Quantum-mechanical description of charged particles with spin $\frac{1}{2}$ in the magnetic field outside of a rectilinear current filament

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The eigenstates of a charged particle with spin $\frac{1}{2}$ in the magnetic field surrounding a rectilinear current filament are determined numerically. As they differ only slightly from local Landau levels, the wave functions may be approximated analytically using stationary perturbation theory. The expectation values of the component parallel to the wire of the velocity operator are calculated for both the exact and the approximated wave functions. They are a measure for the drift of the gyration center parallel to the wire, which is predicted by classical mechanics. Taking into account the quantization of the cyclotron rotation, this drift motion can also be derived by applying the method of adiabatic expansion of the particle propagator. The resulting values for the drift velocities are in excellent agreement with those from classical mechanics if, in the latter, one takes into account energy quantization. [S1050-2947(96)00409-X]

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I. INTRODUCTION

The quantum-mechanical motion of a charged spin $\frac{1}{2}$ particle in a homogeneous magnetic field was first investigated by Landau [1] who, in this case, determined eigenstates (''Landau levels'') and eigenenergies. His results are still of interest in solid-state physics with regard to the quantized Hall effect [2]. In this context, however, as well as in the case of persistent currents in mesoscopic rings [3], deviations from the homogeneous field are of great significance for charge flow. As a result the Pauli equation was solved recently for particles in special nonuniform static field configurations [4–6]. For one of the simplest possible magnetic field configurations, namely, the magnetic field produced by a rectilinear current filament, a detailed quantum-mechanical description is still unavailable. It is the purpose of the present paper to provide such a solution and is an extension of the theoretical [7–10] and experimental [11,12] studies of the bound states of neutral particles possessing magnetic dipole moments in a common field. It is, however, interesting to investigate differences between the quantum-mechanical results and those recently published [13] on the basis of a purely classical theory.

Classically, the motion of a charged particle in a uniform magnetic field consists of a circular motion (''gyration'' or ''cyclotron rotation'') in the plane perpendicular to the field lines, whilst the motion parallel to them is free. The radius of the circular orbit is called the ''gyroradius'' and its center the ''guiding center.'' In the case of a nonuniform magnetic field, the solution of the classical equations of motion is a nontrivial problem. If, however, the distance over which the magnetic field varies appreciably in magnitude or direction is large compared to the local gyroradius, the classical equations of motion may be solved approximately using perturbation methods [14,15]. These methods are based on a decomposition of the motion into a fast gyration perpendicular to the magnetic-field lines and a slow ''drift'' of the guiding center (''guiding center approximation''). The resulting equations of motion for the guiding center can also be derived from Hamiltonian theory [16,17] or from variational principles [18].

It was shown in [13] that the guiding center approximation is applicable to describe the electronic motion outside of a rectilinear current if the kinetic energy of the electron is not too large. The inhomogeneity of the magnetic field causes a uniform drift of the guiding center parallel to the filament. Let us suppose that the wire be directed along the z axis. Within the framework of quantum mechanics, the expectation values of the z component of the velocity operator $\hat{v}_z$ are a measure for the drift motion. After a numerical solution of the time-independent Pauli equation we will use the resulting wave functions to compute the expectation values in various stationary states.

Recently, equations of motion for the guiding center, taking into account the quantization of the cyclotron rotation, were derived for the case of a charged particle which moves in a plane perpendicular to a strong uniform magnetic field in the presence of an external electrostatic field [19]. In this work, the underlying idea is that the Landau levels should become a local concept with their energy spacings depending on the values of the guiding center coordinates. For this purpose, the Born-Oppenheimer method was used to separate the fast variables describing the gyration from the slowly varying coordinates of the guiding center. Assuming that the quantum number n of the local Landau level is not affected by the slow change of the guiding center coordinates, an explicit formula for the path integral can be derived (''adiabatic expansion of the path integral''). It contains an exponent, which represents the effective action function of the guiding center motion for a fixed quantum number of the gyration. Minimization of this action yields equations of motion for the guiding center.

As will be shown in this paper, the adiabatic path-integral expansion may also be applied to the case of a bare inhomogeneous magnetic field, if the guiding center approximation is valid. This method, therefore, allows one to derive the guiding center motion in the magnetic field of a rectilinear current.

The paper is organized as follows: In Sec. II, we investi-

gate symmetries of the Hamiltonian and deduce radial equations for the spin-up and spin-down components of the Pauli spinor. A general formula for the expectation value of the velocity operator $\hat{v}_z$ is given. In Sec. III, we solve the stationary Pauli equation numerically and calculate the expectation values of $\hat{v}_z$ for some of the resulting wave functions. As the eigenstates and eigenvalues deviate only slightly from the case of local Landau levels, in Sec. IV we use stationary perturbation theory to obtain analytic approximations for the wave functions. With their help, we derive analytic formulas for the expectation values of $\hat{v}_z$. In Sec. V, the method of the adiabatic path-integral expansion is used to deduce equations of motion for the guiding center. In each of the Secs. III, IV, and V, the results for the drift velocity are compared with those from classical mechanics. In Sec. VI, a short conclusion is given. Appendix A contains the main results from the classical calculations of Ref. [13] and in Appendix B we summarize the adiabatic path-integral expansion in strong magnetic fields, as derived in Ref. [19].

II. SYMMETRIES AND EXPECTATION VALUES

The Hamiltonian of a nonrelativistic particle of mass M, charge q, and magnetic moment $\boldsymbol{\mu}$ in an external magnetic field $\mathbf{B}(\mathbf{x})=\mathrm{rot}\mathbf{A}(\mathbf{x})$ is given by [20]

$$\hat{H}_P=\frac{1}{2M}\left(\hat{\mathbf{p}}-\frac{q}{c}\mathbf{A}(\mathbf{x})\right)^2-\hat{\boldsymbol{\mu}}\cdot\mathbf{B}(\mathbf{x}). \tag{1}$$

For particles with spin $\frac{1}{2}$, the operator $\hat{\boldsymbol{\mu}}$ of the magnetic moment is related to the vector $\boldsymbol{\sigma}$ of the Pauli matrices by

$$\hat{\boldsymbol{\mu}}=\frac{g}{2}\mu_P\boldsymbol{\sigma}, \tag{2}$$

where $\mu_P=|q|\hbar/2Mc$ denotes the ''magneton'' of the particle and g the gyromagnetic ratio. In the case of electrons, μ_P is given by the Bohr magneton μ_B and the absolute value of g is approximately equal to two.

Outside of a current filament of length L, which is directed along the z axis and whose radial extension can be neglected, the vector potential $\mathbf{A}(\mathbf{x})$ is given by

$$\mathbf{A}(\rho,z)=\frac{I}{c}\left\{\mathrm{arsinh}\left(\frac{L/2+z}{\rho}\right)+\mathrm{arsinh}\left(\frac{L/2-z}{\rho}\right)\right\}\mathbf{e}_z, \tag{3}$$

where I is the strength of the time-independent current. Here, and in what follows, we use cylindrical coordinates (ρ,ϕ,z). If the particle is restricted to a region, whose extension in the z direction is much smaller than L ($|z|\ll L$), the vector potential (3) is approximately equal to

$$\mathbf{A}(\rho)=\frac{2I}{c}\,\mathrm{arsinh}\left(\frac{L}{2\rho}\right)\mathbf{e}_z. \tag{4}$$

If, in addition, the distance ρ of the particle from the z axis remains small compared to L,

$$\rho\ll L \quad\text{and}\quad |z|\ll L, \tag{5}$$

$\mathbf{A}(\mathbf{x})$ may be replaced by

$$\mathbf{A}(\rho)=-\frac{2I}{c}\mathbf{e}_z\ln\frac{\rho}{L}, \tag{6}$$

which agrees with the exact expression (3) up to terms of second order in $|z|/L$ and ρ/L.

The magnetic field $\mathbf{B}(\mathbf{x})=\mathrm{rot}\mathbf{A}(\mathbf{x})$ originating from (6) reads

$$\mathbf{B}(\rho)=\frac{2I}{c\rho}\mathbf{e}_\phi, \tag{7}$$

where $\mathbf{e}_\phi$ denotes the azimuthal unit vector. Note that in (6) the length L of the wire may be replaced by any other length scale ρ_s by adding a constant vector to $\mathbf{A}(\mathbf{x})$. As the magnetic field $\mathbf{B}(\mathbf{x})$ is not influenced by such a modification of $\mathbf{A}(\mathbf{x})$, the special choice of ρ_s is of no physical relevance. Because the region where the charge is localized is restricted to the spatial domain defined by (5), a reasonable length scale is given by the Compton wavelength $\lambda_c=\hbar/Mc$ of the particle under consideration. In this case, $\mathbf{A}(\mathbf{x})$ takes the form

$$\mathbf{A}(\mathbf{x})=\mathbf{A}(\rho)=-\frac{2I}{c}\ln\frac{\rho}{\lambda_c}\mathbf{e}_z. \tag{8}$$

In this paper, we will use the expressions (8) and (7) for vector potential and magnetic field outside of a rectilinear current filament. Note that $\mathbf{A}(\mathbf{x})$ satisfies the Coulomb gauge condition

$$\mathrm{div}\mathbf{A}=0. \tag{9}$$

Applying Eq. (7), the last term on the right-hand side of (1) reads

$$\hat{\boldsymbol{\mu}}\cdot\mathbf{B}=\frac{g\mu_P}{2}\frac{2I}{c\rho}(-\sigma_x\sin\phi+\sigma_y\cos\phi). \tag{10}$$

Defining the operators $\sigma_+:=\frac{1}{2}(\sigma_x+i\sigma_y)$ and $\sigma_-:=\frac{1}{2}(\sigma_x-i\sigma_y)$, Eq. (10) may be transformed into the form

$$\hat{\boldsymbol{\mu}}\cdot\mathbf{B}=\frac{g\mu_P}{2}\frac{2I}{c\rho}i(\mathrm{e}^{i\phi}\sigma_--\mathrm{e}^{-i\phi}\sigma_+). \tag{11}$$

Using Eqs. (8), (9), and (11) in (1) we find for the Hamiltonian $\hat{H}_P$ in cylindrical coordinates

$$\hat{H}_P=-\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\left(\frac{\partial}{\partial z}+i\frac{2Iq}{\hbar c^2}\ln\frac{\rho}{\lambda_c}\right)^2\right]$$
$$-\frac{g\mu_P}{2}\frac{2I}{c\rho}i(\mathrm{e}^{i\phi}\sigma_--\mathrm{e}^{-i\phi}\sigma_+). \tag{12}$$

For particles with spin $\frac{1}{2}$, the z-component $\hat{J}_z$ of the total angular momentum operator $\hat{\mathbf{J}}$,

$$\hat{J}_z=\hat{L}_z+\frac{\hbar}{2}\sigma_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi}+\frac{\hbar}{2}\sigma_z \tag{13}$$

takes the eigenvalues $\hbar\nu:=\hbar(m+1/2), m\in\mathbb{Z}$, and the corresponding eigenfunctions are of the form

$$\Psi(\rho,\phi,z)=f_1(\rho,z)\ \mathrm{e}^{i(\nu-1/2)\phi}\chi_\uparrow+f_2(\rho,z)\ \mathrm{e}^{i(\nu+1/2)\phi}\chi_\downarrow . \tag{14}$$

Here $f_1(\rho,z)$ and $f_2(\rho,z)$ denote arbitrary functions of the cylindrical coordinates ρ and z and $\chi_\uparrow$, $\chi_\downarrow$ are the eigenspinors of σ_z ($\sigma_z\chi_\uparrow=+\chi_\uparrow$, $\sigma_z\chi_\downarrow=-\chi_\downarrow$). Because of cylindrical symmetry, $\hat{J}_z$ commutes with the Hamiltonian $\hat{H}_P$, $[\hat{J}_z,\hat{H}_P]=0$, and thus ν is an exact quantum number.

