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Gauge invariance in quantum mechanics: plane rotor with time-dependent magnetic flux

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Abstract. A plane rotor, which is an electron constrained to move in a circular orbit, has time-dependent magnetic flux on its axis. By Faraday's law, an induced electric field acts on the electron. The induced electric field exerts a torque on the electron and thus changes its kinetic angular momentum. The induced electric field also does work on the electron and changes its energy. These changes are in agreement with generalised Ehrenfest theorems. The kinetic angular momentum and the energy of the electron depend on the instantaneous flux through the orbit. The Schrödinger equation for the plane rotor is solved exactly in a manifestly gauge-invariant way. The probability that the rotor is in an eigenstate of its energy operator is contrasted with the probability that the system is in an eigenstate of the unperturbed Hamiltonian.

1. Introduction

The Schrödinger equation for a plane rotor, which is an electron constrained to a circular orbit, with time-dependent magnetic flux on its axis was recently solved exactly in the Coulomb gauge when the initial wavefunction is an energy eigenstate (Kobe 1982a). In this paper these restrictions are removed. An exact solution to the Schrodinger equation is given when the vector and scalar potentials are in an arbitrary gauge and the initial wavefunction is arbitrary. The manifestly gauge-invariant formulation of quantum mechanics (Yang 1976, Kobe and Smirl 1978) is used to solve the problem, and the method of solution is contrasted with a conventional approach. Because the problem can be solved exactly, questions of approximations do not become involved with questions of principle regarding gauge invariance.

Since the magnetic flux on the axis of the plane rotor is changing in time, there is an induced electric field at the electron by Faraday's law. This induced electric field exerts a torque on the electron, and thus changes its kinetic angular momentum (Peshkin *et al* 1961, Weisskopf 1961). The induced electric field also does work on the electron, and consequently changes its energy.

The energy operator in this time-dependent problem is not in general the same as the Hamiltonian, but is the Hamiltonian without the scalar potential of the time-dependent electromagnetic field (Yang 1976, Kobe and Smirl 1978). The energy operator, which is time dependent, satisfies an eigenvalue problem, which for the plane rotor is solved exactly for arbitrary time dependence of the magnetic flux. The eigenstates and eigenvalues of the energy operator in general depend on the time as a parameter. The eigenvalues of the energy operator depend on the instantaneous flux on the axis of the rotor. When the flux becomes constant the energy eigenvalues

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depend on this constant magnetic flux and are the same as in the bound state Aharonov–Bohm effect (Peshkin 1981a, b).

The probability that the plane rotor is in an eigenstate of the energy operator is shown to be time independent, no matter how the flux changes in time. Therefore, if the plane rotor is in an eigenstate of the energy operator at time zero, the changing magnetic flux will not induce transitions from one state to another. The flux does not have to be varying adiabatically, as some have suggested (Peshkin *et al* 1961).

The observable operators in this problem satisfy generalised Ehrenfest theorems (Yang 1976). An operator corresponding to an observable must be Hermitian and have a gauge-invariant expectation value. To be gauge invariant in this sense implies that a unitary gauge transformation on the operator must induce a gauge transformation on the electromagnetic potentials on which it may depend (Kobe and Yang 1980). A new Ehrenfest theorem is given here for the angular displacement operator. The time rate of change of the average kinetic angular momentum operator is equal to the average of the torque operator. The time rate of change of the average of the energy operator is equal to the average of the power operator.

If the conventional approach to time-dependent problems involving electromagnetic potentials is used, the wavefunction is expanded in terms of the eigenstates of the unperturbed Hamiltonian (Schiff 1968). The expansion coefficients in this case are gauge dependent in general, and not equal to the gauge-invariant probability amplitudes (Yang 1982). In the special case that the Coulomb gauge is used, the conventional expansion coefficients are equal to the gauge-invariant probability amplitudes. In this case, the scalar potential also vanishes in the Coulomb gauge and the Hamiltonian reduces to the energy operator (Yang 1976).

