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Quantum Mechanical Descriptions of an Electron in a Magnetic Field

(Received June 5, 1970)

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Abstract

The various quantum mechanical descriptions for an electron in a constant homogeneous magnetic field are considered for some particular gauges using the elementary methods of solutions. The internal relations between them are investigated by the quantum mechanical operator technique to get the systematic solutions for the wave functions in coordinate space. Then the transformation theory between various solutions is established and further the oscillating motion of a wave packet is analyzed to present another direct example of the theorem due to Ehrenfest.

I. Introduction

Quantum mechanical behaviour of an electron in a uniform constant magnetic field is a well-known problem. Helical orbits are quantized into the famous Landau levels⁽¹⁾. We consider in this paper mainly the relations between the various quantum mechanical descriptions, which are originated owing to the degeneracy of the energy eigenfunctions, or may be interpreted in a classical mechanical language, by the fact that the axes of helical orbits with the same energy may lie anywhere in the plane perpendicular to H . Further the arbitrariness for the vector potential by the gauge transformation makes the problem rather obscure.

Before treating the problem quantum mechanically, we may mention briefly the classical mechanical description. Newtonian equations of motion of an electron in a static homogeneous magnetic field along the z -direction are expressed as

$$m\dot{v}_x = -\frac{eH}{c} v_y, \quad (1-1)$$

$$m\dot{v}_y = +\frac{eH}{c} v_x, \quad (1-2)$$

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$$m\dot{v}_z=0, \quad (1-3)$$

where m is the electronic mass and $-e$, its charge. The motion along the magnetic field is identical as the free motion, and we shall attend to the description for the motion in a plane perpendicular to H , i. e. the x - y plane only. Equations (1-1) and (1-2) are expressed as

$$\dot{v}_x = -\omega v_y, \quad (1-4)$$

$$\dot{v}_y = \omega v_x, \quad (1-5)$$

where $\omega = \frac{eH}{mc}$ is the cyclotron frequency, and we have the solutions,

$$\dot{x} = v_x = r_c \omega \cos(\omega t + \alpha), \quad (1-6)$$

$$\dot{y} = v_y = r_c \omega \sin(\omega t + \alpha), \quad (1-7)$$

and further integration gives,

$$x = \xi + x_0 \quad (1-8)$$

and

$$y = \eta + y_0. \quad (1-9)$$

Here the electronic coordinates are expressed as the sum of two; the coordinates x_0 and y_0 that are identified with the center of the circular orbit, and the relative coordinates ξ and η which describe the relative circular motion to the center x_0 and y_0 , and are related to the velocity components v_y and v_x .

$$\xi = \frac{1}{\omega} v_y = r_c \sin(\omega t + \alpha), \quad (1-10)$$

and

$$\eta = \frac{-1}{\omega} v_x = -r_c \cos(\omega t + \alpha). \quad (1-11)$$

The helical motion is a simple circular motion of the radius r_c with constant speed in a x - y plane centered at the point (x_0, y_0) with angular velocity ω . The energy E of the motion in a x - y plane is expressed only with the radius r_c and the angular frequency ω and therefore independent on the center of the orbit x_0 and y_0 .

$$E = \frac{1}{2} m r_c^2 \omega^2. \quad (1-12)$$

In a quantum mechanical treatment we have to formulate the problem in terms of the Hamiltonian operator which includes the vector potential explicitly rather than the magnetic field, so there appears some uncertainty concerning the gauge transformation. In the following we solve the Schrödinger equations for the stationary state wave functions in the x - y plane for the various gauges by elementary methods, and ask for the internal relations between them. The internal relations are investigated using the quantum mechanical operator formulation to get the systematic solution to the problem. and the meanings of various constants of motion are made clear to get the density of states for particular methods of solutions. Finally the

motion of a wave packet is analyzed to get another example of verification for the theorem due to Ehrenfest.

II. Elementary Solutions for Schrödinger Equations in Various Gauges

We shall now consider the elementary solutions to the free electron problem in a uniform magnetic field in the nonrelativistic quantum mechanics. The Hamiltonian for our problem is

$$\mathcal{H} = \frac{1}{2m} \left(P_x + \frac{e}{c} A_x \right)^2 + \frac{1}{2m} \left(P_y + \frac{e}{c} A_y \right)^2,$$

where we omit the unnecessary part along the field direction (z -component). We now have to specify the vector potential. Since it is the magnetic field that is the observable physical quantity, all vector potentials which produce the same field (O, O, H) should be physically equivalent (gauge invariance). We may take three commonly used forms to the vector potentials.

(1) $A^{(1)} = (-Hy, O, O)$; This gauge is called Landau or linear gauge⁽¹⁾.

(2) $A^{(2)} = (O, Hx, O)$; This is essentially the linear gauge, where roles of x - and y -components are interchanged in contrast to the gauge $A^{(1)}$.

(3) $A^{(3)} = (-\frac{1}{2}Hy, \frac{1}{2}Hx, O)$; This is called symmetrical gauge.

