3} + (1+2\kappa)\frac{\vec{\nabla}^2V}{8m^2} \\ & + (1+2\kappa)\frac{\vec{\sigma}\cdot(\vec{\nabla}V\times\vec{\pi}_{\rm T})}{4m^2} + \frac{e\kappa\vec{\sigma}\cdot\vec{\pi}_{\rm T}\vec{B}_{\rm T}\cdot\vec{\pi}_{\rm T}}{4m^3}. \end{aligned} \tag{87}$$

If we are in a charge-free region, then $\vec{\nabla}^2V = 0$, and we have three contributions,

$$H^{[4]} + H^{[5]} = H_1 + H_2 + H_3. \tag{88}$$

The first is the relativistic correction to the kinetic energy,

$$H_1 = -\frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^4}{8m^3}. \tag{89}$$

It leads to an energy shift $E_1 = \langle H_1\rangle = \langle k\ell ns|H_1|k\ell ns\rangle$ which reads as follows:

$$E_1 = -\frac{\left[\frac{\omega_{(+)}^2\left(n+\frac{1}{2}\right)+\omega_{(-)}^2\left(\ell+\frac{1}{2}\right)}{\omega_{(+)}-\omega_{(-)}} + \frac{\omega_z}{2}\left(k+\frac{1}{2}\right) + \frac{\omega_c s}{2}\right]^2}{2m}$$

$$- \frac{\omega_z^4\left[\left(n+\frac{1}{2}\right)\left(\ell+\frac{1}{2}\right)+\frac{1}{4}\right]}{4m(\omega_{(+)}-\omega_{(-)})^2} - \frac{\omega_z^2}{16m}\left[\left(k+\frac{1}{2}\right)^2+\frac{3}{4}\right]. \tag{90}$$

As compared to Eq. (7.48) of Ref. [9], we take the opportunity to correct an apparent misprint,

$$\underbrace{\left(n+\tfrac{1}{2}\right)\left(\ell+\tfrac{1}{2}\right)-\tfrac{1}{4}}_{\text{[Eq. (7.48) of Ref. 9]}} \to \underbrace{\left(n+\tfrac{1}{2}\right)\left(\ell+\tfrac{1}{2}\right)+\tfrac{1}{4}}_{\text{[Result obtained here]}}. \tag{91}$$

The spin-orbit coupling leads to the term

$$H_2 = (1+2\kappa)\frac{1}{4m^2}\vec{\sigma}\cdot(\vec{\nabla}V\times\vec{\pi}_{\rm T}). \tag{92}$$

The energy shift $E_2 = \langle H_2\rangle = \langle k\ell ns|H_2|k\ell ns\rangle$ reads as follows:

$$E_2 = -\frac{\omega_z^2 s(1+2\kappa)}{4m}\frac{\omega_{(+)}\left(n+\frac{1}{2}\right)+\omega_{(-)}\left(\ell+\frac{1}{2}\right)}{\omega_{(+)}-\omega_{(-)}}. \tag{93}$$

Finally, there is an additional correction due to the higher-order interaction of the electron spin with the magnetic field,

$$H_3 = \frac{e\kappa}{4m^3}(\vec{\sigma}\cdot\vec{\pi}_{\rm T})(\vec{B}_{\rm T}\cdot\vec{\pi}_{\rm T}). \tag{94}$$

The corresponding energy shift $E_3 = \langle H_3\rangle$ is

$$E_3 = -\frac{s\kappa\omega_c\omega_z}{4m}\left(k+\tfrac{1}{2}\right). \tag{95}$$

The terms of fourth and fifth order lead to the joint correction,

$$E^{[4+5]} = E_1 + E_2 + E_3, \tag{96}$$

where the energy corrections E_1, E_2, and E_3 are given in Eqs. (90), (93), and (95), respectively. In terms of the coupling parameters defined in Sec. II C, we can express $E^{[4+5]}$ differently,

$$\begin{aligned} E^{[4+5]} = \alpha_{\rm T}^4 m\Bigg(&-\frac{(1+s+2n)^2}{8}\xi_c^4 \\ &-\frac{(1+2k)[1+2n+s(1+\kappa)]}{8}\xi_c^2\xi_z^2 \\ &-\frac{3+6k(1+k)+4s(1+2n)(1+2\kappa)}{32}\xi_z^4 + O\left(\xi_z^8\right)\Bigg). \end{aligned}$$

The term of order ξ_z^6 vanishes. If the dominant (angular) frequency in the trap is the cyclotron frequency, then we have $\xi_c = 1$ according to Eq. (38).