In addition, the operator $\hat{p}_z$ commutes with $\hat{H}_P$ and thus the z component of the canonical momentum is also a conserved quantity. If we denote the corresponding quantum number by $\hbar k_z$, the solution of the stationary Pauli equation

$$\hat{H}_P\Psi_{k_z\nu}(\mathbf{x})=E_{k_z\nu}\Psi_{k_z\nu}(\mathbf{x}) \tag{15}$$

has the form

$$\Psi_{k_z\nu}(\mathbf{x})=\Psi_{k_z\nu}(\rho,\phi,z)=\frac{1}{2\pi}\mathrm{e}^{ik_zz}[\varphi_\nu^{(+)}(\rho)\ \mathrm{e}^{i(\nu-1/2)\phi}\chi_\uparrow + i\ \mathrm{sgn}(gI)\varphi_\nu^{(-)}(\rho)\ \mathrm{e}^{i(\nu+1/2)\phi}\chi_\downarrow], \tag{16}$$

where k_z is real. The physical meaning of the factor $\mathrm{sgn}(gI)$ in front of the second term on the right-hand side of (16) will be explained later. The eigenfunctions $\Psi_{k_z\nu}(\rho,\phi,z)$ are normalized according to:

$$\langle\Psi_{k_z\nu}|\Psi_{k_z'\nu'}\rangle=\int_0^\infty\rho d\rho\int_0^{2\pi}d\phi\int_{-\infty}^{\infty}dz\Psi_{k_z\nu}^\dagger(\mathbf{x})\Psi_{k_z'\nu'}(\mathbf{x}) =\delta_{\nu\nu'}\delta(k_z-k_z'), \tag{17}$$

which implies that

$$\int_0^\infty\rho d\rho[|\varphi_\nu^{(+)}(\rho)|^2+|\varphi_\nu^{(-)}(\rho)|^2]=1 . \tag{18}$$

Inserting (16) into (15) yields the following set of coupled differential equations for the radial wave functions $\varphi_\nu^{(+)}(\rho)$ and $\varphi_\nu^{(-)}(\rho)$:

$$-\frac{\hbar^2}{2M}\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{(\nu-1/2)^2}{\rho^2}\right]\varphi_\nu^{(+)}(\rho) +\frac{1}{2M}\left(\hbar k_z+\frac{2qI}{c^2}\ln\frac{\rho}{\lambda_c}\right)^2\varphi_\nu^{(+)}(\rho)-\frac{|gI|\mu_P}{c\rho}\varphi_\nu^{(-)}(\rho) =E_{k_z\nu}\varphi_\nu^{(+)}(\rho), \tag{19}$$

$$-\frac{\hbar^2}{2M}\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{(\nu+1/2)^2}{\rho^2}\right]\varphi_\nu^{(-)}(\rho) +\frac{1}{2M}\left(\hbar k_z+\frac{2qI}{c^2}\ln\frac{\rho}{\lambda_c}\right)^2\varphi_\nu^{(-)}(\rho)-\frac{|gI|\mu_P}{c\rho}\varphi_\nu^{(+)}(\rho) =E_{k_z\nu}\varphi_\nu^{(-)}(\rho). \tag{20}$$

Note that the differential operators in (19) and (20) differ only by the centrifugal terms $\hbar^2(\nu\pm1/2)^2/2M\rho^2$. The transformation $\nu\to-\nu$, $\varphi_\nu^{(\pm)}(\rho)\to\varphi_\nu^{(\mp)}(\rho)$, which is equivalent to

$$\Psi_{k_z\nu}(\mathbf{x})\to i\sigma_y\Psi_{k_z\nu}^*(\mathbf{x}), \tag{21}$$

leaves the set of equations invariant. Therefore, $E_{k_z\nu}=E_{k_z-\nu}$, which means that the energy eigenvalues of $\hat{H}_P$ are doubly degenerate (with eigenfunctions $\Psi_{k_z\nu}$ and $i\sigma_y\Psi_{k_z\nu}^*$). In Ref. [21], it is shown that the same degeneracy occurs in the more general case of a magnetic field with negative parity $\mathbf{B}(-\mathbf{x})=-\mathbf{B}(\mathbf{x})$ if $g\ \mathrm{sgn}(q)$ is exactly equal to two. As the magnetic field (7) is of higher symmetry, the energy eigenvalues of $\hat{H}_P$ are doubly degenerate even for arbitrary values of the gyromagnetic ratio. From now on, we will restrict ourselves to the case of non-negative ν.

The equations for $\varphi_\nu^{(\pm)}(\rho)$ are coupled by the terms

$$-\frac{|gI|\mu_P}{c\rho}\varphi_\nu^{(\mp)}(\rho)=:W(\rho)\varphi_\nu^{(\mp)}(\rho) \tag{22}$$

originating from the potential energy $-\hat{\boldsymbol{\mu}}\cdot\mathbf{B}$ of the magnetic dipole moment $\boldsymbol{\mu}$ in the magnetic field $\mathbf{B}$. Owing to the factor $\mathrm{sgn}(gI)$ in the ansatz (16) for the wave functions, the sign of $W(\rho)$ is negative. This implies parallel orientation of $\boldsymbol{\mu}$ and $\mathbf{B}$. From classical mechanics it is known that in this case the force $-\boldsymbol{\nabla}W$ points in the direction of the wire. Neutral particles with a nonvanishing magnetic moment are hence confined in the plane perpendicular to the current filament and it can be shown that quantum mechanically they possess an infinite number of bound states [22,23].

If $\mathrm{sgn}(gI)$ is replaced by $-\mathrm{sgn}(gI)$, $\boldsymbol{\mu}$ and $\mathbf{B}$ point in different directions and $W(\rho)$ becomes positive and the force $-\boldsymbol{\nabla}W$ thus repels the particles from the wire. Consequently, neutral particles are no longer bound in the radial direction. For charged particles, however, the numerical solution of the radial equations shows that bound states still persist. The situation is comparable to the case of a homogeneous magnetic field [1,20]: There, the energy levels for particles with spin $\frac{1}{2}$ depend on the relative orientation of $\boldsymbol{\mu}$ and $\mathbf{B}$,

$$E_n=\left(n+\frac{1}{2}\right)\hbar|\omega_c|\pm\frac{g}{4}\hbar|\omega_c|,\ \text{with}\ \ \omega_c:=\frac{qB}{Mc},n\in\mathbb{N}_0, \tag{23}$$

where the negative (positive) sign in front of the second term belongs to parallel (antiparallel) orientation of magnetic moment and magnetic field. If $g\ \mathrm{sgn}(q)=2$, the Landau levels are doubly degenerate (cf. Fig. 1). Due to the inhomogeneity of the magnetic field (7), in our case this degeneracy is lifted. The difference between the corresponding levels are of the order of the ground-state energy of the radial equations (19), (20).

Equations (19) and (20) contain the z component $\hbar k_z$ of the canonical momentum and therefore, the form of the radial wave functions $\varphi_\nu^{(\pm)}(\rho)$ depends on the choice of the quantum number k_z. (For reasons of notational simplicity, however, we leave out the index "k_z.") Note that the value of this quantum number is gauge dependent: If, for example, the length scale λ_c of the vector potential $\mathbf{A}$ is changed to ρ_s by a gauge transformation

$$\mathbf{A}(\mathbf{x})\to\ \mathbf{A}'(\mathbf{x})=\mathbf{A}(\mathbf{x})+\boldsymbol{\nabla}\chi(\mathbf{x}) \tag{24}$$

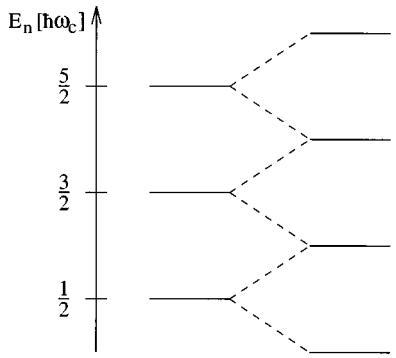

FIG. 1. Energy levels of particles without spin (left) and with spin $\frac{1}{2}$ (right) in a homogeneous magnetic field. If the gyromagnetic ratio g of the particle is equal to two, the energy levels become doubly degenerate.

with a scalar function

$$\chi(\mathbf{x}) = -\frac{2I}{c}\ln\left(\frac{\lambda_c}{\rho_s}\right)z, \tag{25}$$

the eigenvalue equation $\hat{H}'_P\Psi'_{k_z\nu}=E_{k_z\nu}\Psi'_{k_z\nu}$ is solved by the wave functions [20]

$$\Psi'_{k_z\nu}(\mathbf{x}) = \Psi_{k_z\nu}(\mathbf{x})\exp\left[\frac{iq}{\hbar c}\chi(\mathbf{x})\right]. \tag{26}$$

Using (25) and (16), the new eigenfunctions read explicitly

$$\Psi'_{k_z\nu}(\mathbf{x}) = \frac{1}{2\pi}\, e^{\,i[k_z-(2Iq/\hbar c^2)\ln(\lambda_c/\rho_s)]z}[\,\varphi_\nu^{(+)}(\rho)\; e^{\,i(\nu-1/2)\phi}\chi_\uparrow + \mathrm{sgn}(gI)\,\varphi_\nu^{(-)}(\rho)\; e^{\,i(\nu+1/2)\phi}\chi_\downarrow]. \tag{27}$$

Hence a modification $\lambda_c\to\rho_s$ of the length scale of the vector potential $\mathbf{A}(\mathbf{x})$ leads to the substitution

$$k_z\to k'_z = k_z - \frac{2Iq}{\hbar c^2}\ln\left(\frac{\lambda_c}{\rho_s}\right) \tag{28}$$

in the eigenfunctions $\Psi_{k_z\nu}$ of $\hat{H}_P$.

As can be verified directly from the foregoing equation, the radial distance

$$\overline{\rho} = \lambda_c\exp\left(-\frac{\hbar k_z c^2}{2Iq}\right) = \rho_s\exp\left(-\frac{\hbar k'_z c^2}{2Iq}\right) \tag{29}$$

is gauge independent. Classically, $\overline{\rho}$ gives the distance from the z axis at which the particle velocity in the z direction vanishes. Apart from small corrections, $\overline{\rho}$ coincides with the radial coordinate $\rho_{\mathbf{X}}$ of the guiding center (cf. Appendix A).

Let us now introduce new radial functions

$$u_\nu^{(\pm)}(\rho) := \sqrt{\rho}\,\varphi_\nu^{(\pm)}(\rho), \tag{30}$$

which, according to (18), satisfy the normalization condition

$$\int_0^\infty d\rho[|u_\nu^{(+)}(\rho)|^2+|u_\nu^{(-)}(\rho)|^2] = 1\,. \tag{31}$$

Expressing $\varphi_\nu^{(\pm)}(\rho)$ by $u_\nu^{(\pm)}(\rho)$ and taking into account the definition (29) of $\overline{\rho}$, Eqs. (19) and (20) are transformed into

$$-\frac{\hbar^2}{2M}\left[\frac{d^2}{d\rho^2}-\frac{\nu(\nu\mp1)}{\rho^2}\right]u_\nu^{(\pm)}(\rho)+\frac{M}{2}v_{\mathrm{scal}}^2\left(\ln\frac{\rho}{\overline{\rho}}\right)^2 u_\nu^{(\pm)}(\rho) - \frac{|gI|\mu_P}{c\rho}u_\nu^{(\mp)}(\rho) = E_{k_z\nu}u_\nu^{(\pm)}(\rho), \tag{32}$$

where

$$v_{\mathrm{scal}} := \frac{2Iq}{Mc^2} \tag{33}$$

denotes a scaling velocity which plays an important role in classical calculations: As explained in Appendix A, the guiding center approximation is only valid if the kinetic energy of a charged particle is much smaller than E_{scal}: $=(M/2)v_{\mathrm{scal}}^2$ The calculations of the next section will show that this condition is well satisfied for the lowest-lying eigenstates of $\hat{H}_P$.

In a uniform magnetic field, the expectation values for those components of the velocity operator which are perpendicular to the magnetic field vanish if the particle is in a Landau level. This is in agreement with the results of classical mechanics: Since the projection of the particle orbit on the plane perpendicular to the magnetic field is a circle, the time average of the velocity in this plane is zero. In our field configuration, however, a uniform drift motion parallel to the wire is predicted because the time average of the velocity in the z direction does not vanish. We suppose therefore, that in an eigenstate $|\Psi_{k_z\nu}\rangle$ of the Hamiltonian $\hat{H}_P$, the expectation value $\langle\Psi_{k_z\nu}|\hat{v}_z|\Psi_{k_z\nu}\rangle$ for the z component of the velocity operator differs from zero. The general relation $M\hat{\mathbf{v}}=\hat{\mathbf{p}}-(q/c)\,\mathbf{A}$ [20] and the special form (8) of the vector potential yield for $\hat{v}_z$

$$\hat{v}_z = \frac{1}{M}\left(\hat{p}_z+\frac{2Iq}{c^2}\ln\frac{\rho}{\lambda_c}\right). \tag{34}$$

Using the radial functions $u_\nu^{(\pm)}(\rho)$ and the definitions for $\overline{\rho}$ and v_{scal}, the expectation value $\overline{v_z}=\langle\Psi_{k_z\nu}|\hat{v}_z|\Psi_{k_z\nu}\rangle$ takes the form

$$\overline{v_z} = \langle\Psi_{k_z\nu}|\hat{v}_z|\Psi_{k_z\nu}\rangle = v_{\mathrm{scal}}\int_0^\infty d\rho\ln\left(\frac{\rho}{\overline{\rho}}\right)[|u_\nu^{(+)}(\rho)|^2+|u_\nu^{(-)}(\rho)|^2]. \tag{35}$$

In the following section, we will solve the radial equations (32) numerically and compute expectation values of $\hat{v}_z$ for some of the resulting wave functions.