First, we consider the Landau gauge. The Hamiltonian in this gauge is represented as

$$\mathcal{H}^{(1)} = \frac{1}{2m} \left(P_x - \frac{e}{c} Hy \right)^2 + \frac{1}{2m} P_y^2. \quad (2-1)$$

Thus the stationary state wave function $\Psi^{(1)}$ must satisfy the Schrödinger equation,

$$\left\{ \frac{1}{2m} \left(P_x - \frac{e}{c} Hy \right)^2 + \frac{1}{2m} P_y^2 \right\} \Psi^{(1)}(x, y) = E \Psi^{(1)}(x, y). \quad (2-2)$$

It is easy to see that, looking for the solution in the form,

$$\Psi^{(1)}(x, y) = (2\pi)^{-\frac{1}{2}} \exp(ik_x x) \varphi(y), \quad (2-3)$$

we can separate the variables in the Hamiltonian. In other words the coordinate x does not appear in the Hamiltonian (2-1), and P_x is a good quantum number (P_x commutes with the Hamiltonian and its eigen value is denoted as $\hbar k_x$). The equation to be solved for $\varphi(y)$ becomes

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + \frac{1}{2} m \omega^2 (y - k_x \lambda^2)^2 \right\} \varphi(y) = E \varphi(y), \quad (2-4)$$

and

$$\lambda = \left(\frac{\hbar c}{eH} \right)^{\frac{1}{2}}. \quad (2-5)$$

The equation (2-4) is identical with the problem of one-dimensional harmonic

oscillator centered at $y_0 = k_x \lambda^2$. As for the eigenvalues we immediately get from the equation (2-4),

$$E = \hbar \omega (n + \frac{1}{2}), \quad n = 0, 1, 2, \dots, \quad (2-6)$$

and the corresponding eigenfunctions are

$$\varphi = \Phi_n \left(\frac{y - y_0}{\lambda} \right), \quad (2-7)$$

$$\Phi_n(\rho) = (2^n n! \sqrt{\pi} \lambda)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \rho^2 \right) H_n(\rho), \quad (2-8)$$

where $H_n(\rho)$ are the Hermite polynomials. Thus we obtain

$$\Psi_{n, k_x}^{(1)}(x, y) = (2\pi)^{-\frac{1}{2}} \exp(ik_x x) \Phi_n \left(\frac{y - y_0}{\lambda} \right), \quad (2-9)$$

and especially for the ground states

$$\Psi_{0, k_x}^{(1)} = (2\pi)^{-\frac{1}{2}} \exp(ik_x x) (\lambda \sqrt{\pi})^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} \left(\frac{y - k_x \lambda^2}{\lambda} \right)^2 \right\}. \quad (2-9')$$

The length λ defined in the equation (2-5) is called the magnetic radius and determines the order of the cyclotron radius in the quantum mechanical ground state ($n=0$) and is therefore characteristic for the quantum mechanical treatment. In the wave function for stationary states (2-9) and (2-9'), we see the oscillatory motion along the y -direction but not along the x -direction. The probability density $|\Psi_{n, k_x}^{(1)}|^2$ is uniform for the x -direction in contrast to the oscillatory motion in classical treatment.

We shall now determine the degeneracy of levels. First, we observe that just as in the classical description the energy (2-6) is independent on the position of the center y_0 . This means that all the wave functions given in the equation (2-9) with different k_x (or equivalently y_0) belong to the same energy eigenvalue. Since in free space there is no restriction on k_x , we may conclude that each level has an infinite degeneracy. But we consider an electron to be in a cubic box of a dimension L . If we apply the usual periodic boundary condition to the wave function in the x -direction, then the allowed values of k_x are

$$k_x = \frac{2\pi}{L} n_x, \quad (2-10)$$

where n_x is an integer. The center of the orbit, y_0 must be within the normalization length L . The wave functions with centers located within the distance λ from the boundaries may suffer the serious modifications due to the occurrence of the surface states, but the relative number of such states is considered to be very small as long as $\lambda \ll L$. This means $0 \leq k_x = \frac{y_0}{\lambda^2} \leq \frac{L}{\lambda^2}$. Since within the unit length of k_x there are $L/2\pi$ allowed k_x values, the total number of allowed k_x values is $L^2/2\pi \lambda^2$. and this is the degeneracy of each Landau level. The density of states

is $1/2\pi\lambda^2$ per unit surface area. When the magnetic field is so strong that the interval $\hbar\omega$ between the Landau levels becomes very large, we see the phenomena of strong bunching of the allowed levels.

Next, the gauge $A^{(2)}$ is considered with the following Hamiltonian,

$$\mathcal{H}^{(2)} = \frac{1}{2m} P_x^2 + \frac{1}{2m} \left(P_y + \frac{e}{c} Hx \right)^2. \quad (2-11)$$

Following the similar analysis to the case of gauge $A^{(1)}$ we can easily obtain the solution,

$$\psi_{n, k_y}^{(2)}(x, y) = (2\pi)^{-\frac{1}{2}} \exp ik_y y \phi_n \left(\frac{x + k_y \lambda^2}{\lambda} \right), \quad (2-12)$$

with the same expression as (2-6) for the energy eigenvalues. The degeneracy in this case is seen to be identical in the Landau gauge. We see in this gauge the center of the oscillator at $x_0 = -k_y \lambda^2$ and the ground state wave functions are expressed as

$$\psi_{0, k_y}^{(2)} = (2\pi)^{-\frac{1}{2}} \exp ik_y y (\lambda \sqrt{\pi})^{-\frac{1}{2}} \exp \left\{ -\frac{(x + k_y \lambda^2)^2}{2\lambda^2} \right\}. \quad (2-13)$$

Finally, we consider the symmetrical gauge $A^{(3)} = (-\frac{1}{2} Hy, \frac{1}{2} Hx, 0)$. In this gauge the Hamiltonian $\mathcal{H}^{(3)}$ is expressed as

$$\mathcal{H}^{(3)} = \frac{1}{2m} (P_x^2 + P_y^2) + \frac{1}{2} \omega L_z + \frac{1}{8} m\omega^2 (x^2 + y^2). \quad (2-14)$$

In this gauge both P_x and P_y are not constants of motion because we have both coordinates x and y in the Hamiltonian but we have another constant of motion, namely $L_z = (\mathbf{r} \times \mathbf{P})_z$ as is easily seen.

