AAPT PHYSICS EDUCATION
AMERICAN JOURNAL of PHYSICS

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Citation: American Journal of Physics **40**, 1673 (1972); doi: 10.1119/1.1987010
View online: http://dx.doi.org/10.1119/1.1987010
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/40/11?ver=pdfcov
Published by the American Association of Physics Teachers

Geometrical Relations for Charged Particles in a Uniform Magnetic Field

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(Received 9 February 1971; revised 14 February 1972)

By using appropriate gauge transformations one can develop quasiclassical wavefunctions for charged particles in a uniform magnetic field which have large amplitudes only in the neighborhood of classical Larmor orbits centered at arbitrary points in a plane perpendicular to the field. Pairs of such wavefunctions are not orthogonal to each other. Interesting geometrical relationships between these solutions and the degenerate orthonormal sets of wavefunctions in a particular gauge can be found as a result of evaluating overlap integrals. This has been done for both the cylindrical and Landau gauges. In the cylindrical gauge certain of the orthonormal wavefunctions corresponding to different energies give identical probability distributions. Relationships between quantum and classical results, and the effect of the uncertainty principle are discussed.

INTRODUCTION

The importance of gauge transformation **A** of the type

$$\mathbf{A}\rightarrow\mathbf{A}'=A+\nabla\phi \qquad (1)$$

in modifying the equations of motion of a charged particle in a magnetic field has been pointed out in a previous paper[1] hereafter referred to as (I). In Eq. (1) **A** is the vector potential and ϕ an arbitrary scalar function of position, called the transformation function. The magnetic field is given by the relation

$$\mathbf{B}=\mathrm{curl}\mathbf{A}. \qquad (2)$$

In classical physics gauge transformations do not affect particle orbits, but change the canonical momentum **p** defined by the relationship

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

where v is particle velocity, m the mass, and e the electric charge.

Schrödinger's equation is derived by replacing the components of canonical momentum p_i by differential operators

$$p_i\rightarrow(\hbar/i)(\partial/\partial q_i)$$

where q_i are the canonically conjugate space coordinates.

Both the Schrödinger equation itself and the eigenfunctions obtained in solving it are influenced by the choice of gauge and by the choice of coordinate system.

There is, however, a general and readily verified result[2] that if a wave function ψ satisfies Schrödinger's equation in some original gauge, then the wavefunction

$$\psi'=\psi\exp(ie\phi/\hbar) \qquad (3)$$

satisfies Schrödinger's equation in the transformed gauge.

In the case of the motion of a charged particle in a uniform magnetic field the solutions of Schrödinger's wave equation in any gauge are highly degenerate.

This corresponds to the situation in classical physics in which particles with a given energy of motion in the plane perpendicular to the field lines all perform circular orbits with radii equal to the Larmor radius

$$r_L=p_{\perp}/eB \qquad (4)$$

where $p_{\perp}$ is the magnitude of the component of momentum perpendicular to the field. The centers of these orbits, which we shall call guiding centers, may lie anywhere in the plane. The orbits therefore contribute a degenerate set which may be transformed into each other merely by geometrical displacement.

This is, however, not in general the case for the degenerate orthonormal solutions of Schrödinger's equation in a particular gauge; nor do most of these wave mechanical solutions bear any immediate resemblance to the classical orbits, even when the quantum numbers become large.

This paper is concerned to investigate the relationships which do exist between the quantum and classical results.

THE CYLINDRICAL GAUGE

We assume that the uniform magnetic field has a single component B_z in the positive z direction. The basic cylindrical gauge is then defined by the relation

$$\mathbf{A}=\mathbf{A}_c=\tfrac{1}{2}\mathbf{B}\wedge\mathbf{r} \tag{5}$$

where $\mathbf{r}$ is a radius vector from an arbitrary origin, called the gauge center in the plane perpendicular to the z direction.

