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Quantum mechanical magnetic-field-gradient drift velocity: An analytically solvable model

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We present compact analytical solutions for the energy eigenvalues, orthonormalized eigenfunctions, and the gradient B drift velocity including the spin for a single electron (hole) in the quasi-two-dimensional case in a magnetic field $\vec{B}$ of constant direction with arbitrarily strong exponentially depending variation perpendicular to the field direction. In the limit of weak inhomogeneities, the gradient B drift velocity agrees with the classical expression, where the energy is substituted by the energy eigenvalues. Perfect agreement is found with numerical results obtained earlier by other authors.

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The discovery of the integer quantum Hall effect by v. Klitzing[1] and subsequently of the fractional quantum Hall effect[2] stimulated a lot of experimental and theoretical works concerning quasi-two-dimensional (2D) electrons in *homogenous* magnetic fields $\vec{B}$ (a good overview about the quantum Hall effects is given in Refs. 3–5). In contrast to classical plasmas, in the quantum case *inhomogeneous* magnetic fields have hardly been considered, because homogenous (constant) magnetic fields are necessary for the quantum Hall effect. However, besides the quantum mechanical $\vec{E}\times\vec{B}$ drift in constant $\vec{E}$ and $\vec{B}$ fields (cf., e.g., Refs. 3 and 4), I regard the quantum mechanical ∇B drift worthy to be mentioned. In Ref. 6, the Schrödinger equation has been solved numerically for a single spinless 2D electron in a linearly varying magnetic field $B=B_1 y$. The density of states and the ∇B drift velocity have been numerically calculated for special cases.

Hofstetter *et al.*[7] numerically computed the energy spectrum, the electron and the current density for 2D noninteracting electrons in a $\vec{B}$ field with the shape $B_0+B_1\cdot y$. In several theoretical works, 2D electrons were investigated in steplike (abruptly) changing $\vec{B}$ fields having linear[8–13] and circular[14–16] symmetry [magnetic (anti-) dots]. Furthermore, a spatially periodic $\vec{B}$ field was investigated quantum-mechanically in Refs. 9 and 17 and quasiclassically in Refs. 18 and 19, respectively.

Müller and Dietrich[20] studied numerically, the Pauli equation for the case of an infinitely long straight current filament, i.e., for $\vec{B}=(\mu_0 I/2\pi)(1/\rho)\vec{e}_\phi$ (in cylindrical coordinates, with I denoting the total current in the z direction). For further discussion see below.

The theoretical works[6–17,20] have all in common to start from the single-electron Schrödinger and Pauli equation, respectively. Apart from the limiting case of very weak inhomogeneities of the $\vec{B}$ field, the energy spectrum as well as further physical entities like the drift velocity, the electron and current density or the tunneling probability (in case of magnetic barriers) have been calculated without exception only numerically. We also mention that 2D electron systems have been investigated in a number of experimental works (cf., e.g., Ref. 21 and references cited in Ref. 13).

In this paper, I report the completely analytical solution of the Pauli equation for a single 2D electron (hole) in a magnetic field with shape

$$B(x)=B_0 e^{-\kappa x} \quad \text{(in the } z \text{ direction)}, \tag{1}$$

taking into account the spin. Compact analytical expressions are derived for the energy eigenvalues, eigenfunctions, and the ∇B drift velocity.

A $\vec{B}$ field with the local dependence (1) occurs, e.g., inside the London penetration depth of a superconductor of first kind with a homogenous $\vec{B}$ field applied parallel to its (planar) surface. If a semiconductor heterostructure with a narrow quantum well is introduced into a narrow slit of such a superconductor perpendicular to its surface, the magnetic field (1) may be realized in a good approximation for 2D electrons (holes).