In § 2 the potentials for the electromagnetic field due to the changing magnetic flux along the axis of the rotor are obtained, and gauge transformations are discussed. The form invariance of the Schrödinger equation under gauge transformations is shown in § 3. In § 4 the energy operator is defined and its eigenvalue problem is solved. The Schrödinger equation is solved by making an eigenfunction expansion, and the probability of finding the electron in an energy eigenstate is obtained. Generalised Ehrenfest theorems for angular displacement, kinetic angular momentum and energy are given in § 5. A conventional approach to time-dependent problems, which uses eigenstates of the unperturbed Hamiltonian, is applied in § 6. Finally, the conclusions are given in § 7.

2. Electromagnetic potentials

The plane rotor, an electron constrained to move in a circular orbit of radius a, has magnetic flux on its axis. The magnetic induction vector $\boldsymbol{B}$ is zero everywhere except on the axis of the rotor where it is infinite in such a way that the magnetic flux Φ is finite. The vector and scalar potentials for this situation, where the flux Φ can vary in time, are obtained. The potentials are not unique and gauge transformations can be made on the potentials. The problem is most conveniently treated in cylindrical coordinates (ρ, θ, z), where the z axis is taken to be the axis of the rotor.

2.1. *Vector potential*

The magnetic induction $\boldsymbol{B}$ can be expressed in terms of a vector potential $\boldsymbol{A}$ as

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}. \tag{2.1}$$

If (2.1) is integrated over a surface through which the z axis penetrates, we obtain the magnetic flux

$$\Phi = \int_S \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{a} = \oint_C \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{l}, \tag{2.2}$$

by Stokes' theorem, where the closed curve $C = \partial S$, the boundary of the surface S, passes around the z axis. The magnetic flux $\Phi(t)$ can depend on the time t because $\boldsymbol{B}$ is in general time dependent.

A vector potential $\boldsymbol{A}$ which gives a $\boldsymbol{B}$ in the z direction, zero everywhere except on the z axis, and a finite flux Φ, is

$$\boldsymbol{A} = \hat{\theta}\Phi(t) g(\theta, t)/2\pi\rho, \tag{2.3}$$

where $\hat{\theta}$ is a unit vector in the azimuthal direction (Merzbacher 1962). The function $g(\theta, t)$ is an arbitrary periodic function of θ, except that

$$\int_0^{2\pi} \mathrm{d}\theta' \, g(\theta', t) = 2\pi, \tag{2.4}$$

in order for the flux to be given by (2.2).

2.2. *Scalar potential*

Since the flux can change in time, there is an induced electric field $\boldsymbol{E}$ by Faraday's law

$$\oint_C \boldsymbol{E} \cdot \mathrm{d}\boldsymbol{l} = -\dot{\Phi}/c. \tag{2.5}$$

The integral in (2.5) can be evaluated for a circle of radius ρ and the induced electric field is

$$\boldsymbol{E} = -\hat{\theta}\dot{\Phi}/2\pi\rho c, \tag{2.6}$$

where $\dot{\Phi}$ denotes the time derivative of Φ.

Because of Faraday's law, the electric field can be expressed in terms of the vector potential $\boldsymbol{A}$ and scalar potential ϕ by

$$\boldsymbol{E} = -\nabla\phi - \partial\boldsymbol{A}/\partial(ct). \tag{2.7}$$

If we use the vector potential in (2.3), the scalar potential in (2.7) must be

$$\phi = (\dot{\Phi}/2\pi c)[\theta - f(\theta, t)] - (\Phi/2\pi c)\dot{f}(\theta, t), \tag{2.8}$$

where $\dot{f}$ denotes the partial time derivative of f and f is defined as

$$f(\theta, t) = \int_0^{\theta} \mathrm{d}\theta' \, g(\theta', t). \tag{2.9}$$

2.3. *Gauge transformations*

The vector and scalar potentials in (2.3) and (2.8) are not unique, however. The same magnetic induction field in (2.1) and electric field in (2.7) are obtained if the new potentials (Jackson 1975)

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda \tag{2.10}$$

and

$$\phi' = \phi - \partial\Lambda/\partial(ct), \tag{2.11}$$

are used, where we assume that $\nabla\times\nabla\Lambda = 0$ everywhere and that the space and time derivatives of Λ commute.