In cylindrical polars Eq. (5) takes the form

$$\mathbf{A}_c=\tfrac{1}{2}B(0, r, 0), \tag{6}$$

or in Cartesian coordinates,

$$\mathbf{A}_c=\tfrac{1}{2}B(-y, x, 0). \tag{7}$$

Since the origin used in defining r is quite arbitrary we could equally well refer to a different origin and write

$$\mathbf{A}_c=[\tfrac{1}{2}\mathbf{B}\wedge(\mathbf{r}-\mathbf{R})] \tag{8}$$

where $\mathbf{R}$ is a vector displacement of the origin. This shift of origin may be treated[3] as a gauge transformation from Eq. (5) using the transformation function

$$\phi=-(\tfrac{1}{2}\mathbf{B})\cdot(\mathbf{R}\wedge\mathbf{r}). \tag{9}$$

CYLINDRICAL GAUGE SOLUTIONS

All the results in this gauge have been derived on the assumption that e is positive. If e is negative (electron), the sign of l must be changed throughout.

In the basic cylindrical gauge Schrödinger's equation for motion in the (r, θ) plane takes the form

$$\left[-r^{-1}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)-\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} -\frac{2}{i}\left(\frac{eB}{2\hbar}\right)\frac{\partial}{\partial\theta}+\left(\frac{eB}{2\hbar}\right)^2 r^2\right]\psi=\frac{2mE_\perp\psi}{\hbar^2}. \tag{10}$$

Van Vleck[4] has shown how closely this equation is related to the Schrödinger equation for a two-dimensional harmonic oscillator. Using this similarity one easily finds that the allowed values of the energy of motion perpendicular to the field are given by the expressions

$$E_{\perp nl}=(2n+|l|-l+1)(\hbar\omega_L/2) \tag{11}$$

where l is an integer introduced to give single-valued wave functions as functions of θ

$$\psi_{nl}=e^{il\theta}R_{nl}(r) \tag{12}$$

and n is a further positive integer which arises from the boundary conditions on R.

If we write $\alpha^2=(eB/\hbar)$ and $(2mE_\perp/\hbar^2)=\epsilon$ we find

$$\{-(r\partial/\partial r)(r\partial/\partial r) +[l-\tfrac{1}{2}(\alpha^2r^2)]^2\}R=\epsilon r^2R, \tag{13}$$

which has the normalized solutions

$$R_{nl}=C_{nl}r^{-(|l|+2n+2)}\exp(\alpha^2r^2/4)(r^3d/dr)^n \times[r^{2(|l|+1)}\exp(-\alpha^2r^2/2)], \tag{14}$$

for which $\epsilon=\epsilon_n=(2n+|l|-l+1)\hbar^2\alpha^2$ and C_{nl} is the normalization constant given by

$$C_{nl}=\frac{\alpha^{|l|+1}}{[2\pi 2^{(|l|+2n)}n!(|l|+n)!]^{1/2}}. \tag{15}$$

Solutions (14) are an orthonormal set.

From Eqs. (14) and (15) it follows that R_{nl} depends on the modulus of l and not on its sign. Hence, from Eq. (12) $\psi_{nl}^*\psi_{nl}$, the probability density distribution, is the same for given n for azimuthal quantum numbers $+l$ and $-l$.

On the other hand Eq. (11) shows that the energy is different in these two states. Many quantum systems are known which have degenerate states with different probability distributions but the same energy. States with different energies but the same probability distribution are less commonly found. (It is easily verified that the radial probability distributions on orbits of types A and B in Fig. 2 are also identical in the classical limit.)

Equation (13) also shows that for given n all the positive l states are degenerate, i.e., they all have the same energy. When l is negative, however, we find from Eq. (11) that

$$E_{\perp nl}=[2(n+|l|)+1](\hbar\omega_\perp/2).$$

Clearly, each of these states will have the same energy as a state of positive l and quantum number n' such that $n'=n+|l|$. Since n and $|l|$ are both positive integers it follows that at any given energy there are only a finite number of distinct states with negative l. The minimum value of $|l|$ is zero, the maximum value is n' for these states. There are therefore only $(n'+1)$ of them.

