Axial and Landau gauge for a continuum electron in a homogeneous magnetic field

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In an attempt to obtain a suitable access to the quantum description of a continuum electron in a combined Coulomb and homogeneous magnetic field, we first illustrate the complexity of the problem by selected classical trajectories. Subsequently, we examine the properties and consequences of two particular gauges for representing a homogeneous magnetic field, in particular, their usefulness in describing Coulombic bound and continuum states. We show that in the absence of a Coulomb field, the Landau gauge but not the axial gauge allows for a simple construction of asymptotic states that satisfy the requirement of tending to plane waves in the limit of vanishing field strength.

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I. INTRODUCTION

A hydrogenlike atom placed in a homogeneous magnetic field represents one of the simplest possible atomic systems. However, its quantum-mechanical treatment constitutes an exceedingly difficult task. While solutions have been obtained for a large number of special situations, it is fair to say that the full problem still awaits a theoretical description.

The problem has been mostly treated for extremely strong magnetic fields occurring in neutron stars and white dwarfs [1,2] or in the study of chaotic behavior prevalent in highly excited Rydberg states, which are magnetically dominated already for field strengths of a few Teslas [3,4]. The renewed interest derives from the attempts to form antihydrogen in a Penning trap by radiative recombination of antiprotons with positrons and from experiments in an electron cooler ring, where a magnetically guided beam of bare heavy ions merges an electron beam of almost the same velocity so that electrons are radiatively captured into a Coulomb bound state. In contrast to most theoretical treatments, which have dealt with bound or quasibound states, see e.g., [5], both cases of interest require the consideration of continuum electrons.

In Sec. II, we briefly discuss experiments in a cooler ring and attempts to explain the results in terms of classical trajectories, for which two examples are shown. In Sec. III, a quantum description in terms of the axial and the Landau gauge is reviewed, followed by an examination of the corresponding asymptotic continuum states in Sec. IV. Concluding remarks are contained in Sec. V.

II. CLASSICAL TRAJECTORIES

The process of radiative recombination requires a quantum description in order to correctly accommodate photon emission. However, it should be instructive to visualize the corresponding classical trajectories. While we have a good notion of how classical trajectories of continuum electrons look in a Coulomb field alone or in a homogeneous magnetic field alone, we find it difficult to imagine trajectories in a combined Coulomb and magnetic field.

Clearly, we cannot expect that classical trajectories can give a quantitative account of the experimental finding [6] that radiative recombination in the presence of a magnetic field is strongly enhanced compared to theoretical results obtained for the field-free case. For a qualitative understanding, it has been proposed [6] that a low-energy (with respect to the ion) electrons spiralling in the magnetic field may form a quasibound state once they come under the influence of the ion's Coulomb field. This is illustrated in Fig. 1, where the nuclear charge, the magnetic-field strength B and the relative electron energy have been chosen to correspond to the experimental situation. One then would argue that the prolonged presence of the electron in the vicinity of the nucleus will lead to an increased probability for radiative capture and thus explain the observed enhancement [7]. However, in this respect, Fig. 1 is misleading, because the distance of the

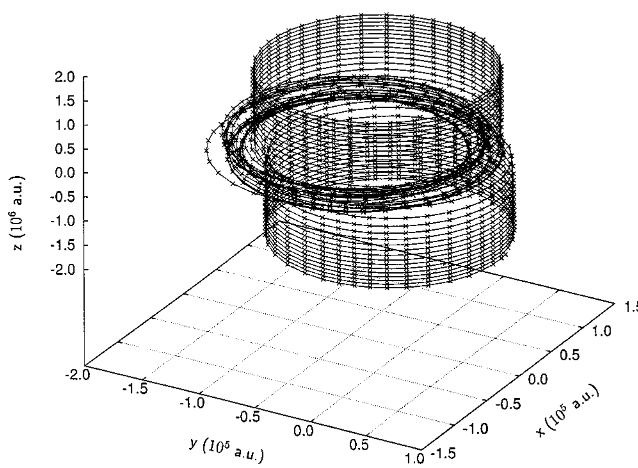

FIG. 1. Classical trajectory of an electron in the combined field of a bare nucleus with charge $Z=6$ and a magnetic field in the z direction of $B_z=42$ mT. The electron has an asymptotic kinetic energy of $E_{\parallel}=1.5$ meV in the direction of the field and of $E_{\perp}=6.0$ meV perpendicular to the field.