In this paper we shall choose the gauge function Λ to be

$$\Lambda(\theta, t) = [\Phi(t)/2\pi] \int_0^\theta d\theta'\,\lambda(\theta', t), \tag{2.12}$$

where λ is a function such that

$$\int_0^{2\pi} d\theta'\,\lambda(\theta', t) = 0. \tag{2.13}$$

Equation (2.13) guarantees that $\nabla\times\nabla\Lambda$ vanishes everywhere, even on the z axis. The value of the curl on the z axis is defined as (Butkov 1968)

$$z\cdot(\nabla\times\nabla\Lambda)|_{\rho=0} = \lim_{\rho\to 0}(\pi\rho^2)^{-1}\oint_C \nabla\Lambda\cdot d\boldsymbol{l} = 0, \tag{2.14}$$

where C is a circle of radius ρ whose axis is the z axis. Equation (2.13) ensures that the integral in (2.14) vanishes.

When (2.12) is used in (2.10) the new vector potential $\boldsymbol{A}'$ is (2.3) with $g' = g + \lambda$ replacing g. When (2.12) is used in (2.11) the new scalar potential ϕ' is (2.8) with f' replacing f. The function f' is obtained from (2.9) with $g' = g + \lambda$ replacing g. It is important to notice that a gauge transformation with $g' = 0$ is not allowed by (2.4) and (2.13) (Bawin and Burnel 1980, Rowe 1980, Wilczek 1982). Otherwise the magnetic field on the axis of the rotor would be reduced to zero by (2.2).

3. Schrödinger equation

An electron of charge q and mass m is constrained to move in a circular orbit of radius a in an electromagnetic field characterised by the vector potential $\boldsymbol{A}$ and scalar potential ϕ. When the electron is minimally coupled to the electromagnetic field, the Schrödinger equation for this system is

$$[(1/2m)(p_\theta - qA_\theta/c)^2 + q\phi]\psi = i\hbar\partial\psi/\partial t, \tag{3.1}$$

where $\psi = \psi(\theta, t)$. When the canonical momentum $p_\theta = -i\hbar\rho^{-1}\partial/\partial\theta$, where $\rho = a$, is used in (3.1) along with (2.3) and (2.8), we obtain

$$\{(\hbar^2/2I)[-i\partial/\partial\theta - \alpha(t)g(\theta, t)]^2 + \hbar\dot\alpha(t)[\theta - f(\theta, t)] - \hbar\alpha(t)\dot f(\theta, t)\}\psi = i\hbar\partial\psi/\partial t, \tag{3.2}$$

where $I = ma^2$ is the moment of inertia and the dimensionless quantity $\alpha(t)$ is defined as

$$\alpha(t) = q\Phi(t)/2\pi\hbar c. \tag{3.3}$$

The Schrödinger equation in (3.1) is form invariant (Yang 1976, Kobe and Smirl 1978) under the gauge transformations in (2.10) and (2.11) if the wavefunction is also transformed,

$$\psi' = \exp(iq\Lambda/\hbar c)\psi. \tag{3.4}$$

For the gauge function (2.12), the new Schrödinger equation is the same form as (3.2) with ψ, g, and f replaced by ψ', g', and f', respectively. In the new gauge $g' = g + \lambda$ and f' is obtained from (2.9) with g replaced by g'.

A technique for solving (3.2) is to transform to the Coulomb gauge where $g' = 1$. A formal solution can then be obtained. This solution can be transformed back to the original gauge in (3.2). Instead of using this method, an expansion in terms of energy eigenfunctions will be used.

4. Energy eigenstates

In order to find the probability that the plane rotor is in an energy eigenstate, it is first necessary to define the energy operator (Yang 1976). The energy operator for a problem in a time-dependent electromagnetic field is not in general the Hamiltonian. The Hamiltonian has a gauge-dependent expectation value so it is not in general an observable. The energy operator, on the other hand, has a gauge-invariant expectation value whose time rate of change is equal to the average of the quantum mechanical power operator. The energy operator for a plane rotor is obtained in this section and its eigenvalue problem is solved. The Schrödinger equation is solved by making an eigenfunction expansion. The probability that the rotor is in an energy eigenstate is time independent.