We next consider those states for which $n=0$ and for which l is negative. For these states $n'=|l|$ and the energy is given by

$$E_{0(l)}=(2|l|+1)(\hbar\omega_L/2). \quad (16)$$

The wavefunction then takes the form

$$\psi_{(0,l)}=\alpha^{|l|+1}/[2\pi 2^{|l|}(|l|)!]^{1/2} \times\exp(-i|l|\theta)r^{|l|}\exp(-\alpha^2r^2/4). \quad (17)$$

It is easily shown[2] that the radial probability density distribution $r\psi_{0,l}{}^*\psi_{0,l}$ derived from Eq. (17) is peaked near

$$r_L=(2|l|+1)^{1/2}/\alpha$$

and has a characteristic radial width

$$\Delta r\sim 1/\alpha. \quad (18)$$

Thus r_L is identical with the classical Larmor orbit radius for a particle whose energy is given by Eq. (16) and the width Eq. (18), is similar to the width of the minimum wavepacket discussed in (I).

We therefore regard Eq. (17) as a quantum mechanical representation of a Larmor orbit centered at the origin. Since this solution is closely analogous to the classical solution for a particle circulating round the origin, we call (17) a "quasiclassical solution" and we expect there to be other solutions corresponding to classical orbits centered at points away from the origin.

We may substitute $[r\exp(i\theta)-R\exp(i\theta_0)]$ directly in place of $re^{i\theta}$ in (15) and obtain another similar wavefunction centered at (R,θ_0) but this will be a solution of Schrödinger's wave equation in a different gauge. The center of the gauge will now also be at the point (R,θ_0).

We cannot, therefore, compare the result of making this substitution directly with solutions (15) for $n\neq 0$, which were derived in the original gauge. If, however, in addition we make a gauge transformation and multiply the displaced wavefunction by the factor $\exp(ie\phi/\hbar)$ where

$$\phi=\tfrac{1}{2}\mathbf{B}(\mathbf{R}\wedge\mathbf{r})=\tfrac{1}{2}B|R||r|\sin(\theta-\theta_0).$$

Equation (9) indicates that we will obtain a wavefunction representing a displaced Larmor orbit centered at the point (R,θ_0) but expressed in the original gauge.[3] By this process the gauge center has been separated from the guiding center of the the Larmor orbit.

The resulting wavefunction is

$$\psi_{0l}(R)=C_{0l}\exp(-i|l|\theta) \times\{r-R\exp[i(\theta-\theta_0)]\}^{|l|} \times\exp(-(\alpha^2/4)\{r^2+R^2-2rR\exp[i(\theta-\theta_0)]\}). \quad (19)$$

The wavefunction in Eq. (19) is not orthonormal to that in Eq. (17) so that in quantum theory displaced orbit solutions are not linearly independent of each other. However, we can investigate the extent to which the solutions (19) overlap with the orthonormal set (14) by expanding Eq. (19) as a linear combination of these solutions. We keep the particle energy constant throughout.

We put

$$\psi_{0l}(R)=\sum_{nl'}A_{nll'}\psi_{nl'}$$

where

$$A_{nll'}=\int_0^\infty\int_0^{2\pi}\psi_{nl'}{}^*\psi_{0l}(R)\,rdrd\theta$$

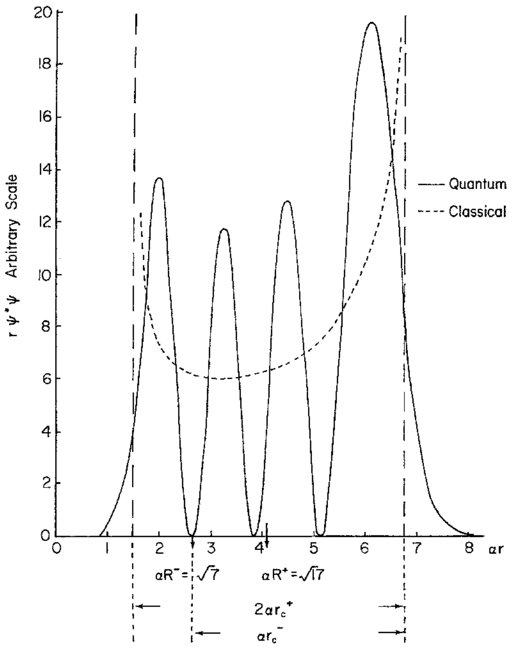

FIG. 1. The radial probability distribution for cylindrical gauge eigenfunctions for $n=3$, $l=\pm 5$. The classical radial probability distribution is also shown.