In order to make the physical situation clear, we may try to solve the corresponding Schrödinger equation in polar coordinates in the form $\psi(\mathbf{r}, \theta) = (\mathbf{r})^{-\frac{1}{2}} F(\mathbf{r}) e^{iM\theta}$, with $F(\mathbf{r})$ obeying the following radial wave equation⁽²⁾:

$$-\frac{\hbar^2}{2m} \frac{d^2 F}{dr^2} + V_{eff} F = E F, \quad (2-15)$$

where

$$V_{eff} = \frac{\hbar^2}{2m} \frac{M^2 - \frac{1}{4}}{r^2} + \frac{1}{2} \hbar\omega M + \frac{1}{8} m\omega^2 r^2. \quad (2-16)$$

We consider the case where M is a very large positive or negative integer, thus the correspondence principle may be applicable. The effective radial potential V_{eff} has a minimum value at

$$r_m = (4M^2 - 1)^{\frac{1}{2}} \lambda, \quad (2-17)$$

and is approximated as

$$V_{eff} = V_0 + \frac{1}{2} m\omega^2 (r - r_m)^2 + \dots, \quad (2-18)$$

where the minimum value of V_{eff} is denoted as V_0 .

$$V_0 = \frac{\hbar^2}{2m} \left\{ M + \frac{1}{2} (4M^2 - 1)^{\frac{1}{2}} \right\} \frac{1}{\lambda^2} \quad (2-19)$$

In the region where the principle of correspondence is applicable, V_0 is approximated as

$$V_0 = \hbar\omega M, \text{ when } M \text{ is a large positive integer,} \quad (2-19')$$

$$\text{or } V_0 = 0, \text{ when } M \text{ is a large negative integer.} \quad (2-19'')$$

Thus we may expect that the eigenvalues of the Hamiltonian (2-14) to be

$$\begin{aligned} \hbar\omega(M + \frac{1}{2}), \hbar\omega(M + \frac{1}{2} + 1), \hbar\omega(M + \frac{1}{2} + 2), \dots, \quad M > 0 \\ \hbar\omega\frac{1}{2}, \hbar\omega(\frac{1}{2} + 1), \hbar\omega(\frac{1}{2} + 2), \dots, \quad M < 0 \end{aligned} \quad (2-20)$$

The eigenvalues as a whole are of course identical to the expression (2-6). The direction of circular motion in the magnetic field is expected to be the origin of the difference due to M values.

The exact solution to this symmetrical gauge problem may be obtained easily rather in the form

$$\Psi^{(3)}(r, \theta) = R(r) e^{iM\theta}, \quad (2-21)$$

where the radial wave function $R(r)$ is investigated by usual polynomial expansion method for the function $R(r)/\exp\left(-\frac{r^2}{4\lambda^2}\right)$. We cite here only the results, the details of which may be found in references⁽³⁾,

$$\Psi_{n,l}^{(3)}(r, \theta) = (2^{-n+l+1} \pi n! l!)^{-\frac{1}{2}} \frac{1}{\lambda} \left(\frac{r}{\lambda}\right)^{n-l} \exp\left\{i(n-l)\theta - \frac{r^2}{4\lambda^2}\right\} L_{n,l}\left(\frac{r^2}{\lambda^2}\right), \quad (2-22)$$

where the polynomial part of the wave function is denoted as

$$L_{n,l}(\rho) = \exp(\rho/2) \left(\frac{d}{d\rho}\right)^n [\rho^l \exp(-\rho/2)]. \quad (2-23)$$

The energy eigenvalues depend only upon n values

$$E_n = \hbar\omega(n + \frac{1}{2}), \quad (2-6)$$

and are degenerate to l values or to M . The quantum number M previously introduced by the equation (2-21) is given by the difference of n and l ,

$$M = n - l, \quad (2-24)$$

where

$$l = 0, 1, 2, 3, \dots \quad (2-25)$$

$$n = 0, 1, 2, 3, \dots$$

The positiveness for the l values is the reflection of (2-20). The ground states are obtained by putting n equal to zero,

$$\Psi_{0,l}^{(3)} = (2^{l+1} \pi l!)^{-\frac{1}{2}} \frac{1}{\lambda} \left(\frac{r}{\lambda}\right)^l \exp\left(-il\theta - \frac{r^2}{4\lambda^2}\right). \quad (2-26)$$

Quantum Mechanical Descriptions of an Electron in a Magnetic Field

The degree of degeneracy or equivalently the state density for the level $E_n = \hbar\omega(n + \frac{1}{2})$ is difficult to obtain in this stage of investigation, where the meaning of the quantum number l is not clear although it has been introduced by the requirement of termination of series for the function $L_{n, l}(\rho)$.

We have now investigated the wave functions in three different gauges. Now we shall proceed to consider the internal relations between them. As is well known the gauge transformation is represented by the canonical transformation for the wave functions in quantum mechanics.

$$\Psi \rightarrow \Psi' = \exp\left(-\frac{ief}{c\hbar}\right)\Psi \quad (2-27)$$

The vector potential appears in the Hamiltonian in the form of combinations of $P + \frac{e}{c}A$ where this quantity is transformed by the canonical transformation (2-27),

$$\begin{aligned} P + \frac{e}{c}A &\rightarrow P' + \frac{e}{c}A' = \exp\left(-\frac{ief}{c\hbar}\right)\left(P + \frac{e}{c}A\right)\exp\left(+\frac{ief}{c\hbar}\right) \\ &= P + \frac{e}{c}(A + \nabla f). \end{aligned} \quad (2-28)$$

Thus the wave function Ψ' is expected to be one for the gauge $A + \nabla f$. Unfortunately we are not able to obtain the simple relation (2-27) for the solutions (2-9), (2-13) and (2-22). For simplicity we consider the ground state wave functions mainly in the following. The linear combinations of the degenerate wave functions that are obtained by the transformation (2-27) are need to obtain the correct wave function. Starting from the wave function $\Psi^{(1)}$ for the Landau gauge, we seek after the solution $\Psi^{(2)}$ in the gauge $A^{(2)}$, where the gauge transformation is

$$A^{(2)} = A^{(1)} + \nabla f' \quad (2-29)$$

and $f' = Hxy$. (2-29')