III. NUMERICAL SOLUTION OF THE PAULI EQUATION

Before turning to the numerical solution of (32), we note that the expressions (6) and (7) for the vector potential and the magnetic field used in the Hamiltonian $\hat{H}_P$ are only valid outside the current filament. Moreover, in $\hat{H}_P$ interactions between the surface of the wire and the charged particle are

neglected. Both assumptions are only justified, if the particle is entirely located outside the wire. To check whether eigenstates of $\hat{H}_P$ exist which satisfy this condition, let us analyze the radial equations (32). They contain a quadratic logarithmic potential of the form

$$V_{\log}(\rho) := \frac{M}{2} v_{\mathrm{scal}}^2 \left(\ln \frac{\rho}{\overline{\rho}} \right)^2 . \tag{36}$$

Its minimum lies at the distance $\overline{\rho}$ from the z axis. According to Eq. (29), the value of $\overline{\rho}$ depends on the quantum number k_z. Therefore, by an appropriate choice of k_z, $\overline{\rho}$ becomes much larger than the radius R of the wire. Suppose that the latter is of magnitude 10^{-4} to 10^{-1} cm. Then, for $\rho > R$, the centrifugal potential $(\hbar^2/2M)(\nu \pm 1/2)^2/\rho^2$ and the coupling term $W(\rho) = -|gI|\mu_P/c\rho$ in (32) are only slowly varying functions of ρ. Consequently, the localization of the particle is determined by $V_{\log}(\rho)$ and hence concentrated around $\overline{\rho} \approx \rho_{\mathbf{X}}$. Thus, if the difference $(\overline{\rho} - R)$ is sufficiently large, the particle is located entirely outside the current filament. In the following calculations, we will restrict ourselves to this situation.

As stated earlier, the operators in Eq. (32) differ from one another only by a term

$$\Delta_\nu(\rho) := \frac{\hbar^2}{2M\rho^2}[\nu(\nu-1) - \nu(\nu+1)] = -\frac{\hbar^2 \nu}{M\rho^2}. \tag{37}$$

In the localization region of the particle, $\Delta_\nu(\rho)$ can be estimated by its value at $\overline{\rho}$,

$$\Delta_\nu(\rho) \approx -\left[\frac{76.2\nu}{\overline{\rho}(\mu\mathrm{m})^2} \frac{m_e}{M} \right] \ \mathrm{neV}, \tag{38}$$

where m_e denotes the electron mass. For values of the quantum number ν up to order of $10^2 \ldots 10^3$, $\Delta_\nu(\rho)$ becomes negligibly small compared to the other terms in the radial equations. Hence the differential operators for $u_\nu^{(+)}(\rho)$ and $u_\nu^{(-)}(\rho)$ are approximately equal. This is also the case for larger values of ν: Because the centrifugal potential increases quadratically with ν, the relative difference of the corresponding terms in (32),

$$\eta_\nu := \frac{2M\Delta_\nu(\rho)}{\hbar^2 \nu(\nu-1)} \approx \frac{2}{\nu}, \tag{39}$$

vanishes as ν^{-1} for $\nu \to \infty$. Therefore, we conclude that in the whole range of definition of ν, the approximation

$$\nu(\nu+1) \approx \nu(\nu-1) \approx \nu^2 \tag{40}$$

does not modify the eigenvalue problem essentially. The differential equations for $u_\nu^{(+)}(\rho)$ and $u_\nu^{(-)}(\rho)$ are then formally equal. Identifying the radial wave functions in (32) by

$$u_\nu^{(+)}(\rho) = u_\nu^{(-)}(\rho) =: u_\nu(\rho) \Leftrightarrow \varphi_\nu^{(+)}(\rho) = \varphi_\nu^{(-)}(\rho) =: \varphi_\nu(\rho), \tag{41}$$

leads to the one-dimensional Schrödinger equation

$$\hat{H} u_\nu(\rho) := \left\{ -\frac{\hbar^2}{2M}\left[\frac{d^2}{d\rho^2} - \frac{\nu^2}{\rho^2} \right] + \frac{M}{2} v_{\mathrm{scal}}^2 \left(\ln \frac{\rho}{\overline{\rho}} \right)^2 - \frac{|gI|\mu_P}{c\rho} \right\} u_\nu(\rho) = E_{k_z \nu} u_\nu(\rho). \tag{42}$$

Note that $\hat{H}$ is the quantum-mechanical counterpart of the classical Hamiltonian H_{class} (A3), if L_z is replaced in (A3) by $\hbar\nu$ and $\mu_\parallel$ by $(|g|/2)\mu_P$.

According to (16) and (41), the total wave function $\Psi_{k_z \nu}(\rho, \phi, z)$ now reads

$$\tilde{\Psi}_{k_z \nu}(\rho, \phi, z) = \frac{1}{2\pi} \mathrm{e}^{ik_z z} \varphi_\nu(\rho) \chi_+(\phi), \tag{43}$$

where $\chi_+(\phi)$ denotes the angle-dependent spinor

$$\chi_+(\phi) = \mathrm{e}^{i(\nu - 1/2)\phi} \chi_\uparrow + i \ \mathrm{sgn}(gI) \ \mathrm{e}^{i(\nu+1/2)\phi} \chi_\downarrow , \tag{44}$$

which is an eigenvector of $\boldsymbol{\sigma} \cdot \mathbf{e}_\phi$ with eigenvalue $\mathrm{sgn}(gI)$,

$$\boldsymbol{\sigma} \cdot \mathbf{e}_\phi \chi_+(\phi) = \mathrm{sgn}(gI) \chi_+(\phi). \tag{45}$$

Thus, the approximation (43) for the total wave function is equivalent to the assumption that the projection of the magnetic moment $\boldsymbol{\mu} = (g/2)\mu_P \boldsymbol{\sigma}$ along the magnetic field $\mathbf{B} = (2I/c\rho)\mathbf{e}_\phi$ remains constant.

The energy eigenvalues of the Schrödinger equation (42) can be estimated with the help of the Bohr-Sommerfeld quantization rule [20]

$$\oint p_\rho d\rho = \left(n_\rho + \frac{1}{2} \right) h, \quad n_\rho \in \mathbb{N}_0, \tag{46}$$

where n_ρ denotes the number of zeros of the corresponding radial wave functions. Taking into account the ''classical'' equations (A4), (A12), and the substitutions $L_z^2 \to (\hbar\nu)^2$ and $\mu_\parallel \to (|g|/2)\mu_P$ mentioned above, the dependence of the momentum p_ρ on the radial coordinate ρ is given by

$$p_\rho = \pm \left[2ME - \frac{\hbar^2 \nu^2}{\rho^2} - M^2 v_{\mathrm{scal}}^2 \left(\ln \frac{\rho}{\overline{\rho}} \right)^2 + \frac{2M|gI|\mu_P}{c\rho} \right]^{1/2}. \tag{47}$$

If the turning points in the radial direction are denoted by $\rho_2 > \rho_1$, Eq. (46) reads

$$2\int_{\rho_1}^{\rho_2} d\rho \left[2ME_{\mathrm{BS}} - \frac{\hbar^2 \nu^2}{\rho^2} - M^2 v_{\mathrm{scal}}^2 \left(\ln \frac{\rho}{\overline{\rho}} \right)^2 + \frac{2M|gI|\mu_P}{c\rho} \right]^{1/2} = \left(n_\rho + \frac{1}{2} \right) h. \tag{48}$$

The integral on the left-hand side of (48) cannot be solved analytically. However, if the parameters M, g, μ_P, I and quantum numbers ν, n_ρ are given, the Bohr-Sommerfeld approximation E_{BS} of the eigenenergies may be determined numerically. For electrons, a current $I = 500$ A and $\overline{\rho} = 1$cm, the results for E_{BS} for $0 \leqslant n_\rho \leqslant 10$ and $\nu = \frac{1}{2}$ are listed in Table I. The large value of I was assumed to ensure that the quantized energy levels can be verified experimentally. To transport a current of 500 A, a wire radius of about

TABLE I. Energy eigenvalues and drift velocities for the lowest electronic eigenstates for $I=500$ A and $\overline{\rho}=1$cm. E_{BS} denotes the Bohr-Sommerfeld approximation of the energy levels, $E_{k_z\nu n_\rho}$ the values from numerical integration of the radial equations (32). The expectation values $\overline{v_z}=\langle\Psi_{k_z\nu}|\hat{v}_z|\Psi_{k_z\nu}\rangle$ are calculated according to formula (35) using the radial functions $u_\nu^{(\pm)}(\rho)$ from the shooting method. To compare with classical mechanics, the drift velocity v_D of a particle with energy $E_{k_z\nu n_\rho}$ is computed with the help of (52). The correspondence of the numerical values for energies and drift velocities is explained in the main text.

n_ρ	ν	E_{BS} (μeV)	$E_{k_z\nu n_\rho}$ (μeV)	$\overline{v_z}$ (cm/s)	v_D (cm/s)
0	1/2	$\approx -10^{-10}$	$\approx -10^{-6}$	$\approx -10^{-4}$	$\approx -10^{-6}$
0	21/2	$\approx 10^{-8}$	$\approx -10^{-6}$	$\approx -10^{-4}$	$\approx -10^{-6}$
0	41/2	$\approx 10^{-7}$	$\approx -10^{-6}$	$\approx -10^{-4}$	$\approx -10^{-6}$
1	1/2	1.158	1.158	1.157	1.158
1	41/2	1.158	1.158	1.157	1.158
2	1/2	2.315	2.315	2.314	2.315
3	1/2	3.473	3.473	3.471	3.473
4	1/2	4.631	4.631	4.628	4.631
5	1/2	5.788	5.788	5.784	5.788
6	1/2	6.946	6.946	6.939	6.946
7	1/2	8.104	8.104	8.098	8.104
8	1/2	9.262	9.261	9.255	9.262
9	1/2	10.42	10.42	10.41	10.42
10	1/2	11.57	11.58	11.57	11.58

1mm is necessary. Therefore, we chose $\overline{\rho}=1$cm to guarantee that the interaction between the electron and the surface of the wire can be neglected. These values for I and $\overline{\rho}$ are used throughout all numerical calculations of this section. The effects of a modification of I and $\overline{\rho}$ will be discussed later.

Moreover, for the lowest-lying states with $n_\rho=0,1$, the influence of the angular motion was investigated by varying the quantum number ν. As can be seen from Table I, the changes in the absolute values of E_{BS} remain very small. They are of the same order as the electronic centrifugal potential at $\overline{\rho}=1$ cm,

$$\frac{\hbar^2\nu^2}{2M\overline{\rho}^2}=[38.1\times10^{-10}\nu^2]\ \mu\,\mathrm{eV}. \tag{49}$$

One may be surprised about the small absolute values of the eigenenergies for $n_\rho=0$. They are a consequence of the different sign of the zero-point energy of the logarithmic potential and the potential energy of the magnetic moment. Due to their small absolute values, the results for the eigenenergies and drift velocities for $n_\rho=0$ cannot be resolved exactly by numerical computations. Therefore, in Table I only orders of magnitudes are given.

Starting with the Bohr-Sommerfeld values E_{BS} as a first estimate of the eigenenergies, the radial equations (32) can be solved numerically by applying the so-called ''shooting method,'' which is described, e.g., in [24]. The forth column of Table I shows the resulting eigenenergies $E_{k_z\nu n_\rho}$. They are in excellent agreement with the Bohr-Sommerfeld results E_{BS}. In Fig. 2, the radial wave functions $u_{\nu n_\rho}^{(+)}(\rho)$ and $u_{\nu n_\rho}^{(-)}(\rho)$ are plotted for $\nu=\frac{1}{2}$ and $0\leqslant n_\rho\leqslant 7$. For fixed n_ρ, the

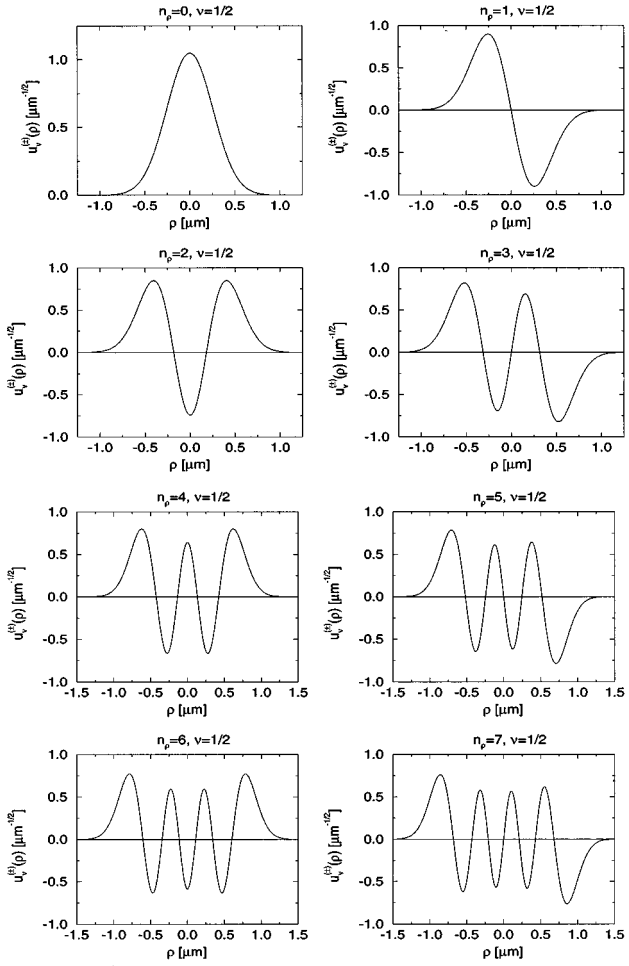

FIG. 2. Normalized radial wave functions $u_\nu^{(\pm)}(\rho)$ for the eight lowest-lying electronic states for $I=500$ A and $\overline{\rho}=1$cm (= origin of the ρ axis). Due to the small difference (37) of the radial equations (32), the components $u_\nu^{(+)}(\rho)$ and $u_\nu^{(-)}(\rho)$ cannot be distinguished graphically.

difference between $u_{\nu n_\rho}^{(+)}(\rho)$ and $u_{\nu n_\rho}^{(-)}(\rho)$ cannot be resolved graphically. Further calculations show that this is also the case for larger values of the quantum number ν. Thus the approximate ansatz (43) for the total wave function, which is based on the identification (41) of $u_{\nu n_\rho}^{(+)}(\rho)$ and $u_{\nu n_\rho}^{(-)}(\rho)$, is confirmed by our numerical results. We will exploit it further in the following sections.