4.1. Energy operator

The energy operator $\mathscr{E}$ for a plane rotor is

$$\mathscr{E} = (\hbar^2/2I)[-\mathrm{i}\partial/\partial\theta - \alpha(t)g(\theta, t)]^2, \tag{4.1}$$

which is the Hamiltonian in (3.2) without the scalar potential term $q\phi$ of the external time-dependent field in (2.8). The Hamiltonian and the energy operator for this time-dependent problem are in general different.

The eigenvalue problem for the energy operator $\mathscr{E}$ is

$$(\hbar^2/2I)[-\mathrm{i}\partial/\partial\theta - \alpha(t)g(\theta, t)]^2\psi_n = \varepsilon_n(t)\psi_n, \tag{4.2}$$

where $\psi_n = \psi_n(\theta, t)$ and time t is a parameter. The flux in (4.2) can depend on the time in an arbitrary way, and there is no restriction that it vary only adiabatically (Klein 1980). The solution to (4.2) is

$$\psi_n(\theta, t) = (2\pi)^{-1/2} \exp\{\mathrm{i}n\theta - \mathrm{i}\alpha(t)[\theta - f(\theta, t)]\}, \tag{4.3}$$

where n is an integer and ψ_n is normalised on $(0, 2\pi)$. Equation (4.3) is single valued,

$$\psi_n(0, t) = \psi_n(2\pi, t), \tag{4.4}$$

since $g(\theta, t)$ in (2.3) is single valued, $g(0, t) = g(2\pi, t)$. We have chosen the standard representation of the kinetic angular momentum in which the wavefunction is single valued, instead of representations with multivalued (or discontinuous) wavefunctions (Kretzschmar 1965, Kobe 1982b). The energy eigenvalue in (4.2) is

$$\varepsilon_n(t) = \hbar^2[n - \alpha(t)]^2/2I, \tag{4.5}$$

in which the time is a parameter.

The energy eigenstate in (4.3) is also an eigenstate of the z component of the kinetic angular momentum

$$L_z = \{\boldsymbol{r} \times (\boldsymbol{p} - q\boldsymbol{A}/c)\}_z = \hbar[-\mathrm{i}\partial/\partial\theta - \alpha(t)g(\theta, t)], \tag{4.6}$$

since L_z and $\mathscr{E}$ in (4.1) commute. The eigenvalue equation is

$$L_z\psi_n = \hbar[n - \alpha(t)]\psi_n. \tag{4.7}$$

The eigenvalue of the kinetic angular momentum is shifted from its value in the absence of flux by an amount which is proportional to the instantaneous flux.

4.2. *Solution to the Schrödinger equation*

By expanding the wavefunction $\psi(t)$ in terms of eigenstates of the energy operator and substituting it into the Schrödinger equation, we obtain an equation for the expansion coefficients which can be solved exactly. By substituting the expression for the expansion coefficients into the wavefunction expansion an exact solution to the Schrödinger equation is obtained.

The wavefunction ψ is expanded in terms of the eigenstates ψ_n of the energy operator

$$\psi(\theta, t) = \sum_n c_n(t)\psi_n(\theta, t), \tag{4.8}$$

where the expansion coefficients at time t are

$$c_n(t) = \langle\psi_n(t)\,|\,\psi(t)\rangle. \tag{4.9}$$

The expansion coefficients in (4.9) are also the probability amplitudes of finding the rotor in an energy eigenstate at the time t. Equation (4.9) is gauge invariant because under a gauge transformation ψ_n transforms in the same way as ψ does in (3.4).