and find

$$A_{nll'} = K_{n|l|l'} R^{|l|+l'} \exp[i(l+l')\theta_0] \times \exp(-\alpha^2 R^2/4), \quad (20)$$

where $K_{n|l|l'}$ involves a sum of definite integrals over r and θ but is independent of R or θ_0.

$|A_{nll'}|^2$ is the probability that a particle with a displaced Larmor orbit-like wavefunction whose guiding center is at (R, θ_0) is simultaneously in the eigenstate $\psi_{nl'}$. This is clearly a function of the position of the guiding center. The *a priori* likelihood of the guiding center lying by chance between a distance R and $R+dR$ from the gauge center, which is an arbitrary point, is simply proportional to the element of area $2\pi R dR$.

The probability of finding a particle in one of the states $\psi_{nl'}$, given that it is in a quasiclassical orbit somewhere in the field, is therefore proportional to

$$P(R)dR = 2\pi R\, |A|_{nll'}{}^2 dR = 2\pi K_{n|l|l'} R^{2(|l|+l')+1} \times \exp(-\alpha^2 R^2/2)\, dR. \quad (21)$$

$P(R)$ is sharply peaked at values of R near to the value

$$R = R_{\max} = [2(|l|+l')+1]^{1/2}/\alpha. \quad (22)$$

But from Eq. (18) $[(2|l|+1)/\alpha]^{1/2} = r_L$, the Larmor radius of the particle. Hence,

$$R_{\max} = [r_L{}^2 + (2l'/\alpha^2)]^{1/2}. \quad (23)$$

It follows that a particle in a quasiclassical state whose guiding center is displaced by a distance close to $R_{\max}$ from the gauge center, and which is therefore closely analogous to a "classical" particle with a guiding center at this point, has a high probability of being found in the state $\psi_{nl'}$. A particle whose guiding center lies elsewhere has a very much lower probability of being in this state.

There is therefore a close relationship between states $\psi_{nl'}$ for which $n \neq 0$ and classical orbits centered away from the gauge center.

Rearranging Eq. (23) one finds

$$l' = \tfrac{1}{2}\alpha^2(R_{\max}{}^2 - r_L{}^2), \quad (24)$$

and we note that $l' > 0$ implies $R_{\max} > r_L$, a guiding center more than one Larmor radius from the gauge center while $l' < 0$ implies $R_{\max} < r_L$, a guiding center less than one Larmor radius from the gauge center.

For $l' < 0$ we have assumed $n + l' = |l|$ and for $l' > 0$, $n = |l|$, in order to ensure that the energies of the states $\psi_{nl'}$ and ψ_{0l} are the same.

Multiplying Eq. (24) on both sides by $\hbar$ yields

$$\hbar l' = (eB/2)(R_{\max}{}^2 - r_L{}^2).$$

Putting $\bar{p}_\theta = \hbar l'$ yields a result identical with what one finds using classical mechanics in the same gauge.

The geometrical relationship between the classical orbits and the probability distributions given by wave mechanics are illustrated in Figs. 1 and 2. The radial width of the probability distributions $r|\psi_{nl'}|^2$ is just $2r_L$.

TIME DEPENDENCE

Including the time dependent factor in the solutions (12) gives the travelling wave expressions

$$\psi_{nl'} = R_{nl'} \exp\{i[l'\theta - (E_{nl'}t/\hbar)]\}. \quad (25)$$

The $R_{nl'}$ are real so that the wavefronts are always radial.