With the help of the radial wave functions, the expectation values for $\hat{v}_z$ in the corresponding eigenstates $|\Psi_{k_z\nu n_\rho}\rangle$ of $\hat{H}_P$ can be computed by numerical integration of (35). The results are listed in the fifth column of Table I. They imply a slow drift motion parallel to the wire, if a particle is in an eigenstate of $\hat{H}_P$.

Within the framework of classical mechanics, a uniform drift motion in the z direction is predicted too [13]. If the total energy E of a particle is small compared to $E_{\mathrm{scal}}=(M/2)v_{\mathrm{scal}}^2$, the guiding center approximation is valid and an analytic expression for the drift velocity v_D can be derived. It is given by (A15)

$$v_D=\frac{v_{\mathrm{scal}}}{2}\,\frac{E+L_z^2/2M\rho_0^2}{E_{\mathrm{scal}}}, \tag{50}$$

where ρ_0 denotes the initial distance of the electron from the z axis and L_z the z component of its angular momentum.

According to Table I, the energies of the lowest-lying electronic states of $\hat{H}_P$ are much smaller than $E_{\mathrm{scal}}^{(\mathrm{el})} = 8.76\times 10^2$ eV. Therefore, we can use (50) to compare classical and quantum-mechanical results for the drift velocity parallel to the wire. Setting

$$E = E_{k_z \nu n_\rho}, \quad L_z = \hbar \nu, \quad \rho_0 \approx \overline{\rho}, \tag{51}$$

Eq. (50) can be written in the form

$$v_D = \frac{v_{\mathrm{scal}}}{2} \frac{E_{k_z \nu n_\rho} + \hbar^2 \nu^2 / 2M\overline{\rho}^2}{E_{\mathrm{scal}}}. \tag{52}$$

The approximation $\rho_0 \approx \overline{\rho}$ is valid in the lowest quantum states because the gyration radii of the corresponding classical orbits are much smaller than $\overline{\rho} = 1$ cm and hence $|\rho_0 - \overline{\rho}|/\rho_0 \ll 1$. The values for v_D resulting from (52) are listed in the last column of Table I. Within deviations of order pars per mile, they agree with the quantum-mechanical expectation values. Thus even for the lowest quantum-mechanical states the drift velocity of electrons can be calculated from (52), if energy quantization is taken into account.

Note that the correspondence of the numerical values for energies and drift velocities listed in Table I occurs only by chance, because for electrons the quotient $v_{\mathrm{scal}}/2E_{\mathrm{scal}}$ is equal to $1\,\mathrm{cm/s}/(\mu\,\mathrm{eV})$, if $I = 500$ A. As the centrifugal energy $\hbar^2\nu^2/2M\overline{\rho}^2$ is only a small correction to the eigenenergies $E_{k_z \nu n_\rho}$, the values for v_D and $E_{k_z \nu n_\rho}$ are approximately equal in the chosen units.

In the preceding numerical calculations we used fixed values for I and $\overline{\rho}$. A variation of these parameters shows that the energy eigenvalues $E_{k_z \nu n_\rho}$ are proportional to the quotient $I/\overline{\rho}$ and only for very large currents I and $\overline{\rho} \approx R$ do deviations from this proportionality occur. In these cases, the radial wave functions $u_{\nu n_\rho}^{(\pm)}(\rho)$ become distinctly different from one another and v_D no longer coincides with the quantum-mechanical expectation values for the drift velocity. However, since for $\overline{\rho} \approx R$ the distance of the charged particle from the wire becomes small, its interaction with the surface of the wire cannot be neglected any more, and the Hamiltonian $\hat{H}_P$ must be modified accordingly. Therefore, we conclude that the results for $I = 500$ A and $\overline{\rho} = 1$ cm are representative for charged particles, which are exposed to the magnetic field of a rectilinear current filament.

IV. PERTURBATION THEORY

The energy eigenvalues $E_{k_z \nu n_\rho}$ of Table I are approximately equidistant. Up to small deviations, their differences agree with those of electronic Landau levels in a uniform magnetic field of strength $B_\phi(\overline{\rho})$ (= local Landau levels at $\overline{\rho}$),

$$\hbar\,|\omega_c(\overline{\rho})| = 1.16\ \ \mu\,\mathrm{eV}, \tag{53}$$

where

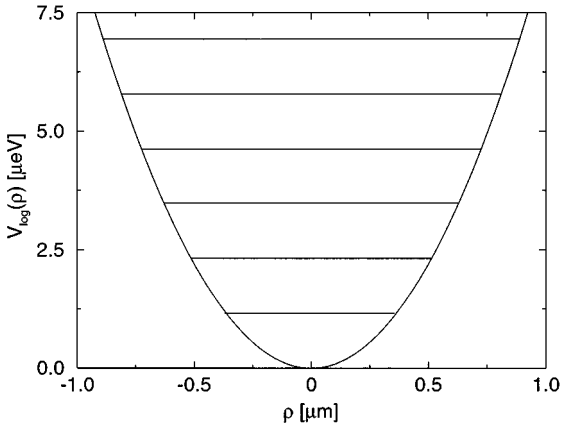

FIG. 3. Quadratic logarithmic potential $V_{\log}(\rho)$ for $I = 500$ A and $\overline{\rho} = 1$ cm (= origin of the ρ axis) in the vicinity of $\overline{\rho}$. The energies of the first six excited electronic states are depicted additionally.

$$\omega_c(\overline{\rho}) := \frac{qB_\phi(\overline{\rho})}{Mc} = \frac{2Iq}{Mc^2\overline{\rho}} = \frac{v_{\mathrm{scal}}}{\overline{\rho}} \tag{54}$$

denotes the corresponding cyclotron frequency. A more detailed analysis of the numerical data shows that, in the localization region of the lowest quantum states, the potential $V_{\log}(\rho) = (M/2)v_{\mathrm{scal}}^2[\ln(\rho/\overline{\rho})]^2$ defined in Eq. (36) can be excellently estimated by the first nonvanishing term of its Taylor expansion around $\overline{\rho}$,

$$V_{\mathrm{osc}}(\rho) := \frac{M}{2} v_{\mathrm{scal}}^2 \left(\frac{\rho}{\overline{\rho}} - 1 \right)^2 = \frac{M}{2} \omega_c^2(\overline{\rho})(\rho - \overline{\rho})^2. \tag{55}$$

As an illustration, Fig. 3 shows the potential $V_{\log}(\rho)$ in the vicinity of $\overline{\rho} = 1$cm for electrons and a current I of 500 A. To visualize their localization region the energies of the first six excited states are also plotted. The difference between $V_{\log}(\rho)$ and $V_{\mathrm{osc}}(\rho)$ cannot be resolved graphically in the depicted region.

As mentioned at the beginning of Sec. III, for $\rho \approx \overline{\rho}$ the centrifugal potential $(\hbar^2/2M)(\nu \pm 1/2)^2/\rho^2$ and $W(\rho) = -|gI|\mu_P/c\rho$ [cf. Eq. (22)] are slowly varying functions of ρ. Leaving them out in the radial equations (32) does not alter the form of the wave functions $u_{k_z \nu n_\rho}^{(\pm)}(\rho)$ significantly. The difference between the new energy eigenvalues and the exact ones is approximately equal to the sum of $W(\overline{\rho})$ and the centrifugal potential at $\overline{\rho}$. Therefore we suppose that the Hamiltonian

$$\hat{H}^{(0)} := -\frac{\hbar^2}{2M}\left[\frac{d^2}{d\rho^2} - \frac{\nu^2}{\overline{\rho}^2}\right] + \frac{M}{2} v_{\mathrm{scal}}^2 \left(\frac{\rho - \overline{\rho}}{\overline{\rho}} \right)^2 - \frac{|gI|\mu_P}{c\overline{\rho}} \tag{56}$$

is a good approximation to $\hat{H}$ and hence $\hat{H}_P$. Note that $\hat{H}^{(0)}$ can be derived from $\hat{H}$ by taking into account only the first nonvanishing terms in the Taylor expansions of $V_{\log}(\rho)$, $W(\rho)$ and the centrifugal potential around $\overline{\rho}$. The Hamiltonian $\hat{H}^{(0)}$ represents a harmonic oscillator of frequency $|v_{\mathrm{scal}}|/\overline{\rho} = |\omega_c(\overline{\rho})|$, whose center lies at $\overline{\rho}$. The domain D of the relative coordinate $\tilde{\rho} := \rho - \overline{\rho}$ is restricted to

$[-\overline{\rho},\infty)$. However, for not too large values of their quantum number, the eigenstates of $\hat{H}^{(0)}$ are localized in a region around $\overline{\rho}$ whose magnitude can be estimated by the oscillator length (e_0 = elementary charge)

$$a_B := [\hbar/M|\omega_c(\overline{\rho})|]^{1/2} = \left[5.74 \left(\frac{\overline{\rho[\mathrm{cm}]}}{I[\mathrm{A}]} \frac{m_e}{M} \frac{e_0}{|q|} \right)^{1/2} \right] \ \mu\mathrm{m}. \tag{57}$$

As a_B is much smaller than $\overline{\rho}$, we can extend D to the whole set of real numbers without great error. The Schrödinger equation

$$\hat{H}^{(0)} u^{(0)}_{\nu n_\rho}(\rho) = E^{(0)}_{k_z \nu n_\rho} u^{(0)}_{\nu n_\rho}(\rho) \tag{58}$$

is then equivalent to the eigenvalue problem of a one-dimensional harmonic oscillator with the solutions

$$u^{(0)}_{\nu n_\rho}(\rho) = \frac{1}{\pi^{1/4} (\beta^{-1/2} \overline{\rho})^{1/2} \sqrt{2^{n_\rho} n_\rho!}} \times \exp\left[-\frac{\beta}{2} \left(\frac{\rho - \overline{\rho}}{\overline{\rho}} \right)^2 \right] H_{n_\rho}\left(\beta^{1/2} \frac{\rho - \overline{\rho}}{\overline{\rho}} \right) \tag{59}$$

and corresponding energy eigenvalues

$$E^{(0)}_{k_z \nu n_\rho} = \hbar |\omega_c(\overline{\rho})| (n_\rho + 1/2) - \frac{|gI|\mu_P}{c\overline{\rho}} + \frac{\hbar^2 \nu^2}{2M\overline{\rho^2}}. \tag{60}$$

In (59), H_{n_ρ} denotes the Hermite polynomial of order n_ρ and the parameter β is defined by

$$\beta := \left(\frac{\overline{\rho}}{a_B} \right)^2 = \frac{M|v_{\mathrm{scal}}|\overline{\rho}}{\hbar}. \tag{61}$$

Its numerical value is $\beta = 3.04 \times 10^6 |I| \overline{\rho}$, if I is given in A and $\overline{\rho}$ in cm. The exponential in the eigenfunctions $u^{(0)}_{\nu n_\rho}(\rho)$ only differs significantly from zero therefore in the immediate vicinity of $\overline{\rho}$.

The differences between the exact radial wave functions $u^{(\pm)}_{\nu n_\rho}(\rho)$ and the approximate solutions $u^{(0)}_{\nu n_\rho}(\rho)$ cannot be resolved graphically. Nevertheless, the expectation values of $\hat{v}_z$ change dramatically, if $u^{(0)}_{\nu n_\rho}(\rho)$ is inserted in (35) instead of $u^{(\pm)}_{\nu n_\rho}(\rho)$. This is a consequence of the symmetry of $u^{(0)}_{\nu n_\rho}(\rho)$ with respect to $\overline{\rho}$.