According to the equation (2-27) we obtain from the equation (2-9'),

$$\Psi_{0, k_x}^{g, k_x} = \text{const} \times \exp\left\{ik_x x - i\frac{xy}{\lambda^2} - \frac{(y - k_x \lambda^2)^2}{2\lambda^2}\right\},$$

for the gauge transformed wave functions. We have further to make the linear combination of the above wave functions which have different k_x values in order to have $\Psi_{0, k_y}^{(2)}$,

$$c(k_y, k_x) = \exp(i\lambda^2 k_x k_y), \quad (2-30)$$

$$\int c(k_y, k_x) \Psi_{0, k_x}^{g, k_x} dk_x \propto \exp\left\{ik_y y - \frac{(x + k_y \lambda^2)^2}{2\lambda^2}\right\} \int \exp\left[-\frac{\lambda^2}{2}\left(k_x - \frac{y + ix + i\lambda^2 k_y}{\lambda^2}\right)^2\right] dk_x. \quad (2-31)$$

This is exactly proportional to the function $\Psi_{0, k_y}^{(2)}$, (2-13). For the excited state

wave functions we can obtain the same coefficients of linear combinations proportional to above $c(k_y, k_x)$ using the generating function for the Hermite functions.

Next, the wave function $\Psi_{0, l=0}^{(3)}$ is obtained from the function $\Psi_{0, k_x}^{(1)}$. In this gauge,

$$A^{(3)} = A^{(1)} + \nabla f'' \quad (2-32)$$

and

$$f'' = \frac{1}{2} H x y, \quad (2-32')$$

then we obtain

$$\Psi_{0, k_x}^{g'} = \text{const} \times \exp \left\{ i k_x x - i \frac{x y}{2 \lambda^2} - \frac{(y - k_x \lambda^2)^2}{2 \lambda^2} \right\}. \quad (2-32'')$$

Taking the coefficient $c'(k_x)$ equal to $\exp \left(-\frac{\lambda^2 k_x^2}{2} \right)$, $\Psi_{0, l=0}^{(3)}$ is easily obtained, i.e., we can see

$$\int c' \Psi_{0, k_x}^{g'} dk_x \propto \exp \left(-\frac{x^2 + y^2}{4 \lambda^2} \right) \int \exp \left\{ -\lambda^2 \left(k_x - \frac{i x + y}{2 \lambda^2} \right)^2 \right\} dk_x \quad (2-33)$$

is exactly proportional to the function $\Psi_{0, l=0}^{(3)}$, (2-26).

III. Systematic Solutions for the Wave Functions

So far we have worked out with the wave functions for a specific vector potential in each case. Now we proceed to work with the systematic treatment. In this formulation the eigenvalue problem can be treated in terms of the relative coordinates and the coordinates of the center of the orbit⁽⁴⁾, and the corresponding eigenfunctions are obtained by factorization procedure, in which the constants of motion may be conveniently used to classify the wave functions.

The Hamiltonian is expressed in terms of the kinetic momenta, π

$$\pi = P + \frac{e}{c} A, \quad (3-1)$$

$$\mathcal{H} = \frac{1}{2m} (\pi_x^2 + \pi_y^2), \quad (3-2)$$

where π_x and π_y satisfy the commutation relation,

$$[\pi_x, \pi_y] = -\frac{e\hbar}{c} H i. \quad (3-3)$$

Relative coordinates ξ and η are introduced quantum mechanically by the definition,

$$\xi = \frac{\pi_y}{m\omega} = \frac{\lambda^2}{\hbar} \pi_y, \quad \eta = -\frac{\pi_x}{m\omega} = -\frac{\lambda^2}{\hbar} \pi_x, \quad (3-4)$$

and therefore, they are not independent variables for each other as in classical treatment, but they have to be considered the canonical variables which are complementary to each other.

$$[\xi, \eta] = -i \lambda^2 \quad (3-5)$$

Quantum Mechanical Descriptions of an Electron in a Magnetic Field

The Hamiltonian (3-2) are expressed in terms of these relative coordinates ξ and η .

$$\mathcal{H} = \frac{1}{2} m \omega^2 (\xi^2 + \eta^2) \quad (3-6)$$

The radius of circular motion r_c is related to these coordinates,

$$r_c^2 = \xi^2 + \eta^2 = \frac{2}{m\omega^2} \mathcal{H}, \quad (3-7)$$

from which we can conclude that r_c is a constant of motion and an eigen state of the Hamiltonian \mathcal{H} may therefore be constructed to become an eigenstate for the operator r_c also. Another set of coordinates are those for the center of the circular orbit x_0 and y_0 , which are defined as

$$\begin{aligned} x_0 &= x - \xi = x - \frac{\lambda^2}{\hbar} \pi_y, \\ y_0 &= y - \eta = y + \frac{\lambda^2}{\hbar} \pi_x. \end{aligned} \quad (3-8)$$

These variables are independent to the relative coordinates, because we may easily see using the relations (3-1), (3-4) and (3-8),

$$[x_0, \xi] = [x_0, \eta] = [y_0, \xi] = [y_0, \eta] = 0. \quad (3-9)$$

and therefore they commute with the Hamiltonian (3-6), but they are not mutually commutable for each other,

$$[x_0, y_0] = i\lambda^2. \quad (3-10)$$

The coordinates of the center, x_0 and y_0 have therefore to be considered as another set of canonical variables in addition to the canonical variables ξ and η .