Wavepackets constructed from solutions (25) travel with an average group angular velocity

$$\omega_g = \hbar^{-1}[d(E_{nl'})/dl']$$

round the gauge center. Using Eq. (11) we find that

$$\omega_g = 0 \quad \text{for} \quad l' > 0,$$
$$\omega_g = -\omega_L \quad \text{for} \quad l' < 0. \qquad (26)$$

This group angular velocity is the closest quantum analog to the classical angular velocity of a particle around the gauge center. We see that the results (26) are consistent with the geometrical picture illustrated in Fig. 2. States for which $l' > 0$ correspond to Larmor orbits which do not embrace the gauge center and therefore the particles concerned appear to remain near a fixed azimuth angle, and $\omega_g = 0$. States for which $l' < 0$ correspond to Larmor orbits which surround the gauge center. Since the period of the classical orbital motion is $2\pi/\omega_L$, the magnitude of the average angular velocity around the gauge center in such orbits is ω_L. The negative sign in Eq. (26) gives the correct sense of rotation for positively charged particles.

A SIMPLE MODEL

As n and l' become larger, the radial probability function $r\psi_{nl'}{}^{*}\psi_{nl'}$ becomes increasingly concentrated into two rings of radii $R \pm r_L$ where R is given by Eq. (22).

We can construct a simple mechanical model of the classical limit of the probability distribution in the following way:

(1) Cover a horizontal tray with a uniform layer of sand.

(2) Represent a particle of given energy circulating about any point by a rotating paddle system which piles up a circular ridge of sand of radius r_L. (To obtain the maximum degree of simulation the paddle should rotate with angular velocity ω_L about the guiding center.) The circular ridge of sand will simulate the probability distribution $[\psi(R, \theta_0)]^2$.

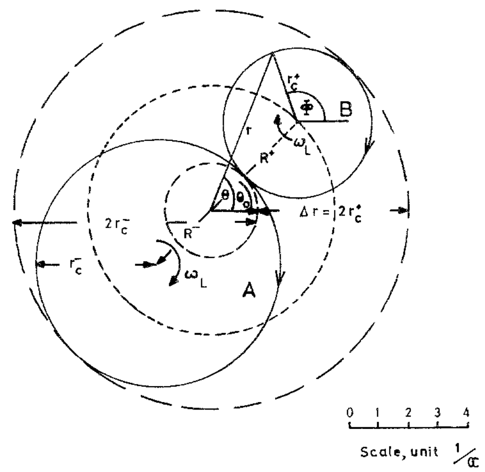

FIG. 2. The geometry of cylindrical gauge wavefunctions. The eigenfunctions for $n=3$, $l=\pm 5$ are approximately bounded by the dashed circles and have identical radial probability distributions. For positively charged particles, eigenfunctions with negative l are closely related to quasiclassical orbits of type A which enclose the origin and eigenfunctions with positive l to the orbits of type B which do not. The reverse is true for negatively charged particles, The magnetic field is assumed to be upwards, perpendicular to the plane of the diagram.

(3) Now attach the center of the rotating paddle system to an arm of length R, one end of which is fixed at the chosen gauge center.

(4) Rotate the arm around the gauge center. The sand will now produce a distribution which looks like $|\psi_{nl}|^2$. (The model does not represent the overlap between $\psi_{nl'}$ and the quasiclassical orbits function centered at radial distances other than R. As the classical limit is approached this overlap becomes smaller and smaller. Nor does it indicate the oscillating probability distribution between $R \pm r_L$. This also decreases in relative importance as n increases.)

LANDAU GAUGE

The same overlap integral technique can be used to see how displaced orbit wavefunctions are related to the Landau gauge wavefunctions [see (I)]. To do this one has to write the displaced orbit wavefunctions in the Landau gauge. The transformation function between the cylindrical and Landau gauges is

$$\phi_{cL} = \tfrac{1}{2}Bxy = \tfrac{1}{2}Br^2 \cos\theta \sin\theta \qquad (27)$$

for which $\mathbf{A}_L = \mathbf{A}_c + \nabla\phi_{cL}$.