Deviations from this symmetry arise, if the next order terms in the Taylor expansions of $V_{\log}(\rho)$, $W(\rho)$ and the centrifugal potential are added to $\hat{H}^{(0)}$. This results in a Hamiltonian of the form

$$\hat{H}^{(0)} + \hat{H}^{(1)}, \tag{62}$$

with

$$\hat{H}^{(1)} = -\frac{\hbar^2}{2M\overline{\rho^2}} (\beta \xi^3 + \alpha \xi), \tag{63}$$

where we have introduced the dimensionless variable

$$\xi := \frac{\rho}{\overline{\rho}} - 1 \tag{64}$$

and a parameter

$$\alpha = 2\nu^2 + \frac{2M|gI|\mu_P \overline{\rho}}{\hbar^2 c}. \tag{65}$$

Within the localization region of the lowest-lying states, $|\xi|$ is much smaller than unity. Because of the small numerical value of $\hbar^2/2M\overline{\rho^2}$, $\hat{H}^{(1)}$ acts in this region as a small ''perturbation'' on $\hat{H}^{(0)}$. Carrying out time-independent perturbation theory, the corrections of the energy eigenvalues and wave functions read in first approximation [20,25]

$$E^{(1)}_{k_z \nu n_\rho} = \langle \nu n_\rho | \hat{H}^{(1)} | \nu n_\rho \rangle, \tag{66}$$

$$u^{(1)}_{\nu n_\rho}(\rho) = \sum_{m_\rho}{}' \ c^{n_\rho}_{m_\rho} u^{(0)}_{\nu m_\rho}(\rho), \tag{67}$$

with coefficients

$$c^{n_\rho}_{m_\rho} = \frac{\langle \nu m_\rho | \hat{H}^{(1)} | \nu n_\rho \rangle}{E^{(0)}_{n_\rho} - E^{(0)}_{m_\rho}} \tag{68}$$

(the prime at the sum means that the term with $m_\rho = n_\rho$ is omitted). Thus, to first order in the perturbation, the eigenfunctions of $\hat{H}^{(0)} + \hat{H}^{(1)}$ are given by

$$\tilde{u}_{\nu n_\rho}(\rho) := [u^{(0)}_{\nu n_\rho}(\rho) + u^{(1)}_{\nu n_\rho}(\rho)] N_{n_\rho}, \tag{69}$$

with a normalization constant

$$N_{n_\rho} = \left(\sqrt{1 + \sum_{m_\rho}{}' \ |c_{n_\rho + k}|^2} \right)^{-1}. \tag{70}$$

The first-order corrections $E^{(1)}_{k_z \nu n_\rho}$ of the energy eigenvalues vanish due to the even parity of the squared wave functions (59). Hence, to first order in perturbation theory, the eigenenergies of $\hat{H}^{(0)} + \hat{H}^{(1)}$ are equal to $E^{(0)}_{k_z \nu n_\rho}$. The matrix elements $\langle \nu m_\rho | \hat{H}^{(1)} | \nu n_\rho \rangle$ may easily be calculated. As a result, we obtain the following coefficients $c^{n_\rho}_{m_\rho}$:

$$c^{n_\rho}_{m_\rho} = 0 \text{, if: } |m_\rho - n_\rho| > 3 \text{ or } m_\rho < 0, \tag{71}$$

$$c^{n_\rho}_{n_\rho - 3} = -\beta^{-1/2} [n_\rho (n_\rho - 1)(n_\rho - 2)/288]^{1/2}, \tag{72}$$

$$c^{n_\rho}_{n_\rho - 2} = 0, \tag{73}$$

$$c^{n_\rho}_{n_\rho - 1} = -\beta^{-1/2} (n_\rho/8)^{1/2} (3n_\rho/2 + \alpha/\beta), \tag{74}$$

$$c^{n_\rho}_{n_\rho + 1} = \beta^{-1/2} [(n_\rho + 1)/8]^{1/2} [3(n_\rho + 1)/2 + \alpha/\beta], \tag{75}$$

$$c^{n_\rho}_{n_\rho + 2} = 0, \tag{76}$$

$$c^{n_\rho}_{n_\rho + 3} = \beta^{-1/2} [(n_\rho + 1)(n_\rho + 2)(n_\rho + 3)/288]^{1/2}. \tag{77}$$

Due to the small factor $\beta^{-1/2}$, their numerical values are even for large quantum numbers n_ρ much smaller than unity. Therefore the first-order correction $u^{(1)}_{\nu n_\rho}(\rho)$ modifies the wave functions by only a small amount and the localization region remains almost unchanged.

Using $\tilde{u}_{\nu n_\rho}(\rho)$ as an approximation to the radial wave functions $u^{(\pm)}_{\nu n_\rho}(\rho)$, we now derive an analytic estimate for the expectation value of $\hat{v}_z$. According to (35), (41), and $u_{\nu n_\rho}(\rho) \approx \tilde{u}_{\nu n_\rho}(\rho)$, $\overline{v_z}$ is approximately equal to

$$\tilde{v}_z := v_{\rm scal} \int_0^\infty d\rho |\tilde{u}_{\nu n_\rho}(\rho)|^2 \ln\frac{\rho}{\overline{\rho}}. \tag{78}$$

As $\tilde{u}_{\nu n_\rho}(\rho)$ is localized in the immediate vicinity of $\overline{\rho}$, we expand the logarithm in the integral around this point

$$\ln\frac{\rho}{\overline{\rho}} = \ln(1+\xi) = \xi - \tfrac{1}{2}\xi^2 + \tfrac{1}{3}\xi^3 + O(\xi^4), \tag{79}$$

where we used the variable ξ as defined in (64). To be consistent with the order in perturbation theory, we have to take into account in the integral in (78) the first three terms of this expansion. This leads to the following expression for $\tilde{v}_z$:

$$\tilde{v}_z = v_{\rm scal} \int_{-\infty}^{\infty} ds \left(\beta^{-1/2} s - \frac{1}{2}\beta^{-1} s^2 + \frac{1}{3}\beta^{-3/2} s^3 \right) \times \exp(s^2) \left[\frac{1}{2^{n_\rho} n_\rho! \sqrt{\pi}} H_{n_\rho}(s) + \sum_{k=-3}^{3} c^{n_\rho}_{n_\rho+k} \frac{1}{2^{n_\rho+k}(n_\rho+k)!\sqrt{\pi}} H_{n_\rho+k}(s) \right]^2 N^2_{n\rho}, \tag{80}$$

where the variable

$$s := \beta^{1/2}\xi \tag{81}$$

has been used.

The analytic solution of the integral on the right-hand side of (80), together with Eqs. (70), (72)–(77), yields $\tilde{v}_z$ as a function of n_ρ, α and β^{-1}. As β^{-1} is a small quantity, a power expansion of $\tilde{v}_z$ with respect to β^{-1} suggests itself. The leading-order term is

$$\tilde{v}_z = \frac{v_{\rm scal}}{2E_{\rm scal}} \left[E^{(0)}_{k_z \nu n_\rho} + \frac{\hbar^2 \nu^2}{2M\overline{\rho^2}} + \frac{217}{3072} \frac{\hbar^2}{2M\overline{\rho^2}} \right]. \tag{82}$$

Up to the small additional term $(217/3072)\hbar^2/2M\overline{\rho^2}$, this expression coincides with formula (52) and hence with the ''classical'' result for the drift velocity parallel to the wire, if $E^{(0)}_{k_z \nu n_\rho}$ is identified with the exact eigenenergy $E_{k_z \nu n_\rho}$.

V. APPLICATION OF THE ADIABATIC EXPANSION OF THE PATH INTEGRAL

The previous two sections confirmed the validity of the assumption that the projection of the particle's magnetic moment parallel to the magnetic field is a constant of motion. Thus the wave functions $\tilde{\Psi}_{k_z \nu}(\rho,\phi,z)$ of Eq. (43) represent an excellent quantum-mechanical description of the electronic state. We now introduce the function

$$\tilde{\psi}_\nu(\rho,z) := e^{ik_z z} \frac{1}{\sqrt{\rho}} \varphi_\nu(\rho) = e^{ik_z z} u_\nu(\rho), \tag{83}$$

which, according to (42) and (29), satisfies the two-dimensional Schrödinger equation

$$\hat{H}_\perp \tilde{\psi}_\nu(\rho,z) = E_\nu \tilde{\psi}_\nu(\rho,z), \tag{84}$$

where $\hat{H}_\perp$ is given by

$$\hat{H}_\perp := -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\rho^2} + \frac{1}{2M}\left(\frac{\hbar}{i}\frac{\partial}{\partial z} + \frac{2Iq}{\hbar c^2} \ln\frac{\rho}{\lambda_c} \right)^2 + \frac{\hbar^2\nu^2}{2M\rho^2} - \frac{|gI|\mu_P}{c\rho}. \tag{85}$$

The Hamiltonian $\hat{H}_\perp$ describes the motion of a charged particle in the plane perpendicular to the magnetic field $\mathbf{B}(\mathbf{x}) = B_\phi(\rho)\mathbf{e}_\phi$, if in addition a scalar potential

$$\phi_0(\rho) := \frac{\hbar^2\nu^2}{2M\rho^2} - \frac{|gI|\mu_P}{c\rho} \tag{86}$$

is present. Note that the effects of azimuthal motion are completely taken into account in $\hat{H}_\perp$ by the centrifugal potential $\hbar^2\nu^2/2M\rho^2$.

As discussed in Sec. III, even for large quantum numbers, the quantum-mechanical eigenenergies are much smaller than the scaling energy $E_{\rm scal}$. Hence, for a classical description of the motion in the corresponding states, the guiding center approximation can be applied. Quantum mechanically, a separation of the slow guiding center motion from the fast gyration can be achieved by applying the Born-Oppenheimer method. However, since the position operators of the guiding center in general do not commute with one another [20], a generalization of this method using the path-integral approach must be employed. This is beautifully handled in Ref. [19], where the motion of a charged particle in the plane perpendicular to a strong uniform magnetic field is investigated, when an electrostatic field is simultaneously present. The corresponding calculations are summarized in Appendix B, to which we will refer in the remainder of this section whenever necessary. One can show that the additional electric field causes a dependence of the energy spacings of the Landau levels on the position of the guiding center. The corresponding eigenfunctions contain the guiding center coordinates as slowly varying parameters [see Eq. (B13)]. An expansion of the particle propagator with respect to these functions leads to a matrix of coefficients, which depend only on the coordinates of the guiding center. If one assumes that the quantum numbers of the Landau levels are not affected by a slow variation of the guiding center position (adiabatic limit), the off-diagonal elements of this matrix vanish [cf. (B15)–(B17)]. The remaining coefficients have the form of path integrals over the guiding center motion for a fixed quantum number of the gyration. The exponential appearing in them represents the effective action of the slow

variables [see (B19)]. Minimization of this action yields classical equations of motion for the guiding center, which take into account the quantization of the gyration.

We will now show that the method described above can also be applied, if a charged particle moves in the inhomogeneous magnetic field outside of a rectilinear current filament. For this purpose, we introduce for arbitrary, but fixed azimuthal angle ϕ a local Cartesian coordinate system, whose z axis is parallel to the wire and whose x axis points in the radial direction. The magnetic field $\mathbf{B}(\mathbf{x})$ is then oriented in positive y direction,

$$\mathbf{B}(\mathbf{x}) = \frac{2I}{cx}\mathbf{e}_y = B_y(x)\mathbf{e}_y . \tag{87}$$

It can be derived from the vector potential

$$\mathbf{A}(\mathbf{x}) = -\frac{2I}{c}\ln\frac{x}{\lambda_c}\mathbf{e}_z = A_z(x)\mathbf{e}_z \tag{88}$$

by the relation $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$. Using the momentum operators $\hat{p}_x := (\hbar/i)(\partial/\partial x)$, $\hat{p}_z := (\hbar/i)(\partial/\partial z)$ and Eqs. (86) and (88), the Hamiltonian $\hat{H}_\perp$ reads in the new coordinate system

$$\hat{H}_\perp = \frac{\hat{p}_x^2}{2M} + \frac{1}{2M}\left(\hat{p}_z - \frac{q}{c}A_z(x)\right)^2 + \phi_0(x). \tag{89}$$

The velocity operators in x- resp. z direction are related to the corresponding momentum operators via

$$\hat{v}_x = \frac{1}{M}\hat{p}_x, \quad \hat{v}_z = \frac{1}{M}\left(\hat{p}_z - \frac{q}{c}A_z(x)\right). \tag{90}$$

Their commutator is different from zero,

$$[\hat{v}_x, \hat{v}_z] = -i\frac{q\hbar}{M^2 c}B_y(x), \tag{91}$$

which means that a charged particle cannot have simultaneously definite values of the velocity components. Using $\hat{v}_x$ and $\hat{v}_z$, the Hamiltonian $\hat{H}_\perp$ can be written in the form

$$\hat{H}_\perp = \frac{M}{2}(\hat{v}_x^2 + \hat{v}_z^2) + \phi_0(x). \tag{92}$$

We now introduce another velocity operator

$$\hat{v}_z^H := \frac{1}{M}\left(\hat{p}_z - \frac{q}{c}A_z^H(x)\right), \tag{93}$$

where $\mathbf{A}^H(\mathbf{x}) = A_z^H(x)\mathbf{e}_z$ is chosen in such a way that the corresponding magnetic field

$$\mathbf{B}^H = B^H\mathbf{e}_y := \nabla \times \mathbf{A}^H(\mathbf{x}) \tag{94}$$

is homogeneous. The magnitude of $\mathbf{B}^H$ will be fixed later in such a way that the absolute value of the difference

$$\hat{v}_z - \hat{v}_z^H = \frac{q}{Mc}[A_z^H(x) - A_z(x)] =: \phi_1(x) \tag{95}$$

remains small within the localization region of the particle compared to its total velocity. The gauge principle implies that velocity operators do not change under gauge transformations. Therefore, $\phi_1(x)$ is also gauge invariant. Setting $\hat{v}_z = \hat{v}_z^H + \phi_1(x)$ and making use of the relation $\hat{v}_z^H\phi_1(x) = \phi_1(x)\hat{v}_z^H$ we obtain for $\hat{H}_\perp$

$$\hat{H}_\perp = \frac{M}{2}[\hat{v}_x^2 + (\hat{v}_z^H)^2] + M\phi_1(x)\hat{v}_z^H + \frac{M}{2}\phi_1^2(x) + \phi_0(x). \tag{96}$$

We now define the position operators

$$\hat{X} := x - \frac{\hat{v}_z^H}{\omega_c}, \quad \hat{Z} := z + \frac{\hat{v}_x}{\omega_c}, \tag{97}$$

where

$$\omega_c := \frac{qB^H}{Mc} \tag{98}$$

is the (constant) cyclotron frequency in the magnetic field $\mathbf{B}^H$. Up to negligible deviations, $\hat{X}$ and $\hat{Z}$ correspond to the coordinates (X,Z) of the guiding center in the x-z plane. If the guiding center approximation is valid, X and Z are slowly varying functions of time compared to the components v_x and v_z of the particle velocity. Note that, owing to the orientation of the coordinate system, X is equal to the radial distance $\rho_{\mathbf{X}}$ of the guiding center from the z axis.