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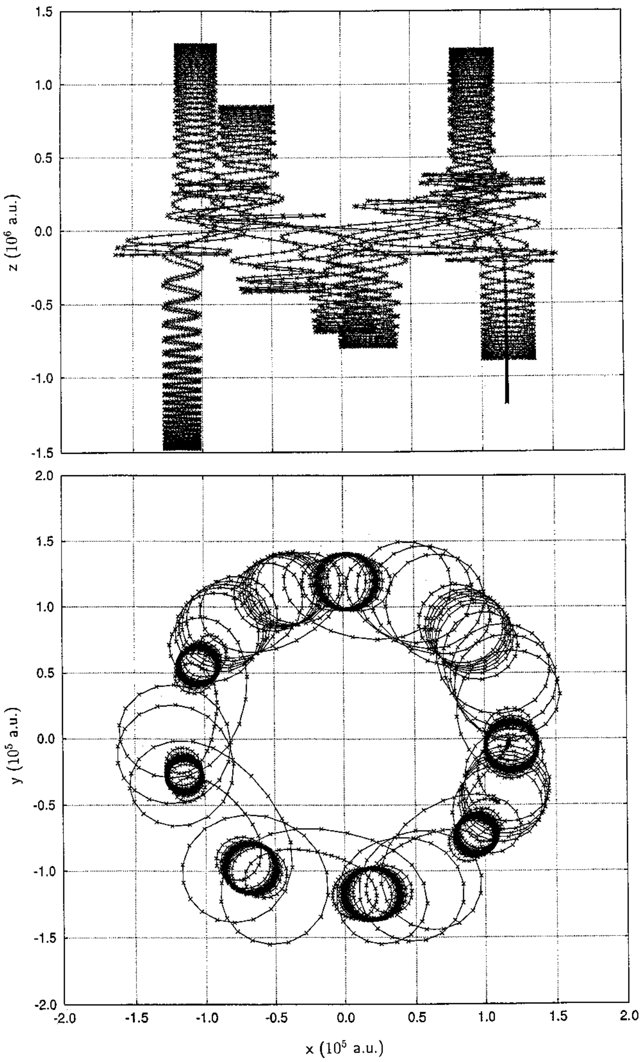

FIG. 2. Classical trajectory of an electron in the combined field of a bare nucleus with charge $Z=6$ and a magnetic field in the z direction of $B_z=42$ mT. The upper part shows the projection in the x-z plane, while the lower part shows the projection in the x-y plane. The electron has an asymptotic kinetic energy of $E_\parallel=0.1$ meV in the direction of the field and of $E_\perp=0.0$ meV perpendicular to the field.

electron from the ion is by orders of magnitude too large for the electron to be radiatively captured and de-excited into a lower state within the time interval in which the electron and the ion beams are merged. Although it is possible to find initial conditions such that electron and ion come close to each other, these are rare and do not have much weight in phase space. In fact, another explanation of the experimental effect has been put forward [8], namely, the occurrence of an induced motional electric field pulse at the beginning and at the end of the merging section of the storage ring. While the observed enhancement of radiative recombination in a cooler ring has been part of the motivation, it is not our intention to explain the effect or to discuss it in detail. Rather, Fig. 1 merely serves as an illustration of a relatively regular trajectory. A quite surprising trajectory is shown in Fig. 2, signalling chaotic behavior. Ion charge and field strength B are the same as before, only the initial condition is changed to a starting velocity parallel to the $\boldsymbol{B}$ field. The upper part of the figure is a projection on a plane containing the vector of the $\boldsymbol{B}$ field, the lower part is a projection on a plane perpendicular to the field. A criterion for the validity of classical trajectories is discussed in Eq. (3.6).

Clearly, the classical trajectories depicted in Figs. 1 and 2, are independent of the gauges discussed in Secs. III and IV. However, they suggest that a description in terms of quasibound states may not be appropriate.