If for the vector potential the gauge

$$\vec{A}=(0,A_y,0) \quad \text{with } A_y=A_y(x)=-\frac{1}{\kappa}B_0 e^{-\kappa x}$$

is chosen, the Hamiltonian reads

$$\hat{H}=\frac{1}{2m^*}\{\hat{p}_x^2+[\hat{p}_y-qA_y(x)]^2\}+\frac{g^*}{2}\mu_B B(x)\sigma_z \tag{2}$$

with the effective mass m^*, the effective Landé factor g^*, the Bohr magneton $\mu_B=\hbar|e|/2m_e$ (m_e and e the electron mass and charge, respectively, and $q=\pm|e|$) and the Pauli matrix σ_z. Since $\hat{H}$, $\hat{p}_y$, and σ_z mutually commute, the ansatz for the wave function in coordinate space

$$\psi(x,y)=\frac{1}{\sqrt{L_y}}e^{ip_y\cdot y/\hbar}\cdot\psi(x) \tag{3}$$

(with $p_y=\hbar k_y$ and the sample width L_y in the y direction) leads to two separate Schrödinger equations

$$\left\{-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}+\frac{1}{2m^*}\left(p_y+q\frac{1}{\kappa}B_0e^{-\kappa x}\right)^2\pm\frac{\hbar|g^*q|}{2m_e}\cdot B_0e^{-\kappa x}-E\right\}\psi(x)=0. \tag{4}$$

From the velocity operator

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$$\hat{v}_y = v_y(x) = \frac{1}{m^*}\left(p_y + \frac{q}{\kappa}B_0 e^{-\kappa x}\right) \tag{5}$$

may be seen that

$$\frac{p_y}{q} < 0 \quad \text{and, thus,} \quad p_y = -\frac{q}{|q|}|p_y| \tag{6}$$

must be valid, so that $v_y(x)$ can change the sign.

The dimensionless variables

$$\xi = \xi(x) \equiv \frac{|q|B_0 e^{-\kappa x}}{\hbar\kappa^2}, \tag{7}$$

$$\xi_0 \equiv \frac{|p_y|}{\hbar\kappa} = \frac{|k_y|}{\kappa} \equiv \frac{|q|B_0 e^{-\kappa x_0}}{\hbar\kappa^2} = \frac{1}{[\kappa l(x_0)]^2} \tag{8}$$

are introduced, with the local magnetic length

$$l^2(x_0) = \frac{\hbar}{|q|B(x_0)} \tag{9}$$

and the parameter

$$\xi_S \equiv \frac{g^*}{4}\frac{m^*}{m_e}, \tag{10}$$

resulting from the Zeeman energy. x_0 is defined by Eq. (8) implicitly in terms of $|p_y|$. Making use of

$$\frac{d\psi[\xi(x)]}{dx} = \frac{\partial\psi}{\partial\xi}\cdot\frac{\partial\xi}{\partial x} = -\kappa\xi\frac{d\psi(\xi)}{d\xi},$$

Eq. (4) is transformed into the new simple Schrödinger equation

$$\left[\frac{d^2}{d\xi^2} + \frac{1}{\xi}\frac{d}{d\xi} - \frac{\beta^2}{\xi^2} + \frac{2(\xi_0 \pm \xi_S)}{\xi} - 1\right]\psi(x) = 0, \tag{11}$$

with

$$\beta^2 \equiv \xi_0^2 - \frac{2m^*}{\hbar^2\kappa^2}E. \tag{12}$$

With the asymptotic solutions of (11) ξ^β and $e^{-\xi}$, for $\xi \to 0$ and $\xi \to \infty$, respectively, and the ansatz $\psi(\xi) = \xi^\beta e^{-\xi} w(\xi)$ the equation

$$z\frac{d^2 w(z)}{dz^2} + (2\beta + 1 - z)\frac{dw(z)}{dz} + \left(\xi_0 \pm \xi_S - \beta - \frac{1}{2}\right)w(z) = 0 \tag{13}$$

for w follows with $z = 2\xi$. In order to have $w(z)$ not destroying the asymptotic behavior

$$\xi_0 \pm \xi_S - \beta^{\pm} - \tfrac{1}{2} = n \tag{14}$$

with $n = 0, 1, 2, \ldots$ must be fulfilled, as is well known, from where, including (12), the energy eigenvalues

$$E^{\mp}_{n,\xi_0} = \frac{\hbar^2\kappa^2}{2m^*}\left\{\xi_0^2 - \left[\xi_0 \pm \xi_S - \left(n + \frac{1}{2}\right)\right]^2\right\}$$
$$= E^{\mp}_{n,|p_y|} = E^{\mp}_{n,x_0} \text{ for } s_z = \pm\frac{1}{2} \tag{15}$$

and for w the confluent hypergeometric function $w(2\xi) = {}_1F_1(-n, 2\beta+1, 2\xi)$ follow as solutions. We suppress the spin dependence of β in the notation of the wave function for the sake of simplicity.