Using position and momentum operators

$$\hat{q} := \frac{\hat{v}_z^H}{\omega_c}, \quad \hat{p} := M\hat{v}_x, \tag{99}$$

$$\hat{Q} := \hat{X}, \quad \hat{P} := M\omega_c\hat{Z}, \tag{100}$$

which satisfy the canonical commutator relations

$$[\hat{P},\hat{Q}] = \frac{\hbar}{i}, \quad [\hat{p},\hat{q}] = \frac{\hbar}{i} \tag{101}$$

(all other commutators vanish), we can write $\hat{H}_\perp$ in the form

$$\hat{H}_\perp = \frac{\hat{p}^2}{2M} + \frac{M\omega_c^2}{2}\hat{q}^2 + M\phi_1(\hat{Q}+\hat{q})\omega_c\hat{q} + \frac{M}{2}\phi_1^2(\hat{Q}+\hat{q}) + \phi_0(\hat{Q}+\hat{q}). \tag{102}$$

The terms ϕ_0, ϕ_1 and ϕ_1^2 are independent of $\hat{P}$ due to the symmetry of the magnetic field. A comparison with Eq. (B8) shows that $\hat{H}_\perp$ is formally equivalent to the Hamiltonian $\hat{H}(\hat{P},\hat{Q};\hat{p},\hat{q})$, which describes the dynamics of a charged particle in the superposition of a uniform magnetic field and an electrostatic field. Consequently, we can use the results of Ref. [19] to derive equations of motion for the guiding center in our field configuration.

According to the remarks at the beginning of Sec. III, the potential $\phi_0(\rho)$ defined in Eq. (86) is a slowly varying function of ρ in the localization region of the particle, which is centered around $\overline{\rho} \approx \rho_{\mathbf{X}} = Q$. By an appropriate choice of the vector potential A_z^H, the same statement holds concerning

ϕ_1. Therefore, in analogy with [19], we expand the potential terms in (102) around the guiding center coordinate Q. Up to second order in $\hat{q}$, $\hat{H}_\perp$ then reads

$$\hat{H}_\perp = \frac{\hat{p}^2}{2M} + \frac{M\omega_c^2}{2}\hat{q}^2 + \left[\frac{M}{2}\phi_1^2(Q) + \phi_0(Q)\right] + \left[M\omega_c\phi_1(Q) + \frac{M}{2}(\phi_1^2)'(Q) + \phi_0'(Q)\right]\hat{q} + \left[2M\omega_c\phi_1'(Q) + \frac{M}{2}(\phi_1^2)''(Q) + \phi_0''(Q)\right]\frac{\hat{q}^2}{2}, \tag{103}$$

where the primes at the potentials denote their derivatives with respect to q. This expansion of $\hat{H}$ is equal to that of $\hat{H}(\hat{P},\hat{Q};\hat{p},\hat{q})$ given in (B25), if the potential terms occurring in (103) and (B25) are identified in the following way:

$$\phi = \frac{M}{2}\phi_1^2 + \phi_0, \tag{104}$$

$$\phi_y = M\omega_c\phi_1 + \frac{M}{2}(\phi_1^2)' + \phi_0', \tag{105}$$

$$\phi_{yy} = 2M\omega_c\phi_1' + \frac{M}{2}(\phi_1^2)'' + \phi_0'', \tag{106}$$

$$\phi_x = \phi_{xy} = \phi_{xx} = 0\,. \tag{107}$$

Here we left out the argument Q on the right-hand sides.

Inserting (104)–(107) into Eqs. (B27), (B28) for the local Landau levels $E_n(P,Q)$, we obtain Landau levels which are independent of P. Therefore, the equation of motion (B23) for the coordinate Q yields

$$\dot{Q} \propto \frac{\partial E_n}{\partial P} = 0\,. \tag{108}$$

This means that the distance $Q = \rho_{\mathbf{X}}$ of the gyration center from the z axis remains constant, in agreement with the results from classical mechanics (cf. Appendix A).

The fact that the x coordinate of the guiding center is time independent implies that the strength $B_y(X)$ of the magnetic field stays constant at this point. If we choose the homogeneous magnetic field $\mathbf{B}^H(\mathbf{x})$ defined in (94) to be equal to the magnetic field at the guiding center position,

$$\mathbf{B}^H = B_y(X)\mathbf{e}_y = \frac{2I}{cX}\mathbf{e}_y\,, \tag{109}$$

the corresponding vector potential $\mathbf{A}^H = A_z^H(x)\mathbf{e}_z$ is given by

$$\mathbf{A}^H(x) = -\frac{2I}{cX}x\ \ \mathbf{e}_z + C\mathbf{e}_z\,. \tag{110}$$

The constant C is determined by the requirement that the difference $\phi_1(x) \propto A_z(x) - A_z^H(x)$ should become as small as possible within the localization region of the particle. This is achieved, if

$$C = -\frac{2I}{c}\left(\ln\frac{X}{\lambda_c} - 1\right), \tag{111}$$

because then

$$\phi_1(x) = \frac{q}{Mc}[A_z^H(x) - A_z(x)] = \frac{2Iq}{Mc^2}\left(\ln\frac{x}{X} - \frac{x}{X} + 1\right) = v_{\mathrm{scal}}\left(\ln\frac{x}{X} - \frac{x}{X} + 1\right) \tag{112}$$

is equal to the difference between the logarithm $\ln(x/X)$ and the first two terms of its Taylor expansion around X.

Evaluating ϕ_0 and ϕ_1 at the point $Q = X$ leads to the following result for ϕ:

$$\phi = \frac{\hbar^2\nu^2}{2MX^2} - \frac{|gI|\mu_P}{cX}. \tag{113}$$

Note that this formula contains no terms originating from ϕ_1, because ϕ_1 and ϕ_1' vanish at X.

To write down the equation of motion for the coordinate $Z = (1/M\omega_c)P$ explicitly, we have to transcribe several quantities defined in Appendix B to our case. First note that, according to (102), $\hat{H}_\perp$ does not depend on $\hat{P}$. Taking into account Eqs. (B20)–(B22), the variables P and Q turn out to be canonical. This is a direct consequence of the symmetry of the magnetic field $\mathbf{B}(\mathbf{x})$. The time development of P is determined by [cf. (B24)]

$$\dot{P} = -\frac{\partial E_n}{\partial Q}, \tag{114}$$

where, according to (B26), the energy E_n can be written in the form

$$E_n(Q) = \hbar\Omega(Q)(n + \tfrac{1}{2}) + E_0(Q), \tag{115}$$

with Ω and E_0 given by (B27) and (B28). Using (113) we obtain for Ω and E_0

$$\Omega = \frac{|v_{\mathrm{scal}}|}{X}\left[1 + \frac{2\epsilon_{3/2}(X)}{Mv_{\mathrm{scal}}^2}\right]^{1/2} = \Omega(X), \tag{116}$$

$$E_0 = \epsilon_{1/2}(X) - \frac{1}{2Mv_{\mathrm{scal}}^2}\epsilon_1^2(X)\left[1 + \frac{2\epsilon_{3/2}(X)}{Mv_{\mathrm{scal}}^2}\right]^{-1} = E_0(X), \tag{117}$$

where the function $\epsilon_\alpha(X)$ is defined by

$$\epsilon_\alpha(x) := \alpha\frac{\hbar^2\nu^2}{2Mx^2} - \frac{|gI|\mu_P}{cx}, \quad \alpha \in \mathbb{R}. \tag{118}$$

Note that by the definitions (22) and (49), $\epsilon_\alpha(x)$ is equal to the sum of $W(x)$ and α times the centrifugal potential. As a result of (114)–(118), the equation of motion for the z coordinate of the guiding center reads

$$\dot{Z}=\frac{1}{M\omega_c}\dot{P}=-\frac{1}{M\omega_c}\frac{\partial E_n}{\partial Q}$$
$$=\frac{\hbar\Omega(X)(n+1/2)}{Mv_{\mathrm{scal}}}\left[1+\frac{\epsilon_3(X)}{Mv_{\mathrm{scal}}^2}\left(1+\frac{2\epsilon_{3/2}(X)}{Mv_{\mathrm{scal}}^2}\right)^{-1}\right]$$
$$+\frac{\epsilon_1(X)}{Mv_{\mathrm{scal}}}\left\{1+\left[\frac{\epsilon_2(X)}{Mv_{\mathrm{scal}}^2}+\frac{\epsilon_3(X)}{Mv_{\mathrm{scal}}^2}\left(1+\frac{2\epsilon_{3/2}(X)}{Mv_{\mathrm{scal}}^2}\right)^{-1}\right]\right.$$
$$\left.\times\left(1+\frac{2\epsilon_{3/2}(X)}{Mv_{\mathrm{scal}}^2}\right)^{-1}\right\}. \tag{119}$$

Since X remains constant, the right-hand side of (119) is time independent. Thus the guiding center motion parallel to the wire is uniform. The drift velocity $\dot{Z}$ depends not only on the quantum numbers n and ν, but also on k_z. This is so because the radial coordinate $X=\rho_{\mathbf{X}}$ of the guiding center is approximately equal to $\overline{\rho}$ (cf. Sec. III), which is related to k_z via Eq. (29).

The basic assumption of the preceding calculations was that the total energy of the charged particle is small compared to E_{scal}. In particular, this implies that the centrifugal energy and the potential energy of the magnetic dipole moment are much smaller than E_{scal} within the localization region of the particle, especially at the position of the guiding center. From Eq. (118), we therefore conclude that the estimation

$$\left|a\frac{\epsilon_\alpha(X)}{Mv_{\mathrm{scal}}^2}\right|\ll 1 \tag{120}$$

is valid for not too large values of the parameters a and α. Hence we expand all terms of the form

$$\left(1+\frac{a\epsilon_\alpha(X)}{Mv_{\mathrm{scal}}^2}\right)^b, \quad b\in\mathbb{Z} \tag{121}$$

appearing on the right-hand side of (119) in power series with respect to $\epsilon_\alpha(X)/Mv_{\mathrm{scal}}^2$ Considering in addition the special form of $\Omega(X)$ given in (116), the leading order term of this expansion reads

$$\dot{Z}=\frac{v_{\mathrm{scal}}}{2}\frac{\hbar|\omega_c|(n+1/2)-|gI|\mu_P/cX+\hbar^2\nu^2/MX^2}{E_{\mathrm{scal}}}. \tag{122}$$

Up to small deviations, which can be neglected in guiding center approximation, the sum of the quantized gyration energy $\hbar|\omega_c|(n+\frac{1}{2})$ and $\hbar^2\nu^2/2MX^2-|gI|\mu_P/cX$ is equal to the total energy $E_{k_z\nu n}$ of the particle. Using again the identification (51) of Sec. III, one can show that (122) is equivalent to the ''classical'' formula (50) for the drift velocity.

V. SUMMARY AND DISCUSSION

In this paper we presented the quantum-mechanical description of electrons (or more generally of pointlike charged particles with spin $\frac{1}{2}$) in the magnetic field of a rectilinear current. The assumption of a rectilinear current of length L represents at the same time a good approximation for a circular current whenever the macroscopic length L exceeds by far the extension of the wave functions in perpendicular direction to the current.

As one can guess from the macroscopic dimension of the field producing current, the classical approximation for the motion of the charged particle is found to be very good, even for low values of the quantum numbers. This is particularly true for the motion of the guiding center. If one treats the gyration quantum mechanically assuming that the quantum numbers of the gyration are adiabatic invariants, one can justify this statement.

The macroscopic dimension of the field producing current implies necessarily that the problem has many similarities with the one of a plasma in an external magnetic field. Therefore, we could use an ingenious method developed in plasma physics [14–18] to take into account the presence of two time scales in the problem, separating the rapid gyration from the slow motion of the guiding center.