We have thus obtained two sets of canonical variables (ξ, η) and (x_0, y_0) and as the Hamiltonian does not contain the one set of variables (x_0, y_0) we may conclude that the eigenfunctions are degenerate by the way in which the eigen functions are expressed in terms of the variables x_0 and y_0 . Thus the variety of the eigen functions is not due to the selection of the gauge to the vector potential, but due to the selection of the wave function for the variables x_0 and y_0 .

We shall proceed to work with the eigenvalues and the eigenfunctions concretely. The annihilation and creation operators for the oscillation of the relative coordinates, a and a^* are defined as

$$\begin{aligned} a &= \frac{1}{\sqrt{2}} \frac{1}{\lambda} (\xi - i\eta) = \frac{i\lambda}{\sqrt{2}} \frac{1}{\hbar} (\pi_x - i\pi_y), \\ a^* &= \frac{1}{\sqrt{2}} \frac{1}{\lambda} (\xi + i\eta) = -\frac{i\lambda}{\sqrt{2}} \frac{1}{\hbar} (\pi_x + i\pi_y). \end{aligned} \quad (3-11)$$

The Hamiltonian is seen to be diagonal in the occupation number representation,

$$a^* a = \frac{1}{2\lambda^2} (\xi^2 + \eta^2) - \frac{1}{2} = \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2}, \quad (3-12)$$

whose diagonal elements,

$$E_n = \hbar\omega(n + \frac{1}{2}), \quad (3-13)$$

are identical to the well known Landau levels. The corresponding eigen functions are obtained from the ground state wave functions which are determined by the requirement $a\Psi_0=0$.

Although the eigenfunctions are determined by the equations,

$$\begin{aligned} \Psi_n &= (n!)^{-\frac{1}{2}} (a^*)^n \Psi_0, \\ a\Psi_0 &= 0, \end{aligned} \quad (3-14)$$

the concrete forms of wave functions are dependent on the variables x_0 and y_0 . Three choices of the wave functions for the center of orbit x_0 and y_0 are considered;

Case I. The wave functions are the eigenfunctions for y_0 .

Case II. The wave functions are the eigenfunctions for x_0 .

Case III. The wave functions are eigenfunctions for $x_0^2 + y_0^2$.

We first consider Case III; the wave functions are the eigen functions for the operator $r_0^2 = x_0^2 + y_0^2$, in which x_0 and y_0 are considered to be canonical variables according to the commutation relation (3-10). Introducing the creation and annihilation operators b^* , and b for these variables,

$$b^* = \frac{1}{\sqrt{2\lambda}} (x_0 - iy_0), \quad (3-15)$$

$$b = \frac{1}{\sqrt{2\lambda}} (x_0 + iy_0),$$

we obtain
$$b^*b = \frac{1}{2\lambda^2} (x_0^2 + y_0^2 + i[x_0, y_0]) = \frac{1}{2\lambda^2} (r_0^2 - \lambda^2), \quad (3-16)$$

and
$$r_0^2 = \lambda^2(2b^*b + 1). \quad (3-17)$$

The eigenvalues of $r_0^2 = x_0^2 + y_0^2$, that is, the squared distance from the origin of the center of the orbit are quantized into the discrete values,

$$\lambda^2, 3\lambda^2, 5\lambda^2, \dots, (2l+1)\lambda^2, \dots \quad (3-17')$$

The degenerate ground state wave functions are classified according to above l -values,

$$\Psi_0(l) = (l!)^{-\frac{1}{2}} (b^*)^l \Psi_0(l=0) = (l!)^{-\frac{1}{2}} \left\{ \frac{1}{\sqrt{2\lambda}} (x - iy) \right\}^l \Psi_0(l=0), \quad (3-18)$$

where the creation operator b^* is equal to $\frac{1}{\sqrt{2\lambda}} (x - iy) - a$ and therefore we may drop the operator a for the ground states $\Psi_0(l)$. The starting ground state in Case III, $\Psi_0(l=0)$ is completely determined by the requirements,

$$a\Psi_0(l=0) = 0, \quad (3-19)$$

and
$$b\Psi_0(l=0) = 0.$$

Quantum Mechanical Descriptions of an Electron in a Magnetic Field

These equations are expressed in terms of π_x and π_y ,

$$\begin{aligned}\pi_x \Psi_0(l=0) &= \frac{\hbar}{2\lambda^2} i(x+iy) \Psi_0(l=0), \\ \pi_y \Psi_0(l=0) &= \frac{\hbar}{2\lambda^2} (x+iy) \Psi_0(l=0),\end{aligned}\tag{3-20}$$

and thus we can obtain the differential equations which the required wave function has to satisfy in the ordinary coordinate space representation.

$$\frac{\partial \Psi_0(l=0)}{\partial x} = \frac{1}{2\lambda^2} \left(-x - iy - i \frac{2A_x}{H} \right) \Psi_0(l=0),\tag{3-21}$$

and

$$\frac{\partial \Psi_0(l=0)}{\partial y} = \frac{1}{2\lambda^2} \left(+ix - y - i \frac{2A_y}{H} \right) \Psi_0(l=0).$$

The solution for the equation (3-21) is confirmed to be

$$\Psi_0(l=0) = (2\pi\lambda^2)^{-\frac{1}{2}} \exp \frac{1}{2\lambda^2} \left\{ -\frac{x^2+y^2}{2} - \frac{i}{H} \left(\int A_x dx + \int A_y dy \right) \right\},\tag{3-22}$$

using the relation $H = \text{rot}_z A$.