III. CHOICE OF GAUGES IN A QUANTUM TREATMENT

We first discuss the problem of a point charge moving in a homogeneous magnetic field $\boldsymbol{B}$. This field, derived from a vector potential $\boldsymbol{A}$ as $\boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}$, defines the z direction of our coordinate system. Among the possible gauges leading to the same $\boldsymbol{B}$ field, the axial or symmetric gauge has been used almost universally in the context of atomic physics problems [3,9–13], while the Landau gauge, originally introduced by Landau in his seminal paper [14] has found much less attention. In order to set up the framework and the definitions, we discuss these two gauges in Secs. III A and III B, respectively, following the elegant formulation by Johnson and Lippmann [15].

It is customary to express the magnetic field $B=\gamma B_0$ in terms of the reference field strength

$$B_0=\frac{2\alpha^2 m_e^2 c^3}{e\hbar}=4.7001\times 10^5 \ \ \mathrm{T}. \tag{3.1}$$

Note that the quantity B_0 is sometimes used for half the value adopted here (i.e., for 2.35×10^5 T) and γ is changed accordingly [3]. Adopting atomic units $e=m_e=\hbar=1$ from now on, the magnetic-field strength can also be characterized by the cyclotron frequency $\omega_c=2\gamma$ or by the cyclotron radius R defined as $R^2=1/\omega_c=1/2\gamma$.

The classical motion of an electron in a uniform magnetic field follows a spiral trajectory with momentum p_z in the direction of the z axis and radius ρ_N around a parallel $x=x_0$, $y=y_0$ to the z axis, where the coordinates x_0 and y_0 specify the guiding center with respect to the origin and with the distance ρ_s from it. These classical quantities play a role also in a quantum description.

A. Axial gauge

The axial or symmetric gauge defined by

$$\boldsymbol{A}^{(a)}=-\tfrac{1}{2}\boldsymbol{r}\times\boldsymbol{B} \tag{3.2}$$

has been applied almost universally in the context of atomic physics. The Hamiltonian describing the electron motion is

$$H_0=\tfrac{1}{2}p^2+\gamma L_z+\tfrac{1}{2}\gamma^2\rho^2, \tag{3.3}$$

where L_z denotes the electron orbital angular momentum operator in the z direction, $\rho^2=x^2+y^2$ and ω_c is the spacing of the Landau levels. We have omitted here the spin part of the Hamiltonian, which only gives rise to a constant energy.

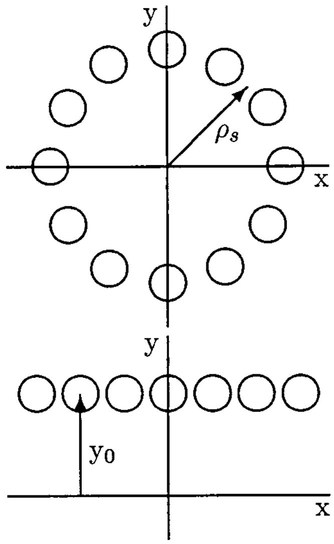

FIG. 3. Gauges and guiding centers. Top: axial gauge. The small circles indicate classical electron orbits with the guiding center located *somewhere* on a circle with radius ρ_s. Bottom: Landau gauge. The guiding center is located *somewhere* on a parallel $y=y_0$ to the x axis.

It is verified that the operators p_z, x_0, y_0, ρ_s^2, ρ_N^2, and L_z commute with H_0 and hence represent constants of motion. However, because the coordinates x_0 and y_0 do not commute [9,15], the location of the guiding center is not well defined. The uncertainties Δx_0 and Δy_0 with $\Delta x_0 \Delta y_0 \geqslant R^2/2$ prevent any accurate experimental determination of the guiding center, from which the orbit may be predicted. While in classical mechanics, for any fixed energy, the coordinates x_0 and y_0 of the guiding center can be independently chosen, and hence constitute a two-dimensional infinite manifold, in quantum mechanics only x_0 or y_0 or some function of x_0 and y_0 can be fixed, corresponding to a one-dimensional infinite manifold.