When trying to apply this method in the quantum-mechanical theory, one faces the difficulty that the variables of the gyration motion are not canonical—physically no surprise in view of the fact that the gyration center does not correspond to a particle. Here the results of a paper by Entelis and Levit [19] were useful for us. This work is based on the path-integral formalism and designed to treat the dynamics of a charged particle in a superposition of a homogeneous magnetic field and a (small) electric field. The same formalism could also be used for our case of a charged particle in an inhomogeneous magnetic field.

The quantum features of our problem become more pronounced as the length L of the current filament is decreased. Since any natural application will be based on a circular current, one should in principle solve the quantum-mechanical problem for the magnetic field produced by a circular current. We note, however, that for not too small length L of the circumference, one can use local curvilinear coordinates and treat the deviations from the rectilinear case as a perturbation.

The most important open questions concern eventual applications of the system we have studied. Is it purely academic or can it be used?

Here we mention some ideas for application, hoping, at the same time, that this list will be extended by the imagination of the reader.

(i) In Ref. [26] we investigated the effect of gravity on an antiproton moving in the magnetic field of a vertical current. This could possibly be used to determine the gravitational mass of the antiproton. Only the classical features of the system would enter this application.

(ii) So far we have only investigated the case where the overlap of the wave functions with the material of the wire are negligible. It is, however, clear that there are also bound states where this overlap is not negligible. Then the particle feels the interaction with the solid, especially its surface, in addition to the magnetic field of the current. If, for instance, these interactions lead to a trapping of the particle in the surface, this could be seen by looking at the electromagnetic transitions.

We note at this point that the rate for spontaneous electromagnetic transitions between the bound states is negligibly small. On the other hand, transitions could probably be

induced in very much the same way as in atomic beam experiments.

(iii) A very different aspect is the possibility to generate chaotic motion of the bound charged particle by subjecting it to the field of a time-dependent electric current. We investigated this classically for the case of an alternating current [26]. In this case, essentially no transition to chaotic motion was observed. Chaotic motion would, however, certainly be produced if the strength and/or the direction of the current changed in a random way. The crucial question is how the dynamical state of the charged particle is observed. Again this could, in principle, be done by inducing transitions.

(iv) An open problem, which we have not yet investigated is that the current contains (statistical and quantum) fluctuations and that the temperature of the wire is finite and cannot be made zero exactly. If the quantum numbers of the particle are such that no overlap occurs with the interior of the wire, these effects are negligible. In the opposite case, they are likely to play an important role. Thus they will have the consequence that the charged particle is never in a pure quantum state but in a mixture of such states. It might even be ejected from the bound states into the continuum by the interactions with the fluctuations of the wire. We note in passing that this problem is also present, and in even more acute form, for neutral particles which are only bound by the coupling of their magnetic moment with the magnetic field.

(v) In applications it is important to know the upper limit of the electronic density which can be reached without losing the electrons on account of their Coulomb repulsion. For this, one has to compare the repulsive Coulomb potential acting on an electron due to the interaction with all the other bound electrons outside of the (neutral) wire with the height of the barrier of the magnetic potential. For a straight wire of length L, this barrier height is given by (A14)

$$V_{\mathrm{bar}}=\frac{M}{2}v_{\mathrm{scal}}^{2}\,\mathrm{arsinh}^{2}\left(\frac{L}{2\rho}\right).$$

The repulsive Coulomb potential has the form

$$V_{\mathrm{Cb}}=e^{2}\int d^{3}\mathbf{x}'\,\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}, \tag{123}$$

where $\rho(\mathbf{x}')$ is the density of the bound particles. As a rough estimate for V_{Cb}, we replace $\rho(\mathbf{x}')$ by a constant charge density in a sphere of radius R around the wire. The outcome of this is that one can attain charge densities of about 3×10^{10}(electrons/cm^3) for large currents of $I=500$ A. The critical charge density is, of course, a function of the strength of the current. For comparison, the charge density in electron lasers is about 10^{10}(electrons/cm^3).

The question of whether stimulated laserlike transitions could be produced suggests itself. We cannot judge whether this is realistic. The interest could be that the lifetime of excited states is not reduced too much by thermal effects as compared to laser transitions in solids at low transition energies.

(vi) A final remark concerns the question of how electrons or other charged particles can be trapped in the magnetic potential. If the particles are ions, i.e., composite, this could be achieved by laser cooling [27]. If the particles to be trapped have no intrinsic excitations, as for the case of electrons, this mechanism does not work. We believe that in this case trapping could be achieved by directing a well collimated low-energy beam of the charged particles tangentially to the wire. The energy must be in the range of the energies of the bound states, i.e., it depends on the strength of the magnetic field which is present.

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APPENDIX A

In this appendix, we briefly review the classical dynamics of a charged particle with spin $\frac{1}{2}$ in the magnetic field outside of a thin rectilinear current, as investigated in [13].

The classical Hamiltonian of this system has the form

$$H_{\mathrm{class}}=\frac{1}{2M}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}(\mathbf{x})\right)^{2}-\boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{x}), \tag{A1}$$

where q denotes the charge of the particle, M its mass, and $\boldsymbol{\mu}$ its intrinsic magnetic moment.

In order to describe the interaction between the particle's magnetic moment $\boldsymbol{\mu}$ and the external magnetic field classically, we assume that the projection of $\boldsymbol{\mu}$ along the field lines is a constant of motion. As shown in [13] and confirmed by the calculations in Sec. III of the present paper, this approximation is valid in the energy range relevant for a comparison between classical and quantum mechanics. In this case, the potential $\boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{x})$ takes the simple form

$$\boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{x})=-\mu_{\parallel}|\mathbf{B}(\mathbf{x})|, \tag{A2}$$

where $\mu_{\parallel}>0$ denotes the (time-independent) component of $\boldsymbol{\mu}$, which points in the direction of the magnetic field. If the latter is produced by a filamentary current, the corresponding force $\boldsymbol{\nabla}(\mu_{\parallel}|\mathbf{B}(\mathbf{x})|)$ attracts the particle to the wire.

Inserting the special forms (6) and (7) for vector potential and magnetic field into (A1), we get for the Hamiltonian

$$H_{\mathrm{class}}(\rho;p_{\rho},p_{\phi},p_{z})=\frac{1}{2M}\left[p_{\rho}^{2}+\frac{p_{\phi}^{2}}{\rho^{2}}+\left(p_{z}+\frac{2Iq}{c^{2}}\ln\frac{\rho}{\lambda_{c}}\right)^{2}\right]-\frac{2|I|\mu_{\parallel}}{c\rho}. \tag{A3}$$

The corresponding Hamiltonian equations of motion read

$$\dot{\rho}=\frac{\partial H_{\mathrm{class}}}{\partial p_{\rho}}=\frac{p_{\rho}}{M}, \tag{A4}$$

$$\dot{\phi}=\frac{\partial H_{\mathrm{class}}}{\partial p_{\phi}}=\frac{p_{\phi}}{M\rho^{2}}, \tag{A5}$$

$$\dot{z}=\frac{\partial H_{\mathrm{class}}}{\partial p_{z}}=\frac{1}{M}\left(p_{z}+\frac{2Iq}{c^{2}}\ln\frac{\rho}{\lambda_{c}}\right), \tag{A6}$$

$$\dot{p}_\rho = -\frac{\partial H_{\rm class}}{\partial \rho} = -\frac{2Iq}{c^2\rho}\dot{z} + \frac{p_\phi^2}{M\rho^3} - \frac{2|I|\mu_\parallel}{c\rho^2}, \tag{A7}$$

$$\dot{p}_\phi = -\frac{\partial H_{\rm class}}{\partial \phi} = 0 \Rightarrow p_\phi = \text{const} =: L_z, \tag{A8}$$

$$\dot{p}_z = -\frac{\partial H_{\rm class}}{\partial z} = 0 \Rightarrow p_z = \text{const} =: P_z. \tag{A9}$$

Due to the symmetry of the magnetic field, the canonical momenta p_ϕ and p_z are conserved quantities. According to (A6), the velocity in z direction, however, is not constant. It vanishes, if the particle is at a distance

$$\overline{\rho} = \lambda_c \exp\left(-\frac{P_z c^2}{2Iq}\right) \tag{A10}$$

from the z axis.

Using the scaling velocity $v_{\rm scal} = 2Iq/Mc^2$ defined in (33) and taking into account (A8)–(A10) we obtain for the Hamiltonian

$$H_{\rm class}(\rho;p_\rho) = \frac{p_\rho^2}{2M} + \frac{L_z^2}{2M\rho^2} + \frac{M}{2}v_{\rm scal}^2\left(\ln\frac{\rho}{\overline{\rho}}\right)^2 - \frac{2|I|\mu_\parallel}{c\rho}. \tag{A11}$$

Equations (A11) and (A4), together with the fact that the energy of the system is conserved, $H_{\rm class}(\rho;p_\rho,p_\phi,p_z) = E = \text{const}$, lead to the following relation between $\dot{\rho}$ and ρ:

$$\dot{\rho} = \pm\frac{1}{M}\left[2ME - \frac{L_z^2}{\rho^2} - M^2 v_{\rm scal}^2\left(\ln\frac{\rho}{\overline{\rho}}\right)^2 + \frac{4M|I|\mu_\parallel}{c\rho}\right]^{1/2}$$

$$=: \pm\frac{1}{M}\sqrt{D(\rho)}. \tag{A12}$$

To learn something about the classically allowed region in radial direction, the function $D(\rho)$ must be analyzed. As a result, one finds that in the field configuration given by (6) charged particles cannot move arbitrarily far away from the wire.

If the condition $\rho \ll L$ is no longer valid, the expression (4) for the vector potential has to be used instead of (6). Except for a modification of the magnetic field, which is negligible for the determination of the classically allowed region, the quadratically logarithmic potential $(M/2)v_{\rm scal}^2[\ln(\rho/\overline{\rho})]^2$ in (A11) has to be replaced by

$$\frac{M}{2}v_{\rm scal}^2\left[\operatorname{arsinh}\left(\frac{L}{2\overline{\rho}}\right) - \operatorname{arsinh}\left(\frac{L}{2\rho}\right)\right]^2. \tag{A13}$$

This potential approaches a finite boundary value for $\rho \to \infty$,

$$V_{\rm bar} := \frac{M}{2}v_{\rm scal}^2 \operatorname{arsinh}^2\left(\frac{L}{2\overline{\rho}}\right). \tag{A14}$$

Consequently, the motion in radial direction is no longer bound, if the total energy of the particle exceeds $V_{\rm bar}$.

Note that in the vicinity of $\overline{\rho}$, where the lowest quantum states are localized, $(M/2)v_{\rm scal}^2[\ln(\rho/\overline{\rho})]^2$ and the expression (A13) coincide. Therefore, the simpler form (6) of the vector potential was taken as a basis for the quantum-mechanical calculations of this paper.

If the total energy of the particle is small compared to $E_{\rm scal} = (M/2)v_{\rm scal}^2$, one can show that the motion consists of a rapid gyration around the magnetic field lines and a drift of the guiding center parallel to the wire. In this case, the time integration of Eqs. (A12) and (A6) can be carried out analytically. As a result, one gets the following formula for the drift velocity v_D in z direction:

$$v_D = \frac{v_{\rm scal}}{2}\frac{E + L_z^2/2M\rho_0^2}{E_{\rm scal}}, \tag{A15}$$

where ρ_0 denotes the radial coordinate of the particle at the beginning of the motion.

Equation (A15) is in agreement with general results for the guiding center motion, which are derived, e.g., in [16–18]. Especially, one can show (see [26]) that up to small deviations, which can be neglected in guiding center approximation, the radial coordinate $\rho_{\mathbf{X}}$ of the guiding center is equal to $\overline{\rho}$.

APPENDIX B

For a charged particle moving in a strong homogeneous magnetic field in the presence of an electrostatic potential a separation of the slow guiding center motion from the fast gyration was carried out quantum mechanically by Entelis and Levit [19]. As we make direct use of their method in Sec. V of the present paper, the relevant calculations of Ref. [19] are summarized in this appendix.

To this end, consider a particle with mass M and charge q, confined to the x-y plane, which is exposed to a homogeneous magnetic field $\mathbf{B} = B\mathbf{e}_z$ and an electrostatic potential $\phi(x,y)$. The two-dimensional Hamiltonian of this system is given by

$$\hat{H} = \frac{1}{2M}\left[\left(\hat{p}_x - \frac{q}{c}A_x(x,y)\right)^2 + \left(\hat{p}_y - \frac{q}{c}A_y(x,y)\right)^2\right] + \phi(x,y), \tag{B1}$$

where $\mathbf{A}(x,y) = A_x(x,y)\mathbf{e}_x + A_y(x,y)\mathbf{e}_y$ denotes the vector potential.

