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Motion of a Wave Packet Constructed from Landau Gauge Solutions

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The eigensolutions of the Schrödinger equation for the motion of a charged particle in a uniform magnetic field depend on the choice of electromagnetic gauge. In the Landau gauge it is hard to discern a relationship between the eigensolutions and the circular or helical orbits of classical theory. In this paper a wave packet is constructed from the Landau gauge eigensolutions which simulates the classical motion in the plane perpendicular to the magnetic field. Some properties of the wave packet are discussed.

INTRODUCTION

The motion of a nonrelativistic charged particle in a magnetic field may be derived from the Hamiltonian

$$H=(1/2m)(\mathbf{p}-e\mathbf{A})^2 \tag{1}$$

where $\mathbf{p}$ is the canonical momentum, m is the mass of the particle, e its electric charge, and $\mathbf{A}$ is the vector potential defined by

$$\mathbf{B}=\text{curl }\mathbf{A}. \tag{2}$$

where $\mathbf{B}$ is the magnetic field vector.

Since, for any scalar function ϕ, $\text{curl}(\nabla\phi)=0$, it follows that the same magnetic field $\mathbf{B}$ can be derived from a wide variety of vector potential fields $\mathbf{A}$. The choice of a particular field $\mathbf{A}$ which satisfies Eq. (2) is called the choice of electromagnetic "gauge."

If the magnetic field is uniform we may choose a Cartesian coordinate system (x, y, z) in which $\mathbf{B}=(0, 0, B_z)$. The Landau gauge is then defined by the choice

$$\mathbf{A}=\mathbf{A}_L=(0, B_x, 0). \tag{3}$$

We obtain the time independent Schrödinger equation from Eq. (1) by writing $H\psi=E\psi$, where E is the kinetic energy of the particle, and setting $p_i=(\hbar/i)(\partial/\partial x_i)$.

It is easily shown that the equation can be separated into an equation containing functions only of z and an equation containing functions of x and y.

We put $\psi=Z(z)F(x, y)$ and find

$$Z=\exp(ik_z z) \tag{4}$$

independent of the strength of the magnetic field, while F is a solution of the equation

$$\frac{\partial^2F}{\partial x^2}+\frac{\partial^2F}{\partial y^2}-2i\left(\frac{eB}{\hbar}\right)x\frac{\partial F}{\partial y}-\frac{e^2B^2}{\hbar^2}x^2F+\frac{2mE_\perp F}{\hbar^2}=0 \tag{5}$$

where $E_\perp=E-(\hbar^2k_z^2/2m)$.

As is well known,[1] normalized eigensolutions of Eq. (5) take the form

$$F_{k_y,n}(x,y)=\left(\frac{\alpha}{2^n\pi^{1/2}n!}\right)^{1/2}L_y^{-1/2}H_n\left[\alpha\left(x-\frac{k_y}{\alpha^2}\right)\right]\times\exp\left[ik_yy-\tfrac{1}{2}\alpha^2\left(x-\frac{k_y}{\alpha}\right)^2\right] \tag{6}$$

where $\alpha^2=(eB/\hbar)$, L_y is the y dimension of the system, and H is a Hermite polynomial defined by

$$H_n(\xi)=(-n)^n\exp(+\xi^2)\times(\partial/\partial\xi)^n[\exp(-\xi^2)]. \tag{7}$$

In order to satisfy periodic boundary conditions in y we must have $k_y = r(2\pi/L_y)$ where r is an integer. $E_\perp$ must take one of the values

$$E_\perp = (n+\tfrac{1}{2})(\hbar^2\alpha^2/m) = (n+\tfrac{1}{2})\hbar\omega_L \qquad (8)$$

where $\omega_L = (eB/m)$, is the Larmor angular frequency of the particle.

Since $E_\perp$ is independent of k_y, the solutions (6) are highly degenerate. This is related to the fact that classically the guiding center of the particle motion may be located anywhere in the magnetic field without affecting the particle energy.

CONSTRUCTION OF A WAVEPACKET

The solutions (6), apart from the factor $\exp(ik_y y)$, are identical with the eigensolutions of the one-dimensional oscillator equation for oscillator potentials centered at $x = x_0 = (k_y/\alpha^2)$.