C. Sixth-order corrections

For the Penning trap, the sixth-order terms assume the form

$$\begin{aligned} H^{[6]} = &\frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^6}{16m^5} - \frac{5i}{128m^4}[(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, \{\vec{\sigma}\cdot\vec{\nabla}V, \vec{\sigma}\cdot\vec{\pi}_{\rm T}\}] \\ &- \frac{3i}{64m^4}\{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, [\vec{\sigma}\cdot\vec{\pi}_{\rm T}, \vec{\sigma}\cdot\vec{\nabla}V]\} + \frac{(\vec{\nabla}V)^2}{8m^3}. \end{aligned} \tag{97}$$

One has two further useful relations. The first of these is

$$[(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, \{\vec{\sigma}\cdot\vec{\nabla}V, \vec{\sigma}\cdot\vec{\pi}_{\rm T}\}] = i\left[\vec{\pi}_{\rm T}^2, \left[\vec{\pi}_{\rm T}^2, V\right]\right], \tag{98}$$

and the second,

$$\begin{aligned} \{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, [\vec{\sigma}\cdot\vec{\pi}_{\rm T}, \vec{\sigma}\cdot\vec{\nabla}V]\} = -i\{&(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, \vec{\nabla}^2 V \\ &+ 2\vec{\sigma}\cdot\vec{\nabla}V\times\vec{\pi}_{\rm T}\}. \end{aligned} \tag{99}$$

Hence, one can express the sixth-order terms as follows:

$$\begin{aligned} H^{[6]} = &\frac{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^6}{16m^4} + \frac{5}{128m^4}\left[\vec{\pi}_{\rm T}^2, \left[\vec{\pi}_{\rm T}^2, V\right]\right] \\ &- \frac{3}{64m^4}\{(\vec{\sigma}\cdot\vec{\pi}_{\rm T})^2, [\vec{\sigma}\cdot\vec{\pi}_{\rm T}, \vec{\sigma}\cdot\vec{\nabla}V]\} + \frac{(\vec{\nabla}V)^2}{8m^3}. \end{aligned} \tag{100}$$

Overall, in the sixth order, one has two terms, which are as follows: (i) directly due to the sixth-order Hamiltonian and (ii) due to a second-order effect, involving the fourth-order Hamiltonian,

$$\begin{aligned} E^{[6]} = &\langle k\ell ns|H^{[6]}|k\ell ns\rangle \\ &+ \langle k\ell ns|H^{[4]}\left(\frac{1}{E_0 - H_0}\right)' H^{[4]}|k\ell ns\rangle, \end{aligned} \tag{101}$$

where $[1/(E_0 - H_0)]'$ is the reduced Green's function. A remark is in order. For a Penning trap, the unperturbed eigenstates are separately eigenstates of the Hamiltonian $H^{[3]}$, and so, a conceivable additional sixth-order term vanishes

$$\left\langle k\ell ns\middle|H^{[3]}\left(\frac{1}{E_0 - H_0}\right)' H^{[5]}\middle|k\ell ns\right\rangle = 0. \tag{102}$$

The exact expression for $\langle H^{[6]}\rangle$ is very lengthy, however, an expansion into the coupling parameters defined in Sec. II C leads to the compact expression,

$$\begin{aligned} \langle H^{[6]}\rangle = \alpha_{\rm T}^6 m\Bigg(&\frac{(1+s+2n)^3}{16}\xi_c^6 \\ &+ \frac{3(1+2k)(1+2n+s)^3}{32}\xi_c^4\xi_z^2 \\ &+ \frac{3}{64}\Big([5+6k(1+k)](1+2n) \\ &+ [5+6k(1+k)+8n(1+n)]s\Big)\xi_c^2\xi_z^4 \\ &+ \frac{1}{128}(1+2k)[13+10k(1+k) \\ &+ 6(1+2n)s]\xi_z^6 + O\left(\xi_z^8\right)\Bigg]. \end{aligned} \tag{103}$$