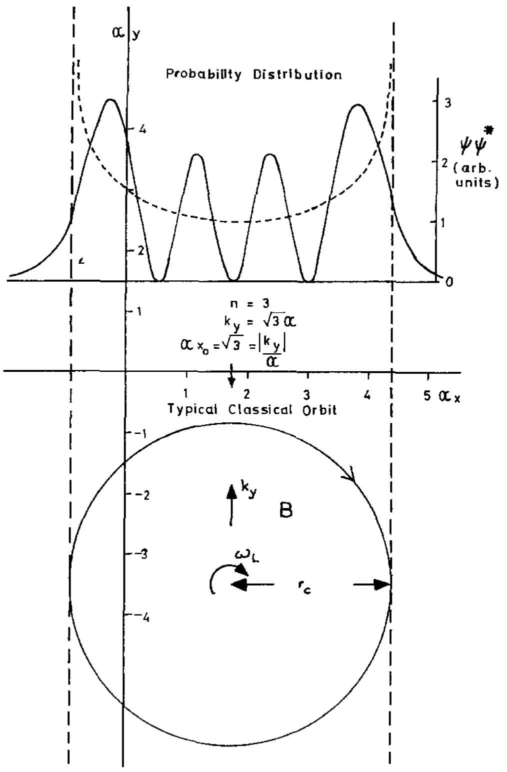

FIG. 3. A typical "strip" wavefunction in the Landau gauge. It is approximately bounded by the dashed lines. One of the corresponding classical orbits is shown. The quantum and classical probability distributions in the x direction are shown. The probability distribution is uniform in the y direction in this gauge for all eigenfunctions.

One has therefore to multiply Eq. (19) by $\exp(ie\phi_{cL}/\hbar)$ and change to Cartesian coordinates. The geometrical relations between the Landau wavefunctions and the quasiclassical displaced Larmor orbit wavefunctions which give the maximum overlap are illustrated in Fig. 3.

The Landau gauge solutions are similar to what one would get by moving the gauge center in the cylindrical gauge to an infinite distance along the x axis.

GENERAL COMMENTS

The probability distributions $r\psi_{nl'}{}^*\psi_{nl'}$ are independent of "θ", i.e., they are uniform in azimuth around the gauge center. Similarly, the Landau wavefunctions give uniform probability distributions in the "y" direction.

These results are simple consequences of the fact that the state $\psi_{nl'}$ corresponds to an exact value for the canonical momentum $p_\theta=\hbar l'$, and the Landau states give exactly defined values to $p_y=\hbar k_y$. It follows from the uncertainty principle that the respective canonically conjugate position coordinates, θ and y, are indeterminate.

The probability distributions in the other coordinates, r and x, are confined to belts whose widths are closely similar to the diameters of the classical orbits $2r_L$. As the quantum numbers increase the distributions are increasingly concentrated on two narrow strips separated by $2r_L$.

Only the basic cylindrical gauge wavefunctions ψ_{0l} and the displaced orbit wavefunctions derived from them are geometrically similar to individual classical orbits. The other wavefunctions cannot be interpreted as describing the range of motion of a single particle, since a particle is not expected to be found far from the region of its classical orbit. The large geometrical size of the $\psi_{nl'}$ is merely the result of lack of information about the initial location and direction of motion of the "particle." No information about these has been inserted into Schrödinger's equation and its solution beyond setting bounds to the "box" containing the particle. To obtain a close wave mechanical analogy to the motion of a single particle one must insert some additional information about the initial conditions by the construction of an initial wavepacket. This is done in Ref. 1 and the result is indeed to show that such a wavepacket rather closely follows the motion of a classical particle within the limits of precision set by the uncertainty principle.

ACKNOWLEDGMENTS

Mr. J. Kavulu helped in programming the computer to produce the probability distributions in Figs. 1 and 3. Professor T. W. B. Kibble assisted by discussing this paper with me.

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