If (4.8) is substituted into the Schrödinger equation in (3.2), we obtain

$$\mathrm{i}\hbar\dot{c}_n - \varepsilon_n(t)c_n = \sum_m \langle\psi_n\,|\,(q\phi - \mathrm{i}\hbar\partial/\partial t)\psi_m\rangle c_m, \tag{4.10}$$

with the help of (4.2). The matrix element on the right-hand side of (4.10) can be explicitly evaluated,

$$\langle\psi_n\,|\,(q\phi - \mathrm{i}\hbar\partial/\partial t)\psi_m\rangle = 0, \tag{4.11}$$

when (4.3) and (2.8) are used. Equation (4.10) thus becomes

$$\mathrm{i}\hbar\dot{c}_n - \varepsilon_n(t)c_n = 0, \tag{4.12}$$

the solution of which is

$$c_n(t) = \exp\left(-(\mathrm{i}/\hbar)\int_0^t \mathrm{d}t'\,\varepsilon_n(t')\right)c_n(0). \tag{4.13}$$

The initial wavefunction $\psi(\theta, 0)$ must be known to solve the time-dependent Schrödinger equation in (3.2), so $c_n(0)$ in (4.9) at time $t = 0$ is known.

The solution to the Schrödinger equation in (3.2) is then obtained by substituting (4.13) and (4.3) into (4.8), which gives explicitly

$$\psi(\theta, t) = \exp\{-\mathrm{i}\alpha(t)[\theta - f(\theta, t)]\} \times \sum_n c_n(0) \exp\left(-(\mathrm{i}/\hbar) \int_0^t \mathrm{d}t'\, \varepsilon_n(t')\right)(2\pi)^{-1/2} \exp(\mathrm{i}n\theta). \tag{4.14}$$

That (4.14) is a solution to the Schrödinger equation in (3.2) may be checked by direct substitution.

The probability for finding the system in the state n at time t is

$$P_n(t) = |c_n(t)|^2 = P_n(0), \tag{4.15}$$

by (4.13). If the plane rotor has a probability $P_n(0)$ of being in the state n at time zero, it will have the same probability for all time. There are no transitions between energy eigenstates no matter how the flux changes in time. Equation (4.15) is gauge invariant because (4.13) is gauge invariant.

5. Ehrenfest theorems

In this section generalised Ehrenfest theorems (Yang 1976) are used to show the relationship between quantum theory and classical theory for the plane rotor. The time rate of change of the expectation value of a periodic function of the angular displacement, the kinetic angular momentum operator, and the energy operator are considered.

5.1. Angular displacement

The analogue of the expectation value of linear displacement is the expectation value of the angular displacement $\langle\psi|\theta\psi\rangle$. The time rate of change of $\langle\psi|\theta\psi\rangle$ is not $\langle\psi|(L_z/I)\psi\rangle$ as one might expect, where L_z/I can be defined as the angular velocity operator. For L_z to be a self-adjoint operator the wavefunction ψ must be periodic with period 2π. Therefore the function $\theta\psi$ is not in the domain of the operator L_z (Biedenharn and Louck 1981).

Instead, we shall consider $\exp(\mathrm{i}\theta)$, which is a periodic function of θ, so that if ψ is in the domain of L_z so is $\exp(\mathrm{i}\theta)\psi$. It can be shown that

$$\mathrm{d}\langle\psi|\exp(\mathrm{i}\theta)\psi\rangle/\mathrm{d}t = \langle\psi|\mathrm{i}\exp(\mathrm{i}\theta/2)(L_z/I)\exp(\mathrm{i}\theta/2)\psi\rangle. \tag{5.1}$$

This equation is an Ehrenfest theorem corresponding to the classical equation for the time derivative of $\exp(\mathrm{i}\theta)$. In the classical case L_z commutes with $\exp(\mathrm{i}\theta/2)$ and we obtain the form expected classically. The operator $\exp(\mathrm{i}\theta)$ is not Hermitian, so it cannot be considered as an observable. To obtain Hermitian operators, the real and imaginary parts of (5.1) can be taken.