The total wave function in coordinate space reads, up to a normalization constant C,

$$\psi_{n,p_y}(x,y) = \frac{1}{\sqrt{L_y}}e^{ip_y\cdot y/\hbar}C\cdot[\xi(x)]^\beta e^{-\xi(x)}$$
$$\times {}_1F_1[-n, 2\beta+1, 2\xi(x)]. \tag{16}$$

Solely from the selfadjointness of $\hat{H}(\xi)$ and from the Schrödinger equation follows [cf. (11) in Ref. 22) for the expectation value of $\hat{v}_y$,

$$\langle v_y\rangle^{\mp}_{n,p_y} = \frac{\partial E^{\mp}_{n,|p_y|}}{\partial p_y} = \frac{\partial E^{\mp}_{n,|p_y|}}{\partial\xi_0}\frac{\partial\xi_0}{\partial|p_y|}\frac{\partial|p_y|}{\partial p_y} = v^{\mp}_{D,n,p_y}$$

from where for the ∇B drift velocity

$$v^{\mp}_{D,n} = -\frac{|q|}{q}\frac{\hbar\kappa}{m^*}\left(n + \frac{1}{2} \mp \xi_S\right) \tag{17}$$

is derived, which is independent from x_0 and $|p_y|$, respectively, for the B field (1).

Equations (15)–(17) contain the most important results of this paper. Subsequently, these results shall be completed and discussed. Taking into account Eqs. (8) and (9), for the energy (15) may also be written

$$E^{\mp}_{n,x_0} = \hbar\omega_C(x_0)\left[1 - \tfrac{1}{2}\kappa^2 l^2(x_0)\left(n + \tfrac{1}{2} \mp \xi_S\right)\right] \times \left(n + \tfrac{1}{2} \mp \xi_S\right), \tag{18}$$

including the local cyclotron frequency

$$\omega_C(x_0) = \frac{|q|}{m^*}B(x_0). \tag{19}$$

The degeneration of the energy concerning x_0 or $|p_y|$ is lifted, as expected.

Using (17) for the drift velocity, further useful expressions for the energy can be gained

$$E^{\mp}_{n,x_0} = \hbar\omega_C(x_0)\left(n + \frac{1}{2} \mp \xi_S\right) - \frac{m^*}{2}(v^{\mp}_{D,n})^2, \tag{20}$$

$$E^{\mp}_{n,x_0} = \hbar\omega_C(x_0)\left[1 - \kappa^2 l^2(x_0)\left(n + \frac{1}{2} \mp \xi_S\right)\right] \times \left(n + \frac{1}{2} \mp \xi_S\right)$$
$$+ \frac{m^*}{2}(v^{\mp}_{D,n})^2. \tag{21}$$

These expressions may directly compare to analogous ones in case of the $\vec{E}\times\vec{B}$ drift.[3,4] It can be seen very easily from Eq. (18) that in the case

$$\tfrac{1}{2}\kappa^2 l^2(x_0)\left(n+\tfrac{1}{2}\mp\xi_S\right)\ll 1 \quad \text{(weak inhomogeneity)} \tag{22}$$

the energy takes the form

$$E^{\mp}_{n,x_0}\simeq \hbar\omega_C(x_0)\left(n+\tfrac{1}{2}\mp\xi_S\right). \tag{23}$$