Specifically, in the axial gauge (3.2), the operators

$$H_0, \quad p_z, \quad \rho_N^2, \quad \text{and} \ \rho_s^2 \tag{3.4}$$

form a set of mutually commuting operators. While the radius ρ_N is well defined, the guiding center is only known to be located on a circle with radius ρ_s around the origin, see Fig. 3. Hence, the uncertainty in locating points on the orbit is solely due to locating the center of the orbit.

Instead of using ρ_N^2 and ρ_s^2 for specifying a quantum state, it is also possible to refer to the orbital angular momentum about the z axis,

$$L_z = \tfrac{1}{2}\omega_c(\rho_N^2 - \rho_s^2) \tag{3.5}$$

for classifying the eigenstates [9,15,16].

The uncertainty relation for the location of the guiding center may be used to derive a necessary criterion for the validity of a classical description of electron trajectories in a magnetic field. Classical trajectories constitute a good approximation, if the uncertainty in the position of the guiding center is small compared to the radius of the orbit, i.e.,

$$\frac{R^2}{\rho_N^2} = \frac{\hbar\omega_c}{m_e v_\perp^2} \ll 1, \tag{3.6}$$

where $\rho_N = v_\perp/\omega_c$ and $v_\perp$ is the electron velocity in the x-y plane. Hence a classical description is valid, if the spacing ω_c of Landau levels in a magnetic field is small compared to the transverse kinetic energy of the electrons. This is valid for the trajectories shown in Figs. 1 and 2.

The eigenvalues of the Hamiltonian H_0 in the form (3.3) can be labeled by the quantum number k denoting the longitudinal momentum k_z and two quantum numbers for the transverse motion. For the latter, we may use the set $\{N,s\}$ corresponding to the operators ρ_N^2 and ρ_s^2 with the eigenvalues $R^2(2N+1)$ and $R^2(2s+1)$, respectively, with $N,s = 0,1,2,\ldots$, or, alternatively, the set $\{n,m\}$, where the quantum numbers $m=N-s$ are the eigenvalues of the operator L_z in Eq. (3.5) [15]. For $m=0$, $R_N=R_s$, the electron orbit passes through the origin.

The eigenenergy of an electron in a magnetic field [10] is composed of the kinetic energy of free motion in the z direction and the Landau energy of a harmonic oscillator in the x-y plane with principal quantum number N,

$$\begin{aligned} E_{Nk} &= \tfrac{1}{2}k_z^2 + \omega_c(N+\tfrac{1}{2}), \\ &= \tfrac{1}{2}k_z^2 + \omega_c[n+\tfrac{1}{2}(|m|+m+1)] = E_{nmk}. \end{aligned} \tag{3.7}$$

The solution of the eigenvalue equation

$$H_0\Psi_{nmk}^{(a)}(\rho,\varphi,z) = E_{nmk}\Psi_{nmk}^{(a)}(\rho,\varphi,z) \tag{3.8}$$

in cylindrical coordinates (ρ,φ,z) is

$$\Psi_{nmk}^{(a)}(\rho,\varphi,z) = (2\pi)^{-1/2} e^{ik_z z}\Phi_{nm}^{(a)}(\rho,\varphi). \tag{3.9}$$

Here, k_z is the momentum in the z direction (this is the only possible free motion), n counts the number of radial nodes, and m is the magnetic quantum number, i.e., $L_z\Phi_{nm}^{(a)}(\rho,\varphi) = m\Phi_{nm}^{(a)}(\rho,\varphi)$.

The normalized Landau states for a charged particle in a magnetic field are given by

$$\begin{aligned} \Phi_{nm}^{(a)}(\rho,\varphi) = \sqrt{\frac{\gamma}{\pi}}\left(\frac{n!}{(n+|m|)!}\right)^{1/2} (\gamma\rho^2)^{(1/2)|m|} e^{-(1/2)\gamma\rho^2} \\ \times L_n^{|m|}(\gamma\rho^2) e^{im\varphi}, \end{aligned} \tag{3.10}$$

where $L_p^q(x)$is a Laguerre polynomial [17].