The real part of (5.1) gives

$$\mathrm{d}\langle\psi|\cos\theta\psi\rangle/\mathrm{d}t = -\langle\psi|[\sin(\theta/2)(L_z/I)\cos(\theta/2) + \cos(\theta/2)(L_z/I)\sin(\theta/2)]\psi\rangle. \tag{5.2}$$

In the classical case L_z commutes with $\cos(\theta/2)$ and $\sin(\theta/2)$, and we obtain $-\sin\theta(L_z/I)$, which is the form expected classically. The imaginary part of (5.1) gives

$$\mathrm{d}\langle\psi|\sin\theta\psi\rangle/\mathrm{d}t = \langle\psi|[\cos(\theta/2)(L_z/I)\cos(\theta/2) - \sin(\theta/2)(L_z/I)\sin(\theta/2)]\psi\rangle. \tag{5.3}$$

In the classical case where L_z commutes with $\cos(\theta/2)$ and $\sin(\theta/2)$, we obtain $\cos\theta(L_z/I)$ which is the form expected classically. All the operators in (5.2) and (5.3) are Hermitian. Therefore (5.2) and (5.3) are Ehrenfest theorems for sinusoidal functions of the angular displacement operator. Equation (5.1) is satisfied by the wavefunction in (4.8) which can be shown by direct substitution (see appendix, § A1).

5.2. *Kinetic angular momentum*

The z component of the kinetic angular momentum in (4.6) also satisfies a generalised Ehrenfest theorem (Yang 1976)

$$\mathrm{d}\langle\psi|L_z\psi\rangle/\mathrm{d}t=\langle\psi|\tau_z\psi\rangle. \tag{5.4}$$

In this case the z component of the torque operator, $\boldsymbol{\tau}=\boldsymbol{r}\times q\boldsymbol{E}$, is

$$\tau_z=\rho qE_\theta=-\hbar\dot{\alpha}(t), \tag{5.5}$$

by (2.6) and (3.3). Equation (5.5) is independent of the coordinates, and so the torque on the electron is the same regardless of the size of the orbit. Equation (5.4) is satisfied by the wavefunction in (4.8), which can be shown by direct substitution (see appendix, § A2).

5.3. *Energy*

The energy operator $\mathscr{E}$ in (4.1) can be written in terms of the z component of the kinetic angular momentum L_z in (4.6) as

$$\mathscr{E}=L_z^2/2I, \tag{5.6}$$

where $I=ma^2$ is the moment of inertia. Equation (5.6) has the same form as the classical energy, and is equal to the Hamiltonian only when the scalar potential of the time-dependent electromagnetic field vanishes. The energy operator also satisfies a generalised Ehrenfest theorem (Yang 1976)

$$\mathrm{d}\langle\psi|\mathscr{E}\psi\rangle/\mathrm{d}t=\langle\psi|P\psi\rangle. \tag{5.7}$$

The power operator P in this case is

$$P=qE_\theta v_\theta=\tau_zL_z/I, \tag{5.8}$$

where $v_\theta=\hat{\theta}\cdot\boldsymbol{v}$ is the azimuthal component of the velocity operator $\boldsymbol{v}=(\boldsymbol{p}-q\boldsymbol{A}/c)/m$, the torque operator τ_z is given in (5.5) and the kinetic angular momentum operator L_z is given in (4.6). By substituting (4.8) into (5.7) it can be shown to be satisfied (see appendix § A3).

6. Conventional procedure for probability amplitudes

The Schrödinger equation in (3.2) is the equation for a charged particle in a time-dependent electromagnetic field. The conventional procedure for solving such problems is to expand the quadratic term in the Hamiltonian, and treat all the time dependence as a perturbation (Schiff 1968). This procedure destroys the manifest gauge invariance of the Schrödinger equation. When the wavefunction is expanded in terms of the eigenstates of the unperturbed Hamiltonian H_0, the expansion coefficients are dependent on the choice of the gauge, and cannot be interpreted in general as probability amplitudes (Yang 1982).