The phase integral $\int A_x dx + \int A_y dy$ is related to the gauge transformation $A = A^{(3)} + \nabla f$, where we have defined the general gauge relative to the symmetrical gauge, $A^{(3)} = (-\frac{1}{2}Hy, \frac{1}{2}Hx, 0)$ using the scalar function f .

$$2f = \int A_x dx + \int A_y dy\tag{3-23}$$

The wave function (3-22) becomes finally to

$$\Psi_0(l=0) = \frac{1}{\lambda\sqrt{2\pi}} \exp \left(-\frac{x^2+y^2}{4\lambda^2} \right) \exp \left(-i \frac{f}{H\lambda^2} \right).\tag{3-22'}$$

The factor $\exp \left(-i \frac{f}{H\lambda^2} \right)$ is identical to the canonical transformation (2-27). The degenerate ground state wave functions are obtained in Case III in coordinate space using the relation (3-18),

$$\Psi_0(l) = \frac{1}{\sqrt{l!}} \left\{ \frac{1}{\sqrt{2}} \frac{(x-iy)}{\lambda} \right\}^l \frac{1}{\lambda\sqrt{2\pi}} \exp \left(-\frac{x^2+y^2}{4\lambda^2} \right) \exp \left(-i \frac{f}{H\lambda^2} \right),\tag{3-18'}$$

which confirms the result (2-26) for the arbitrary gauge.

From the expressions (3-17) and (3-17') we can obtain the meaning of the quantum number l , that is the measure for the distance of the center of the orbit from the origin. Considering the specimen to be a circle of radius R and neglecting the boundary effects to the number of states we may obtain for the density of states per unit surface area for the very large value of R ,

$$\frac{1}{\pi R^2} l_{max} = \frac{1}{2\pi R^2} \left(\frac{R^2}{\lambda^2} - 1 \right) \rightarrow \frac{1}{2\pi\lambda^2}.$$

The form (3-18') confirms that the angular momentum $l_z = \frac{\hbar}{i} \frac{\partial}{\partial \theta}$ is a constant of motion only in the symmetrical gauge $A^{(3)}$, where f is equal to zero as is pointed out previously. The solution for the Landau gauge $A^{(1)}$ should be obtained if we put f equal to $-\frac{1}{2}Hxy$ but the function $\frac{1}{\lambda\sqrt{2\pi}} \exp\left(-\frac{x^2+y^2}{4\lambda^2}\right) \exp\left(-i\frac{xy}{2\lambda^2}\right)$ is the wave function corresponding to $l=0$ and $n=0$ in the Landau gauge. In order to get the wave function of the form (2-9) and (2-9') we have to proceed to Case I.

Next we consider the wave functions in Case I, where the ground state wave functions are classified according to the eigenvalues y_0' . The wave function $\Psi_0(y_0')$ is obtained from the wave function $\Psi_0(y_0'=0)$ using the displacement operator for y_0 , i.e., $\exp\left(i\frac{y_0'x_0}{\lambda^2}\right)$. We can easily see the function

$$\Psi_0(y_0') = \exp\left(i\frac{y_0'x_0}{\lambda^2}\right) \Psi_0(y_0'=0) \quad (3-24)$$

is the eigenfunction of y_0 with eigenvalue y_0' using the relation

$$\begin{aligned} y_0 \Psi_0(y_0'=0) &= 0, \\ \exp\left(-i\frac{y_0'x_0}{\lambda^2}\right) y_0 \exp\left(i\frac{y_0'x_0}{\lambda^2}\right) &= y_0 + y_0'. \end{aligned} \quad (3-24')$$

The starting wave function in Case I is therefore determined by the requirements,

$$\begin{aligned} a \Psi_0(y_0'=0) &= 0, \\ y_0 \Psi_0(y_0'=0) &= 0. \end{aligned} \quad (3-25)$$

The equations (3-25) are transformed into the following form in terms of π_x and π_y ,

$$\begin{aligned} \pi_x \Psi_0(y_0'=0) &= -\frac{\hbar}{\lambda^2} y \Psi_0(y_0'=0), \\ \pi_y \Psi_0(y_0'=0) &= \frac{\hbar}{\lambda^2} i y \Psi_0(y_0'=0), \end{aligned} \quad (3-25')$$

and finally into the form of differential equations in coordinate space.

$$\begin{aligned} \frac{\partial}{\partial x} \Psi_0(y_0'=0) &= \frac{1}{\lambda^2} \left(-yi - i\frac{A_x}{H}\right) \Psi_0(y_0'=0), \\ \frac{\partial}{\partial y} \Psi_0(y_0'=0) &= \frac{1}{\lambda^2} \left(-y - i\frac{A_y}{H}\right) \Psi_0(y_0'=0). \end{aligned} \quad (3-26)$$

The solution of the equations (3-26) is expressed in terms of scalar function f previously defined,

$$\Psi_0(y_0'=0) = (2\pi\sqrt{\pi} \lambda^2)^{-\frac{1}{2}} \exp\left\{-\frac{y^2}{2\lambda^2} - i\left(\frac{f}{\lambda^2 H} + \frac{xy}{2\lambda^2}\right)\right\}. \quad (3-27)$$

In order to get $\Psi_0(y_0')$ from the solution (3-27) using the relation (3-24), we notice

Quantum Mechanical Descriptions of an Electron in a Magnetic Field

$$x_0 \exp \left\{ -i \left(\frac{f}{\lambda^2 H} + \frac{xy}{2\lambda^2} \right) \right\} = \exp \left\{ -i \left(\frac{f}{\lambda^2 H} + \frac{xy}{2\lambda^2} \right) \right\} \left(x - \frac{\lambda^2}{\hbar} P_y \right),$$

and we may therefore move the factor $\exp \left\{ -\frac{i}{\lambda^2 H} (f + \frac{1}{2} Hxy) \right\}$ through the operator x_0 to the left,

$$\begin{aligned} \Psi_0(y_0') &= (2\pi \sqrt{\pi} \lambda^3)^{-\frac{1}{2}} \exp \left\{ -\frac{i}{\lambda^2 H} \left(f + \frac{Hxy}{2} \right) \right\} \exp \left\{ \frac{iy_0'}{\lambda^2} \left(x - \frac{\lambda^2}{\hbar} P_y \right) \right\} \exp \left(-\frac{y^2}{2\lambda^2} \right) \\ &= \exp \left\{ -\frac{i}{\lambda^2 H} \left(f + \frac{Hxy}{2} \right) \right\} (2\pi \lambda^2)^{-\frac{1}{2}} \exp \left(i \frac{y_0' x}{\lambda^2} \right) (\lambda \sqrt{\pi})^{-\frac{1}{2}} \exp \left\{ -\frac{(y - y_0')^2}{2\lambda^2} \right\}. \end{aligned} \quad (3-28)$$