The axial gauge outlined here is particularly adequate for localized states. This is so because for atomic bound states, the angular momentum projection m is a good quantum number, a property that is retained in the axial gauge. Therefore, the space of solutions for a combined Coulomb and magnetic field separates into subspaces, each characterized by a specific value of m. The resulting simplification has led to the universal use of this gauge in atomic and molecular problems.

B. Landau gauge

In the Landau gauge [14], the vector potential yielding the same magnetic field is taken as $A_x^{(L)}=-By$ and $A_y^{(L)}=A_z^{(L)}=0$. Here, the x and y coordinates are treated unsymmetrically and can be interchanged. The Hamiltonian replacing Eq. (3.3) is

$$H_0=\tfrac{1}{2}\omega_c^2(y-y_0)^2+\tfrac{1}{2}p_y^2+\tfrac{1}{2}p_z^2,$$

$$y_0=\frac{p_x}{\omega_c}, \tag{3.11}$$

where y_0 is the coordinate of the guiding center, which is located on a parallel to the x axis, but its position on this line is unknown. This is illustrated in Fig. 3.

While in the axial gauge the operators (3.4) form a set of mutually commuting operators, in the Landau gauge this set is replaced by

$$H_0, \quad p_z, \quad \rho_N^2, \quad \text{and } y_0. \tag{3.12}$$

Here, the angular momentum L_z about the z axis is not a good quantum number.

The energy eigenvalue is given by

$$E_{Nk}=\tfrac{1}{2}k_z^2+\omega_c(N+\tfrac{1}{2}) \tag{3.13}$$

and is degenerate with respect to y_0.

The corresponding eigenfunction is

$$\Psi_{Ny_0k}^{(L)}(x,y,z)=(2\pi)^{-1/2}e^{ik_zz}\Phi_{Ny_0}^{(L)}(x,y),$$

$$\Phi_{Ny_0}^{(L)}(x,y)=e^{i\omega_c y_0 x}\chi_{Ny_0}(y), \tag{3.14}$$

with

$$\chi_{Ny_0}(y)=\mathcal{N}_N \exp\left[-\frac{(y-y_0)^2}{2R^2}\right]H_N\left(\frac{y-y_0}{R}\right),$$

$$\mathcal{N}_N=\frac{1}{\pi^{1/4}R^{1/2}\sqrt{2^N N!}}, \tag{3.15}$$

where H_N is a Hermite polynomial [17,18]. Because, in contrast to the axial gauge, m is not a good quantum number, the Landau gauge is less suitable for localized bound states, which can be classified by the angular momentum projection m, but it may be appropriate for nonlocalized scattering states corresponding to the classical trajectories shown in Figs. 1 and 2.

C. Transformation between the axial and the Landau gauge

If one wishes to calculate matrix elements between bound and continuum states as is the case for the cross section for radiative recombination in a combined Coulomb and magnetic field, one will need an expansion in terms of zero-order states $\Psi_{nmk}^{(a)}$ in the axial gauge for the bound states, while for the continuum states an expansion in terms of zero-order states $\Psi_{Ny_0k}^{(L)}$ in the Landau gauge will be more appropriate, see Eqs. (3.9) and (3.14), respectively. Therefore, we need matrix elements connecting states defined in different gauges and hence an expansion of states given in one gauge in terms of states given in the other gauge.

The axial and the Landau gauge are related by

$$\boldsymbol{A}^{(a)}=\boldsymbol{A}^{(L)}+\boldsymbol{\nabla}\chi, \tag{3.16}$$

where the gauge function is

$$\chi=\tfrac{1}{2}\omega_c xy=\gamma xy. \tag{3.17}$$

As a result, wave functions are related by

$$\Psi^{(a)}=\Psi^{(L)}e^{-i\omega_c xy/2}. \tag{3.18}$$

Taking the dipole operator $D=\hat{\boldsymbol{u}}\cdot\boldsymbol{r}$ as an example, one has transition matrix elements of the form

$$D_{nmk,Ny_0k}=\langle\Psi_{nmk}^{(a)}|e^{-i\omega_c xy/2}D|\Psi_{Ny_0k}^{(L)}\rangle. \tag{3.19}$$

In order to evaluate matrix elements of this kind, it is useful to expand transformed eigenstates of the axial gauge in terms of the Landau gauge. Specifically, for $m=0$ it can be shown that an eigenstate in the axial gauge can be expressed [19] by eigenstates in the Landau gauge with expansion coefficients given by a finite multiple sum over elementary functions and coefficients. In this way, it is possible to calculate matrix elements needed for describing radiative recombination in a magnetic field.