The condition (22) for the drift velocity (17) (note $\kappa=-\nabla B/B$) yields

$$\vec{v}^{\mp}_{D,n}=\frac{|q|}{q}\left(\frac{\vec{B}}{B}\times\frac{\nabla B}{B}\right)_{x_0}\frac{\hbar}{m^*}\left(n+\frac{1}{2}\mp\xi_S\right)$$
$$\simeq\frac{1}{q}\left(\frac{\vec{B}}{B}\times\frac{\nabla B}{B^2}\right)_{x_0}E^{\mp}_{n,x_0}. \tag{24}$$

This expression corresponds to the classical guiding center approximation, if the classical energy is plugged into (24) (cf., e.g., Ref. 23). A closer look towards the "potential" energy in (4) yields further physical insights. It represents the expression for the kinetic energy $(m^*/2)v_y^2(x)$ in the present problem. At the same time, this expression may be regarded as a real potential energy of a strongly anharmonic one-dimensional oscillator (where v_D loses its meaning and $\xi_S=0$ must be set).

From Eq. (4), with (8), (9), and (19) one gets for the potential energy

$$V(x)=\frac{1}{2m^*}\left(p_y+\frac{q}{\kappa}B_0e^{-\kappa x}\right)^2=\frac{m^*}{2}\omega_C^2(x_0)\left[\frac{1-e^{-\kappa(x-x_0)}}{\kappa}\right]^2$$
$$=\frac{1}{2}\hbar\omega_C(x_0)\left[\frac{1-e^{-\kappa l(x_0)\frac{x-x_0}{l(x_0)}}}{\kappa l(x_0)}\right]^2. \tag{25}$$

x_0 and $|p_y|$, respectively, determine the zero point ("center") of the potential. This reveals that for small κ a harmonic potential and thus the familiar (local) Landau levels follow.

In order not to let a charge to escape towards $x\to\infty$,

$$E^{\mp}_{n,x_0}<\frac{1}{2}\frac{\hbar\omega_C(x_0)}{[\kappa l(x_0)]^2} \tag{26}$$

must be fulfilled, from where straightforwardly

$$\beta\pm\xi_S=\frac{1}{[\kappa l(x_0)]^2}-\left(n+\frac{1}{2}\mp\xi_S\right)>0 \tag{27}$$

follows, which guarantees a correct asymptotic behavior of the wave function for $\xi\to 0$.

The normalization condition reads with Eq. (16)

$$C^2\int_{-\infty}^{+\infty}dx[\xi(x)]^{2\beta}e^{-2\xi(x)}\{{}_1F_1[-n,2\beta+1,2\xi(x)]\}^2$$
$$=C^2\int_0^{+\infty}\frac{d\xi}{\kappa\xi}\xi^{2\beta}e^{-2\xi}[{}_1F_1(-n,2\beta+1,2\xi)]^2=1. \tag{28}$$

In the last expression, relation $\xi=\xi(x)$ after Eq. (7) has been utilized.

Fortunately, the integrals in (28) have been analytically calculated in the mathematical appendix (f) of Ref. 22. Therefore, the orthonormalized eigenfunctions may be directly given

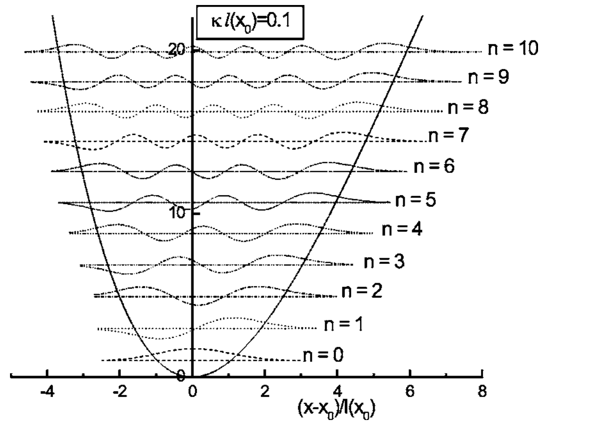

FIG. 1. The potential $V(x)$, Eq. (25), together with the energy eigenvalues E_{n,x_0}, Eq. (18), both in units of $\hbar\omega_C(x_0)/2$, and the normalized eigenfunctions $\psi_{n,x_0}(x), n=0,\ldots,10$, Eq. (29) vs $x-x_0/l(x_0)$ for $\kappa l(x_0)=0.1$ and for $\xi_S=0$.