By analogy with the well known technique for constructing a wavepacket from harmonic oscillator eigenfunctions (1) we consider a wavepacket whose form at time $t=0$ is given by the equation

$$\psi(0) = \alpha\pi^{-1/2}\exp[-\tfrac{1}{2}\alpha^2(x-x_0)^2 - \tfrac{1}{2}\alpha^2 y^2 + iKy]. \qquad (9)$$

In order to study the motion of this wavepacket we expand it as a linear combination of the solutions (6) and make use of the orthonormality rule. Setting $k_y = k$ we write

$$\psi(0) = \sum_k \sum_n A_{kn} F_{kn}$$

and find

$$A_{kn} = \int_\infty^\infty \int_\infty^\infty F_{kn}{}^*\psi(0)\,dx\,dy$$

$$= \left(\frac{2}{\alpha}\right)^{1/2} \frac{\alpha^n}{(2^n n! L_y)^{1/2}} \left(x_0 - \frac{k}{\alpha^2}\right)^n \times \exp\left[-\tfrac{1}{4}\alpha^2\left(x_0 - \frac{k}{\alpha^2}\right)^2 - \frac{(K-k)^2}{2\alpha^2}\right]. \qquad (10)$$

As time elapses each eigenfunction F_{kn} must be multiplied by the time dependent factor

$$\exp(-iE_\perp t/\hbar) = \exp[-i(n+\tfrac{1}{2})\omega_L t]$$

and we obtain

$$\psi(t) = \sum_k \sum_n A_{kn}\psi_{kn}(0)\exp[-i(n+\tfrac{1}{2})\omega_L t]. \qquad (11)$$

If one substitutes

$$\xi = \alpha[x - (k/\alpha^2)]$$

and

$$\lambda = \tfrac{1}{2}\alpha[x_0 - (k/\alpha^2)]\exp(-i\omega_L t),$$

the sum over n leads directly to the generating function for the Hermite polynomials[1]

$$\sum_n H_n(\xi)(\lambda^n/n!) = \exp[-\lambda^2 + 2\lambda\xi].$$

We then replace the summation over k values by $(L_y/2\pi)$ times an integration between limits $-\infty$ and ∞ and find that

$$\psi^*(t)\psi(t) = F\exp\{(-\alpha^2/D) \times [A(x' - x_0'\cos\omega_L t)^2 + B(y + x_0'\sin\omega_L t)^2 + 2C(x' - x_0'\cos\omega_L t)(y + x_0'\sin\omega_L t)]\} \qquad (12)$$

where

$$x' = [x - (K/\alpha^2)],$$
$$x_0' = [x_0 - (K/\alpha^2)],$$
$$A = 1 + (1-\cos\omega_L t)^2 + 2(1-\cos^2\omega_L t),$$
$$B = 1 + (1-\cos\omega_L t)^2,$$
$$C = \sin\omega_L t\cos\omega_L t,$$
$$D = [1 + (1-\cos\omega_L t)^2]^2 + (1-\cos^2\omega_L t)(2-\cos\omega_L t)^2,$$

and F is a constant.

The maximum value of $\psi^*(t)\psi(t)$ lies on the curve $x' = x_0'\cos\omega_L t$, $y = -x_0'\sin\omega_L t$, i.e., on a circle of radius $r_L = x_0'$. It moves round this circle with angular velocity $-\omega_L$ at the same rate as a "classical" particle of positive charge. (A wavepacket associated with a negatively charged particle circulates in the opposite direction.)

The expectation value of the tangential linear momentum p_T at time $t=0$ is readily found to be