IV. ASYMPTOTIC PLANE-WAVE STATES

In order to define a differential cross section for a reaction in a magnetic field, it is necessary to consider asymptotic plane-wave states in the limit of vanishing field strength B. That is, we seek an asymptotic solution in the form

$$\chi(\boldsymbol{r})=(2\pi)^{-3/2}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tag{4.1}$$

with the decomposition $\boldsymbol{k}=(\boldsymbol{k}_\perp,k_z)$ and $\boldsymbol{k}_\perp=(k_\perp,\varphi_k)$. If the total energy $E=E_\perp+E_\parallel$ is given, we identify the transverse energy $E_\perp$ with a corresponding Landau state characterized by the principal quantum number N, i.e.,

$$E_\perp=\tfrac{1}{2}k_\perp^2=\omega_c(N+\tfrac{1}{2})=\omega_c[n+\tfrac{1}{2}(|m|+m+1)],$$

$$E_\parallel=E-E_\perp=\tfrac{1}{2}k_z^2=E-\omega_c(N+\tfrac{1}{2}), \tag{4.2}$$

In the following, we discuss asymptotic plane waves in the axial and the Landau gauge.

A. Axial gauge

So far, all attempts to construct asymptotic plane waves, have been performed in the axial gauge [20,21]. Zarcone *et al.* [21] argue that the adiabatic limit $\omega_c\to 0$ needed to obtain plane-wave states (4.1) can be performed only if the magnetic field is restricted to a finite area in the x-y plane with zero field outside. For finite values of $|m|\leqslant|M|<\infty$ and n given by Eq. (4.2) for a fixed transverse energy $\frac{1}{2}k_\perp^2$, the expansion with the required limit is

$$\psi_{Nmk}^{(a)}(\boldsymbol{r})=L^{-3/2}\sum_{m=-\infty}^{N} i^{|m|}e^{im\varphi}e^{ik_z z}\Phi_{n(N),m}^{(a)}(\rho,\varphi), \tag{4.3}$$

where L is a normalization length. The goal is to achieve the plane-wave limit in the field-free region, that is

$$\chi(\boldsymbol{r})=L^{-3/2}e^{ik_z z}\sum_{m=-\infty}^{\infty} i^{|m|}e^{im(\varphi-\varphi_k)}J_{|m|}(k_\perp\rho), \tag{4.4}$$

where $J_{|m|}(x)$ is a Bessel function. For $\omega_c\to 0$, Eq. (4.2) states that $n\to\infty$ and m remains bounded. Furthermore, for the wave function (4.3) to tend to the limit (4.4), certain constraints have to be satisfied, notably the limitation of the magnetic field to an axial extension of $\rho<L$ and $k_\perp/\omega_c<L$. It should be pointed out that in Ref. [21], the transition from the spatial field-free region to a given value $B\neq 0$ satisfying $\boldsymbol{\nabla}\cdot\boldsymbol{B}=0$, is not considered, although it may influence the form of the wave function.

We may conclude, that the axial gauge, which is suitable for bound states with a specified magnetic quantum number m, meets with difficulties when trying to define scattering states, which require a partial-wave expansion.