$$\psi_{n,p_y}(x,y)=\frac{1}{\sqrt{L_y}}e^{ip_y\cdot y/\hbar}\frac{1}{\sqrt{l(x_0)}}$$
$$\times\left[\frac{\Gamma(2\beta+n+1)\kappa l(x_0)}{\Gamma(2\beta+1)\Gamma(2\beta)\Gamma(n+1)}\right]^{1/2}[2\xi(x)]^{\beta}$$
$$\times e^{-\xi(x)}{}_1F_1[-n,2\beta+1,2\xi(x)], \tag{29}$$

with β according to Eq. (14) (note that β depends on the spin orientation), $\xi(x)$ according to (7), and p_y according to (6).

In Figs. 1 and 2, the potential (25) is shown together with the energy eigenvalues (18) and the normalized eigenfunctions (29) for different values of $\kappa l(x_0)$ and $\xi_S=0$. The increasing asymmetry of the potential with increasing $\kappa l(x_0)$ and the respective asymmetry of the eigenfunctions may be clearly seen as well as the more weakly with n increasing energy levels (which are gradually more strongly renormalized due to the anharmonicity).

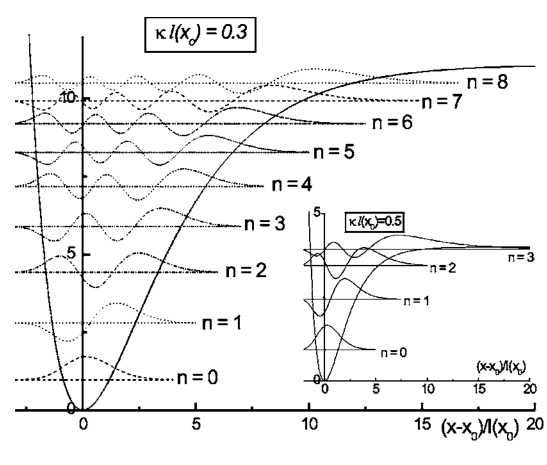

FIG. 2. The same as in Fig. 1 for $\kappa l(x_0)=0.3$ and $\kappa l(x_0)=0.5$ (inset).

Finally, the number of states with given n has to be considered. Since the Hamiltonian (2) [or (4), respectively] is independent of the y coordinate, $dN=L_y|dp_y|/h$, or, with (8) and (9) $dN=L_y|dx_0|/2\pi l^2(x_0)$, for $0<x_0<L_x$ is valid, i.e., the local density of the centers x_0 is determined by the local magnetic length. For one state (with n given) the "territory" $2\pi l^2(x_0)$ is necessary (cf. the case B=const. in Ref. 3).

If the initial data for the numerical calculations in Ref. 20 are taken as a basis, $\kappa l(x_0)=2.57\times10^{-5}$ follows. According to that, extremely weak inhomogeneity is present. An asymmetry of the wave function regarding x_0 with $V(x_0)=0$ is therefore invisible by graphical means. For electrons in vacuum, $m^*=m_e$, $g^*=2$ and, thus, $\xi_S=\frac{1}{2}$ is valid. In semiconductors, on the other hand, $\xi_S\ll\frac{1}{2}$ is usually implemented. With the initial data in Ref. 20 full numerical consistency with (23) for the energy and with (24) for the drift velocity is obtained.

To summarize, I found compact strictly analytical solutions for the energy eigenvalues, the orthonormalized eigenfunctions and the ∇B drift velocity for electrons and holes, taking account for the spin, in the quasi-two-dimensional case for an arbitrarily strong exponentially depending $\vec{B}$ field [cf. Eq. (1)]. In the limiting case of weak inhomogeneities [cf. condition (22)] the possibility of a local description followed, which in the classical case merges into the guiding center approximation for the ∇B drift velocity. A comparison with the special numerical results in Ref. 20 leads to total consistency. The derived solutions simultaneously describe a strongly anharmonic quantum mechanical oscillator in closed form.

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