The function (3-28) is identical to the function (2-9'), where we remark the relation $y_0' = k_x \lambda^2$, and $f + \frac{1}{2} Hxy$ is equal to zero for the gauge $A^{(1)}$.

The wave function $\Psi_0(y_0')$, (3-28) is changed into the form

$$\Psi_0(y_0') \propto \exp \left(-i \frac{f}{\lambda^2 H} \right) \exp \left(-\frac{x^2 + y^2}{4\lambda^2} \right) \exp \frac{(x - iy + 2iy_0')^2}{4\lambda^2}. \quad (3-28')$$

In the form (3-28') the last factor is the function of $(x - iy)$, the power series expansion of which thus may give the expansion of $\Psi_0(y_0')$ by the wave function $\Psi_0(l)$. We notice here that the states of even l may appear for the state $\Psi_0(y_0' = 0)$ but states of all l 's may appear for the general state $\Psi_0(y_0')$, and further that the same expansion formula may apply for the excited state wave functions because they can be obtained by repeated application of the creation operator a^* to them. The state $\Psi_0(y_0')$ is an eigenstate of the operator y_0 and the operator x_0 consequently has infinitely large uncertainty as is required by the commutation relation (3-10). This is the reason why $|\Psi_{n, kx}^{(1)}|^2$ has uniform charge density for the x -direction.

Finally we can treat Case II similarly. The wave function $\Psi_0(x_0' = 0)$ is determined by the requirements,

$$a\Psi_0(x_0' = 0) = 0, \quad (3-29)$$

and

$$x_0\Psi_0(x_0' = 0) = 0,$$

whose solution is

$$\Psi_0(x_0' = 0) = (2\pi \sqrt{\pi} \lambda^3)^{-\frac{1}{2}} \exp \left\{ -\frac{x^2}{2\lambda^2} - i \left(\frac{f}{\lambda^2 H} - \frac{xy}{2\lambda^2} \right) \right\}. \quad (3-30)$$

The displacement operator $\exp \left(-i \frac{x_0' y_0}{\lambda^2} \right)$ generates the function $\Psi_0(x_0')$ from the function $\Psi_0(x_0' = 0)$,

$$\begin{aligned} \Psi_0(x_0') &= \exp \left(-i \frac{x_0' y_0}{\lambda^2} \right) \Psi_0(x_0' = 0) \\ &= \exp \left\{ -\frac{i}{\lambda^2 H} \left(f - \frac{Hxy}{2} \right) \right\} (2\pi \lambda^2)^{-\frac{1}{2}} \exp \left(-i \frac{x_0' y_0}{\lambda^2} \right) (\lambda \sqrt{\pi})^{-\frac{1}{2}} \exp \left\{ -\frac{(x - x_0')^2}{2\lambda^2} \right\}, \end{aligned} \quad (3-31)$$

and the analogous one for the equation (3-28') is

$$\Psi_0(x_0') \propto \exp\left(-i \frac{f}{\lambda^2 H}\right) \exp\left(\frac{x^2 + y^2}{4\lambda^2}\right) \exp\left\{-\frac{(x - iy - 2x_0')^2}{4\lambda^2}\right\},$$

which may give the expansion of $\Psi_0(x_0')$ by the function $\Psi_0(l)$.

IV. Conclusion and Further Discussions

We have developed the theory for the wave functions in the general vector potential, and reached the conclusion that the differences in the wave functions originate from the differences which constants of motion we chose to classify the degenerate wave functions. The different vector potentials may give the different constants of motion at first sight in terms of r and P but, as our previous treatment in terms of π shows, we can obtain the same constants of motion in the general gauge although they become obscure for the particular gauge. The remaining problem is to find out the transformation theory in quantum mechanics from the general point of view. As two sets of the canonical variables are (ξ, η) and (x_0, y_0) for our Hamiltonian, we may work out the transformation theory in the ξ and y_0 representation. We can obtain the wave functions in this representation.

Case I.

$$\Psi_n(y_0') = |n\rangle \delta(y_0 - y_0'), \quad (4-1)$$

where $|n\rangle$ is the n -th oscillator wave function as a function of ξ to the Hamiltonian, $\mathcal{H} = \frac{1}{2} m\omega^2(\xi^2 + \eta^2)$.

Case II.

$$\Psi_n(x_0') = |n\rangle (2\pi\lambda^2)^{-\frac{1}{2}} \exp\left(-i \frac{x_0' y_0}{\lambda^2}\right), \quad (4-2)$$

where we have used the commutation relation $[x_0, y_0] = i\lambda^2$, and normalized the wave functions for the continuous variable x_0' , as is done for Case I for the variable y_0' .

Case III.

$$\Psi_n(l) = |n\rangle Y_l(y_0), \quad (4-3)$$

where $Y_l(y_0) = (2^l l! \sqrt{\pi} \lambda)^{-\frac{1}{2}} H_l(\lambda y_0) \exp\left(-\frac{y_0^2}{2\lambda^2}\right)$ is the normalized wave function for the operator $x_0^2 + y_0^2$ whose eigenvalues are $\lambda^2(2l+1)$ in y_0 representation.