B. Landau gauge

We next consider the problem in the Landau gauge, adopting the wave function $\Psi_{Ny_0k}^{(L)}(x,y,z)$ given by Eq. (3.14) and relating the transverse energy to the principal quantum number by $E_\perp=\omega_c(N+\frac{1}{2})$. Without loss of generality, we can take $\boldsymbol{k}_\perp=k_y\hat{\boldsymbol{e}}_y$ in the y direction, so that $\frac{1}{2}k_y^2=\omega_c(N+\frac{1}{2})$. For a given value of k_y we have

$$N=\frac{k_y^2}{2\omega_c}-\frac{1}{2}\Rightarrow \mathrm{int}\left(\frac{k_y^2}{2\omega_c}-\frac{1}{2}\right)\approx \mathrm{int}\left(\frac{k_y^2}{2\omega_c}\right)$$
$$\text{for}\quad \omega_c\to 0,\quad N\to\infty. \tag{4.5}$$

In taking the asymptotic limit $N\to\infty$ of the Hermite polynomials contained in the wave function $\chi_{Ny_0}(y)$ defined in Eq. (3.15), we have to treat even and odd orders separately. Defining N as even, $N=2n$, and combining an even with an odd function, we can write a Landau wave function in the asymptotic form

$$\lim_{N\to\infty}\Psi_{Ny_0k}^{(L)}(\boldsymbol{r})=(2\pi)^{-1/2}e^{ik_z z}e^{i\omega_c y_0 x}\frac{(-1)^n\sqrt{(2n)!}}{\pi^{1/4}R^{1/2}2^n n!}$$
$$\times\left[C_{2n}\cos\left(\sqrt{4n+1}\frac{y-y_0}{R}\right)\right.$$
$$\left.+C_{2n+1}\sin\left(\sqrt{4n+3}\frac{y-y_0}{R}\right)\right]. \tag{4.6}$$

For large values of n, the arguments of the angular functions can be taken as equal, and according to Eq. (4.5),

$$\sqrt{4n}/R=\sqrt{2N\omega_c}=k_y\,. \tag{4.7}$$

Choosing

$$C_{2n}=\frac{(-1)^n}{\sqrt{2\pi}}\frac{\pi^{1/4}R^{1/2}2^n n!}{\sqrt{(2n)!}},\quad C_{2n+1}=iC_{2n}, \tag{4.8}$$

we find that a linear combination of two Landau wave functions $N=2n$,

$$\tilde{\Psi}_{N=2n,y_0,k}^{(L)}(x,y,z)=\frac{(-1)^n}{2\pi}e^{ik_z z}e^{i\omega_c y_0 x}\frac{\pi^{1/4}R^{1/2}2^n n!}{\sqrt{(2n)!}}$$
$$\times[\chi_{2n,y_0}(y)+i\chi_{2n+1,y_0}(y)], \tag{4.9}$$

with $\chi(y)$ defined by Eq. (3.14), has the property of smoothly merging into a plane wave

$$\lim_{N\to\infty}\tilde{\Psi}_{N=2n,y_0,k}^{(L)}(x,y,z)=\frac{e^{i\omega_c y_0 x}}{2\pi}e^{ik_y y}e^{ik_z z}, \tag{4.10}$$

propagating in the y-z plane, for $\omega_c\to 0$, or $B\to 0$, $\gamma\to 0$. In this limit, and for y_0 and x finite, the phase factor $\exp(i\omega_c y_0 x)$ tends to unity.

We see in this section, that the Landau gauge offers a simple possibility to construct asymptotic states for an electron in a homogeneous magnetic field that satisfy the requirement of tending to plane waves for a vanishing magnetic field B. In this way, one avoids the problems one has to cope with in the axial gauge used so far [20,21]. For a pure Coulomb field, a continuum state is described as a plane wave multiplied by a confluent hypergeometric function. If we substitute our solution (4.9) for the plane-wave part, we obtain a wave function that is exact for $Z=0$, B finite and for $B=0$, Z finite [19]. However, it remains to be seen how good the wave function is between these limits.

V. SUMMARY

We have shown by classical trajectory calculations that the description of low-energy continuum electrons in a combined Coulomb and magnetic field constitutes an extremely complex problem. A quantum description of scattering (not quasibound) states in a homogeneous infinitely extended magnetic field has to cope with the problem of defining the asymptotic incoming states. After discussing the conventional axial and the Landau gauge we have demonstrated that the latter, in contrast to the former, allows for a simple construction of asymptotic states that tend to plane waves in the limit of vanishing field strength.

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