After expansion in ξ_z, the second-order shift is

$$\left\langle k\ell ns\left|H^{[4]}\left(\frac{1}{E_0-H_0}\right)'H^{[4]}\right|k\ell ns\right\rangle = \alpha_{\rm T}^6 m\left[-\frac{1}{32}(1+2k)[1+s+2n(1+n+s)]\xi_c^4\xi_z^2 - \frac{1}{64}[5+6k(1+k)](1+2n+s)\xi_c^2\xi_z^4 - \frac{1}{512}(1+2k)[45+17k(1+k)+24(1+2n)s]\xi_z^6 + O\left(\xi_z^8\right)\right]. \quad (104)$$

The total sixth-order energy shift is obtained as the sum of the results given in Eqs. (103) and (104),

$$E^{[6]} = \alpha_{\rm T}^6 m\left[\frac{1}{16}(1+2n+s)^3\xi_c^6 + \frac{(1+2k)[10n(1+n+s)+2+5s+3s^2]\xi_c^4\xi_z^2}{32} + \frac{[5+6k(1+k)][(1+2n+s)+12n(1+n)s]\xi_c^2\xi_z^4}{32} + \frac{1}{512}(1+2k)[7+23k(1+k)]\xi_z^6 + O\left(\xi_z^8\right)\right]. \quad (105)$$

We leave the evaluation of the seventh-order corrections for a Penning trap to a future investigation. These, otherwise, also include higher-order corrections to the Lamb shift (self-energy) of the quantum states.

V. CONCLUSIONS

The main results of the current investigation can be summarized as follows. We have carried out in Sec. III A the full iterative Foldy-Wouthuysen transformation of the single-particle Dirac Hamiltonian, coupled to general electromagnetic fields, up to seventh order in the momenta. The results, for the 4×4 matrices that combine the particle and antiparticle states, are given in Eqs. (63)–(73). The effective Hamiltonian for the particle (as opposed to the antiparticle) is given in Eqs. (75)–(79). We have clarified that the standard Foldy-Wouthuysen method, iteratively applied, reproduces the effective Hamiltonian, to order α^7, which has been derived based on NRQED methods in Ref. [12]. So, we have shown that the Hamiltonian first obtained by a nonstandard Foldy-Wouthuysen transformation in Ref. [5], and then augmented by an additional unitary transformation given in Eq. (19) of Ref. [6], is exactly equal to the gauge-covariant Hamiltonian used recently in Eq. (7) of Ref. [11]. It is instructive to recall that the kinetic momentum $\vec{\pi}$ is gauge covariant but not gauge invariant because $\vec{A}$ transforms nontrivially under gauge transformations. As a result of the investigations reported here, complete agreement between the various methods has been achieved, and the calculations have been extended to the seventh order in α, including effects due to strong magnetic fields.

Our results are valid for cases where the binding of the electron proceeds in strong external fields, such as those encountered in Penning traps. In such cases, the term $|e|B_{\rm T}/m = \omega_c$ (cyclotron frequency), where $B_{\rm T}$ is the trap magnetic field, is of order $\alpha_{\rm T}^2 m$ where $\alpha_{\rm T}$ is a suitably defined coupling constant for the trap [see Eq. (35)]. In a Penning trap, the magnetic field is not an external perturbation but provides the decisive energy scale for the bound states inside the trap. After an initial discussion of the separation of the electron Hamiltonian inside the trap, carried out in Sec. II A, and the discussion of scaling relations in Sec. II C, we discuss the relevant expressions for relativistic corrections to electron energy levels in quantum cyclotrons in Sec. IV.

Our results, given for the Penning trap in Eqs. (90)–(95), (97), and (105), enable a more accurate evaluation of the relativistic corrections to quantum cyclotron states, which are important for the determination of the fine-structure constant [7,14–18]. Terms of seventh order in $\alpha_{\rm T}$ can be obtained from Eq. (79) under the substitutions $\vec{\pi} \to \vec{\pi}_{\rm T}$ and $e\vec{E} \to -\vec{\nabla}V$. However, these are of the same order as the relativistic corrections to the Lamb shift, notably, to the relativistic Bethe logarithm (order $\alpha_{\rm T}^7 m$). Hence, we leave these terms for a future work. We do not indicate them separately.

In a more general context, our calculations show that it is possible to generalize the standard direct calculation of the Foldy-Wouthuysen transformation to seventh order in the coupling parameters under the intensive use of computer algebra [22].

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