The coefficients of transformations between them are easily obtained in this representation taking the inner product between the above wave functions.

Case I and Case II

$$\langle \Psi_n(y_0') | \Psi_{n'}(x_0') \rangle = \delta_{n,n'} \frac{1}{\sqrt{2\pi} \lambda} \exp\left(-i \frac{x_0' y_0'}{\lambda^2}\right) \quad (4-4)$$

Case I and Case III

$$\langle \Psi_n(y_0') | \Psi_{n'}(l) \rangle = \delta_{n,n'} (2^l l! \sqrt{\pi} \lambda)^{-\frac{1}{2}} H_l(\lambda y_0') \exp\left(-\frac{y_0'^2}{2\lambda^2}\right) \quad (4-5)$$

Quantum Mechanical Descriptions of an Electron in a Magnetic Field

Case II and Case III

$$\langle \Psi_n(x_0') | \Psi_n(t) \rangle = \delta_{n,n'} (2^{l!} \sqrt{\pi} \lambda)^{-\frac{1}{2}} H_l(\lambda x_0') \exp\left(-\frac{x_0'^2}{2\lambda^2}\right) \quad (4-6)$$

As a final interesting example the motion of a wave packet in a constant magnetic field is shown to have an exact solution as in a one dimensional harmonic oscillator problem⁽⁵⁾. As for the initial state wave function of a packet, the function

$$\Psi(x, y; t=0) = \frac{1}{\sqrt{\pi} \lambda} \exp\left(ikx - \frac{x^2 + y^2}{2\lambda^2}\right) \quad (4-7)$$

is chosen and we will try to look for the time evolution of the packet. The form of the wave function (4-7) means that an electron is localized near the origin and has the initial mean velocity $\frac{\hbar k}{m}$ along the x -direction.

The function is expanded in terms of the eigenfunctions of the Hamiltonian for which we use $\mathcal{H}^{(1)}$, (2-1) of the Landau gauge for simplicity, thus the time development is easily achieved by the factor $\exp\left(-i\frac{E_n t}{\hbar}\right)$.

$$\Psi(x, y; t) = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk' \Psi_{n,k'}^{(1)} A_{n,k'} \exp(-in\omega t) \exp\left(-\frac{i}{2}\omega t\right) \quad (4-8)$$

The coefficients $A_{n,k'}$ are obtained by the inner product between the function $\Psi(x, y; t=0)$ and the eigenfunctions $\Psi_{n,k'}^{(1)}$, (2-9).

$$\begin{aligned} A_{n,k'} &= (\Psi_{n,k'}^{(1)} | \Psi(x, y; t=0)) \\ &= \left(\frac{\lambda}{\sqrt{\pi}}\right)^{\frac{1}{2}} \exp\left(-\frac{\lambda^2(k-k')^2}{2}\right) \frac{(-\lambda k')^n}{(2^n n!)^{\frac{1}{2}}} \exp\left\{-\left(\frac{k'\lambda}{2}\right)^2\right\} \end{aligned} \quad (4-9)$$

With these coefficients $A_{n,k'}$, we can sum up over n using the property of the generating function for the Hermite functions and then the integration over k' can be performed with use of the Gaussian integral formula.

$$\begin{aligned} \Psi(x, y; t) &= \frac{1}{\pi\sqrt{2}} \int_{-\infty}^{\infty} dk' \exp\left\{ik'x - \frac{\lambda^2}{2}(k'-k)^2 - \frac{1}{4}(\lambda k' e^{-i\omega t})^2 - k'(y-k'\lambda^2)e^{-i\omega t}\right. \\ &\quad \left. - \frac{1}{2\lambda^2}(y-k'\lambda^2)^2 - \frac{i}{2}\omega t\right\} \\ &= \frac{\sqrt{2}}{\lambda} \left\{ \pi(5-4e^{-i\omega t} + e^{-2i\omega t}) \right\}^{-\frac{1}{2}} \exp\left[\frac{\{k\lambda^2 + ix + y(1-e^{-i\omega t})\}^2}{\lambda^2(5-4e^{-i\omega t} + e^{-2i\omega t})} - \frac{y^2}{2\lambda^2} - \frac{(k\lambda)^2 + i\omega t}{2}\right] \end{aligned} \quad (4-10)$$

The moving wave packet (4-10) gives the position probability density proportional to $\exp(2F)$ as a function of space coordinates,

$$\lambda^2 F = \frac{\{k\lambda^2 + ix + y(1 - e^{-i\omega t})\}^2}{2(5 - 4e^{-i\omega t} + e^{-2i\omega t})} + \frac{\{k\lambda^2 - ix + y(1 - e^{i\omega t})\}^2}{2(5 - 4e^{i\omega t} + e^{2i\omega t})} - \frac{1}{2}y^2, \quad (4-11)$$

where F is a quadratic function for the x and y . The equations which gives the center of our oscillating wave packet are obtained by the requirement that F has a maximum value and are written down after some rearrangement.

$$\begin{aligned} x(5 - 4 \cos \omega t + \cos 2\omega t) + y \sin 2\omega t &= k\lambda^2(4 \sin \omega t - \sin 2\omega t) \\ x \sin 2\omega t + y(7 - 4 \cos \omega t - \cos 2\omega t) &= k\lambda^2(9 - 10 \cos \omega t + \cos 2\omega t) \end{aligned} \quad (4-12)$$

The equations (4-12) have obviously the solution,

$$\begin{aligned} x &= k\lambda^2 \sin \omega t, \\ y &= k\lambda^2(1 - \cos \omega t), \end{aligned} \quad (4-13)$$

which shows that the packet represented by the equation (4-10) oscillates exactly as in classical mechanics. Thus we have another direct example of the theorem due to Ehrenfest.

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