Introducing the velocity operators

$$\hat{v}_x = \frac{1}{M}\left(\hat{p}_x - \frac{q}{c}A_x\right), \quad \hat{v}_y = \frac{1}{M}\left(\hat{p}_y - \frac{q}{c}A_y\right) \tag{B2}$$

and the operators of the guiding center coordinates (cf. [20])

$$\hat{X} = x + \frac{\hat{v}_y}{\omega_c}, \quad \hat{Y} = y - \frac{\hat{v}_x}{\omega_c}, \tag{B3}$$

one can write $\hat{H}$ in the form

$$\hat{H} = \frac{M}{2}(\hat{v}_x^2 + \hat{v}_y^2) + \phi\left(\hat{X} - \frac{\hat{v}_y}{\omega_c}, \hat{Y} + \frac{\hat{v}_x}{\omega_c}\right). \tag{B4}$$

If the magnetic field **B** is strong compared to the electric field $\mathbf{E}(x,y)=-\boldsymbol{\nabla}\phi(x,y)$, the classical guiding center approximation is valid. This implies that the velocity of the particle changes rapidly in time compared to the position of the gyration center. The Hamiltonian $\hat{H}$ thus contains motions on two different time scales via the operators $\hat{v}_x$, $\hat{v}_y$ (fast) and $\hat{X}$, $\hat{Y}$ (slow). Therefore, an application of the Born-Oppenheimer method to describe the dynamics of the particle suggests itself. As, however, $\hat{X}$ and $\hat{Y}$ do not commute with one another, the guiding center coordinates cannot be specified simultaneously and a generalization of the Born-Oppenheimer method is needed. It can be obtained by applying the path-integral formalism [28,29].

To cast the corresponding formulas into a conventional form, the operators

$$\hat{q}:=\frac{\hat{v}_x}{\omega_c},\quad \hat{p}:=M\hat{v}_x, \tag{B5}$$

$$\hat{Q}:=\hat{Y},\quad \hat{P}:=M\omega_c\hat{X} \tag{B6}$$

are defined, which satisfy the commutation relations

$$[\hat{P},\hat{Q}]=\frac{\hbar}{i},\quad [\hat{p},\hat{q}]=\frac{\hbar}{i}. \tag{B7}$$

As all other commutators vanish, $\hat{q}$, $\hat{p}$ and $\hat{Q}$, $\hat{P}$ can be considered as canonically conjugate position and momentum operators. Using (B4)–(B6), the Hamiltonian $\hat{H}$ reads

$$\hat{H}(\hat{P},\hat{Q};\hat{p},\hat{q})=\frac{\hat{p}^2}{2M}+\frac{M\omega_c^2\hat{q}^2}{2}+\phi\left[\frac{1}{M\omega_c}(\hat{P}-\hat{p}),\hat{Q}+\hat{q}\right]. \tag{B8}$$

According to (B7) and (B8), the classical variables q and Q can be interpreted as (generalized) coordinates. Quantum mechanically, their time development is determined by the propagator

$$\langle Q_f,q_f,t_f|Q_i,q_i,t_i\rangle:=\langle Q_f q_f|\,\mathrm{e}^{-i\hat{H}(t_f-t_i)}|Q_i q_i\rangle=\int_{(Q_i,q_i)}^{(Q_f,q_f)}DQ(t)Dq(t)\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}L(Q,q;\dot{Q},\dot{q})dt\right], \tag{B9}$$

where the indices ''i'' resp. ''f'' denote the values of the variables at the beginning resp. end of the time interval under consideration. In the path integral, the coordinates $Q(t)$, $q(t)$ are time-dependent functions and the Lagrangian L is given by

$$L(Q,q;\dot{Q},\dot{q})=P\dot{Q}+p\dot{q}-H(P,Q;p,q), \tag{B10}$$

where p resp. P are classical momenta conjugate to q resp. Q. Due to the definitions (B5) and (B6), the variables P and Q are slowly varying in time compared to p and q.

In analogy with the ansatz for the total wave function in the Born-Oppenheimer method, we now split up the path integral in the following way:

$$\langle Q_f,q_f,t_f|Q_i,q_i,t_i\rangle=\int_{Q_i}^{Q_f}DP(t)DQ(t)\exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f}P\dot{Q}dt\right)\int_{q_i}^{q_f}Dp(t)Dq(t)\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}[p\dot{q}-H(P,Q;p,q)]dt\right], \tag{B11}$$

which means that we carry out first the path integration over the fast variables at fixed trajectory $\{P(t),Q(t)\}$ and then integrate over all paths of the guiding center motion. Formally, (B11) is equal to [30]

$$\langle Q_f,q_f,t_f|Q_i,q_i,t_i\rangle=\int_{Q_i}^{Q_f}DP(t)DQ(t)\exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f}P\dot{Q}dt\right)\left\langle q_f\left|T\exp\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{H}'[P(t),Q(t);\hat{p},\hat{q}]dt\right\}\right|q_i\right\rangle. \tag{B12}$$

The Hamiltonian $\hat{H}'$ appearing in the time-ordered exponential has the same form as $\hat{H}$, but contains the variables P and Q as slowly varying functions of time and not as operators.

We will now derive an explicit expression for the propagator of the fast variables using the complete set of eigenstates of $\hat{H}'$ for fixed parameters P and Q, which we denote by $|n(P,Q)\rangle$. The corresponding wave functions $\psi_n(q;P,Q)$ are according to (B8) solutions of the stationary Schrödinger equation

$$\left\{\frac{1}{2M}\frac{\partial^2}{\partial q^2}+\frac{M\omega_c^2q^2}{2}+\phi[(P+i\hbar\partial/\partial q)/M\omega_c,Q+q]\right\}\psi(q;P,Q)=E_n(P,Q)\psi(q;P,Q), \tag{B13}$$

where the energy eigenvalues $E_n(P,Q)$ can be interpreted as local Landau levels, whose distance depends on the position of the guiding center. An expansion of the second factor in the path integral (B12) with regard to the eigenstates $|n(P,Q)\rangle$ at the parameter values P_i, Q_i and P_f, Q_f yields

$$\left\langle q_f \left| T\exp\left\{ -\frac{i}{\hbar}\int_{t_i}^{t_f} \hat{H}'[P(t),Q(t);\hat{p},\hat{q}]dt \right\} \right| q_i \right\rangle$$
$$= \sum_{n,m} \psi_n^*(q_f;P_f,Q_f)\langle n(P_f,Q_f)|T\exp\left\{ -\frac{i}{\hbar}\int_{t_i}^{t_f} \hat{H}'[P(t),Q(t);\hat{p},\hat{q}]dt \right\}|m(P_i,Q_i)\rangle \psi_m(q_i;Q_i,Q_f)$$
$$=: \sum_{n,m} \psi_n^*(q_f;P_f,Q_f)K_{nm}(t_f;t_i)\psi_m(q_i;Q_i,Q_f). \tag{B14}$$

If one assumes that the quantum numbers of the eigenstates of $\hat{H}'$ are not affected by a slow time variation of the parameters P and Q (adiabatic approximation), the matrix elements $K_{nm}(t_f;t_i)$ are of the form [31]

$$K_{nm}(t_f;t_i) = \delta_{nm}\exp\left\{ \frac{i}{\hbar}\int_{t_i}^{t_f} dt[f_n(P,Q)\dot{Q} + g_n(P,Q)\dot{P} - E_n(P,Q)] \right\}, \tag{B15}$$

with the functions

$$f_n(P,Q) := i\hbar\langle n(P,Q)|\partial/\partial Q|n(P,Q)\rangle, \tag{B16}$$

$$g_n(P,Q) := i\hbar\langle n(P,Q)|\partial/\partial P|n(P,Q)\rangle. \tag{B17}$$

As a result, the adiabatic expansion of the total particle propagator (B9) is given by

$$\langle Q_f q_f t_f|Q_i q_i t_i\rangle \simeq \sum_n \int DP(t)DQ(t)\psi_n^*(q_f;P_f,Q_f)\psi_n(q_i;P_i,Q_i)$$
$$\times \exp\left\{ \frac{i}{\hbar}\int_{t_i}^{t_f} dt[P\dot{Q} + f_n(P,Q)\dot{Q} + g_n(P,Q)\dot{P} - E_n(P,Q)] \right\}. \tag{B18}$$

The integral in the exponential can be interpreted as the effective action of the guiding center motion for fixed quantum number n of the Landau level,

$$S_n^{\rm eff}(P_f,Q_f;P_i,Q_i) := \int_{t_i}^{t_f} dt[f_n(P,Q)\dot{Q} + g_n(P,Q)\dot{P} - E_n(P,Q)]. \tag{B19}$$

Here, $E_n(P,Q)$ plays the role of a Hamiltonian and the Berry phase term $f_n\dot{Q} + g_n\dot{P}$ modifies the structure of the (P,Q) phase space: the Poisson bracket of the originally canonical variables Q and P are changed into

$$\{P,Q\} = \frac{1}{R_n(P,Q)}, \tag{B20}$$

where the function $R_n(P,Q)$ takes the form

$$R_n(P,Q) = 1 + \frac{\partial f_n}{\partial P}(P,Q) - \frac{\partial g_n}{\partial Q}(P,Q). \tag{B21}$$

Note that according to general results in connection with the Berry phase [32], the difference $\partial f_n/\partial P - \partial g_n/\partial Q$ can be calculated using the formula

$$\frac{\partial f_n}{\partial P}(P,Q) - \frac{\partial g_n}{\partial Q}(P,Q) = \hbar\ \mathrm{Im}\left\{ \sum_{m\neq n} \frac{\left\langle n\left|\frac{\partial \hat{H}'}{\partial P}\right|m\right\rangle\left\langle m\left|\frac{\partial \hat{H}'}{\partial Q}\right|n\right\rangle - \left\langle n\left|\frac{\partial \hat{H}'}{\partial Q}\right|m\right\rangle\left\langle m\left|\frac{\partial \hat{H}'}{\partial P}\right|n\right\rangle}{[E_n(P,Q) - E_m(P,Q)]^2} \right\}. \tag{B22}$$

Minimization of the effective action $S_n^{\rm eff}$ yields the classical equations of motion

$$\dot{Q}=\frac{1}{R_n}\frac{\partial E_n}{\partial P}, \tag{B23}$$

$$\dot{P}=-\frac{1}{R_n}\frac{\partial E_n}{\partial Q} \tag{B24}$$

for the guiding center coordinates $X=P/M\omega_c$ and $Y=Q$. They can be written down in closed form, whenever the dependence of the local Landau levels $E_n(P,Q)$ on the variables P and Q is explicitly known. For this purpose, an analytic solution of the Schrödinger equation (B13) is needed, which in general cannot be given.

If, however, the potential $\phi(x,y)$ is slowly varying within the localization region of the particle, which can be estimated by the quantum-mechanical oscillator length $a_B=(\hbar/M|\omega_c|)^{1/2}$ ($\omega_c=qB/Mc$ denotes the cyclotron frequency corresponding to the uniform magnetic field **B**), an expansion of $\phi(x,y)$ around the guiding center position (X,Y) is possible. Up to second order in the operators $\hat{p}/M\omega_c$ and $\hat{q}$, the Hamiltonian $\hat{H}'(P,Q;\hat{p},\hat{q})$ reads

$$\begin{aligned}\hat{H}'(P,Q;\hat{p},\hat{q})\simeq&\frac{\hat{p}^2}{2M}+\frac{M\omega_c^2\hat{q}^2}{2}+\phi-\phi_x\frac{\hat{p}}{M\omega_c}+\phi_y\hat{q}\\&+\frac{\phi_{xx}}{2(M\omega_c)^2}\hat{p}^2-\frac{\phi_{xy}}{2M\omega_c}(\hat{q}\hat{p}+\hat{p}\hat{q})\\&+\frac{1}{2}\phi_{yy}\hat{q}^2,\end{aligned} \tag{B25}$$

where the indices ''x'' and ''y'' denote partial derivatives of $\phi(x,y)$ with respect to the corresponding variables. The functions ϕ, ϕ_x, etc., have to be evaluated at the point $(X,Y)=(P/M\omega_c,Q)$.

After an elimination of the term $-(\phi_{xy}/2M\omega_c)(\hat{q}\hat{p}+\hat{q}\hat{p})$ in (163) by a Bogoliubov transformation, the eigenenergies of $\hat{H}'$ take the form

$$E_n(P,Q)=\hbar|\Omega(P,Q)|(n+1/2)+E_0(P,Q), \tag{B26}$$

with an oscillator frequency

$$\Omega=\omega_c\left(1+\frac{1}{M\omega_c^2}(\phi_{xx}+\phi_{yy})+\frac{1}{M^2\omega_c^4}(\phi_{xx}\phi_{yy}-\phi_{xy}^2)\right)^{1/2} \tag{B27}$$

and an energy constant

$$\begin{aligned}E_0=&\phi-\phi_x^2\frac{1+\phi_{yy}/M\omega_c^2}{2M\Omega^2}-\phi_y^2\frac{1+\phi_{xx}/M\omega_c^2}{2M\Omega^2}\\&+\phi_x\phi_y\frac{\phi_{xy}}{M^2\omega_c^2\Omega^2}.\end{aligned} \tag{B28}$$

Starting from (B26)–(B28), an analytic expression for the guiding center equations (B23) and (B24) can be derived if, in addition, the approximation

$$\frac{\partial f_n}{\partial P}(P,Q)-\frac{\partial g_n}{\partial Q}(P,Q)\approx\frac{\phi_{xy}^2-\phi_{xx}\phi_{yy}}{(M\omega_c\Omega)^2} \tag{B29}$$

is used. The latter is obtained by neglecting in (B22) all matrix elements but the ones with $m=n\pm1$ and inserting the expansion (B25) for $\hat{H}'$.

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