$$\langle p_T\rangle = eB[x_0 - (K/\alpha^2)] = x_0' eB. \qquad (13)$$

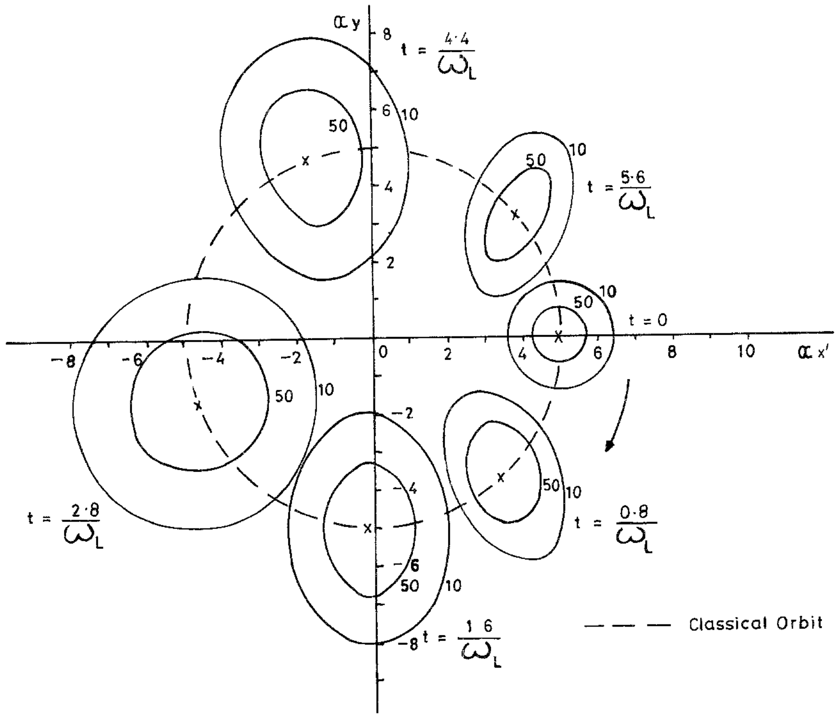

FIG. 1. The form and position of a typical wavepacket for which $\rho = \alpha r_L = 5$ as a function of time. The wavepacket starts from the position $(r_L, 0)$ at $t = 0$. The positions where $\psi^*(t)\psi(t)$ is a maximum and contours at which $\psi^*(t)\psi(t)$ falls to 50% and 10% of its maximum values are shown.

It follows that $r_L = x_0'$ is equal to the radius of the orbit of a classical particle of momentum $\langle p_T \rangle$. Note, however, that $\langle p_T \rangle \neq \hbar K$.

DISCUSSION

The expressions (11) and (12) give further information about the shape of the wavepacket at different points around the orbit. When $\omega_L t = 0$, $A = B = D = 1$ and $C = 0$ making Eqs. (11) and (12) consistent with Eq. (9).

The initial shape of the wavepacket is circular and its characteristic radius is $(1/\alpha)$.

Since, classically, the tangential component of linear momentum $p_T = eBr_L$ where r_L is the Larmor radius, we easily find that the initial spread in tangential momentum Δp_T and the initial spread Δs in azimuthal position in the wavepacket are related by the expression

$$(\Delta p_T \Delta s)_{t=0} \sim (eB/\alpha^2) = \hbar. \qquad (14)$$

The initial wavepacket is therefore one of the "minimum" wavepackets allowed by the Heisenberg uncertainty principle.

Figure 1 shows how the form of the wavepacket changes during the subsequent motion. The following features implicit in Eqs. (11) and (12) are confirmed by Fig. 1:

(1) The wavepacket resumes its initial position and form for all times satisfying the equation $\omega_L t = 2\pi q$ where q is an integer. This follows from the fact that A, B, C, and D are all periodic functions of $\omega_L t$.

(2) The wavepacket is again circular for $\omega_L t = (2q+1)\pi$ since here $A = B = 5$ and $C = 0$. However, since $D = 25$, the characteristic radius is now $(5)^{1/2}/\alpha$ instead of $(1/\alpha)$.

(3) At intermediate values of $\omega_L t$ the shape is distorted owing to the fact that $C \neq 0$ and $A \neq B$, but never spreads appreciably outside the limits $r_L \pm (5)^{1/2}/\alpha$. The behavior of the wavepacket is

therefore intermediate between that of a free particle wavepacket, which spreads without limit, and a harmonic oscillator wavepacket, which propagates without change of form.[1]

(4) The "area" of the minimum wavepacket depends on B but not on the energy of the particle

$$\alpha^{-2} \simeq 6.6 \times 10^{-16} B \text{ m}^2$$

where B is in tesla (1 tesla $= 10^4$ gauss).

(5) One may regard $\rho = \alpha r_L$, the ratio between the Larmor radius and the initial radius of a minimum circular wavepacket, as measuring the approach to the classical limit. Large ρ means that the spread of the wavepacket is small compared with the radius of the classical orbit:

$$\rho^2 = (2mE_\perp / \hbar eB) \tag{15}$$

where m is the mass of the particle.

When $E_\perp$ is measured in electron volts and B in teslas we find, for electrons,

$$\rho \simeq 132 (E_\perp / B)^{1/2}. \tag{16}$$

Figure 1 is plotted for $\rho = 5$ and so corresponds to $E_\perp \sim 1.5 \times 10^{-3}$ eV in a field $B = 1$ tesla.

For electrons at the Fermi surface in a typical metal $E_\perp \sim 5$ eV. Hence, $\rho \sim 300 B^{-1/2}$. In fields of about 1 tesla, one can therefore "localize" a wavepacket simultaneously in azimuth and in radius for these electrons within a few tenths of a percent of the classical Larmor radius throughout the motion.

Elementary arguments from the uncertainty principle would lead one to suppose that one could start from a noncircular initial wavepacket. One could, for example, narrow the radial spread, and hence the uncertainty in azimuthal momentum, at the expense of a greater initial spread of azimuthal position.

The computations involved in analyzing the motion are, however, significantly more difficult for a noncircular initial wavepacket and have not been pursued.

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[1] D. Bohm, *Quantum Theory* (Prentice-Hall, New York, 1951), mainly Sec. 13.15, p. 306 *et seq.*