6.1. Expansion coefficients

The quadratic term in the Hamiltonian in (3.2) can be expanded, which gives the Schrödinger equation

$$\{H_0+(\mathrm{i}\hbar^2/I)\alpha(t)g(\theta,t)\partial/\partial\theta+(\mathrm{i}\hbar^2/2I)\alpha(t)\partial g(\theta,t)/\partial\theta+(\hbar^2/2I)[\alpha(t)g(\theta,t)]^2 \\ +\hbar\dot{\alpha}(t)[\theta-f(\theta,t)]-\hbar\alpha(t)\dot{f}(\theta,t)\}\psi=\mathrm{i}\hbar\partial\psi/\partial t. \quad (6.1)$$

The unperturbed Hamiltonian H_0 in (6.1) is

$$H_0=-(\hbar^2/2I)\partial^2/\partial\theta^2, \quad (6.2)$$

which is the Hamiltonian of a plane rotor in the absence of flux in a gauge in which the potentials are zero. The eigenvalue problem for the unperturbed Hamiltonian is

$$-(\hbar^2/2I)\partial^2\phi_n/\partial\theta^2=e_n\phi_n. \quad (6.3)$$

The eigenfunctions ϕ_n in (6.3) are

$$\phi_n(\theta)=(2\pi)^{-1/2}\exp(\mathrm{i}n\theta), \quad (6.4)$$

where n is an integer, which are single valued and normalised on $(0,2\pi)$. The eigenvalue e_n in (6.3) is

$$e_n=(n\hbar)^2/2I, \quad (6.5)$$

which is the energy of the plane rotor in the absence of magnetic flux.

In the conventional procedure, the wavefunction $\psi(\theta,t)$ in (6.1) is expanded in terms of the eigenfunctions of the unperturbed Hamiltonian

$$\psi=\sum_n a_n\phi_n, \quad (6.6)$$

where the expansion coefficients a_n are

$$a_n(t)=\langle\phi_n|\psi(t)\rangle. \quad (6.7)$$

When (6.6) is substituted into (6.1) and the resulting equation is simplified, the equation for the expansion coefficients is

$$\mathrm{i}\hbar\dot{a}_n-e_na_n=\sum_k\langle\phi_n|\{(\mathrm{i}\hbar^2/I)\alpha(t)g(\theta,t)\partial/\partial\theta \\ +(\mathrm{i}\hbar^2/2I)\alpha(t)\partial g(\theta,t)/\partial\theta+(\hbar^2/2I)[\alpha(t)g(\theta,t)]^2 \\ +\hbar\dot{\alpha}(t)[\theta-f(\theta,t)]-\hbar\alpha(t)\dot{f}(\theta,t)\}\phi_k\rangle a_k. \quad (6.8)$$

The solution to this equation depends on the arbitrary function g, so it depends on the gauge chosen. If (6.8) is solved exactly subject to the initial conditions and substituted into (6.6) a correct solution of the Schrödinger equation is obtained.

The exact solution to (6.8) gives the expansion coefficients in (6.7), where ψ is the solution to the Schrödinger equation in (3.2). The expansion coefficient a_n depends on the gauge because the wavefunction ψ depends on the gauge. Conventionally $|a_n(t)|^2$ is interpreted as the probability for finding the rotor in the state ϕ_n. Since $|a_n(t)|^2$ is gauge dependent, different results for the same physical quantity are obtained in different gauges. The answer to this dilemma is that eigenfunctions of the unperturbed Hamiltonian do not have any physical significance for the problem because H_0 is not an operator corresponding to an observable. It is only meaningful to obtain the probability that the rotor is in an eigenstate of an operator corresponding to an observable, like the energy (Kobe and Wen 1980, 1982). The probability amplitude that the rotor is in an eigenstate n of the energy operator is given in (4.9). It is not equal to (6.7) except when the latter is in the Coulomb gauge.

6.2. Coulomb gauge

In the Coulomb gauge the conventional approach to time-dependent problems simplifies, and the expansion coefficients become the gauge-invariant probability amplitudes of (4.9). This simplification occurs because the Hamiltonian and the energy operator are the same in the Coulomb gauge. The Coulomb gauge condition is $\nabla \cdot \boldsymbol{A}^{c} = 0$, where the superscript c indicates the Coulomb gauge. Equation (2.3) shows that in the Coulomb gauge $g^{c} = 1$ and (2.9) shows that $f^{c} = \theta$. The scalar potential in (2.8) in the Coulomb gauge is $\phi^{c} = 0$.

The eigenfunctions ψ_n^{c} of the energy operator in the Coulomb gauge are

$$\psi_n^{c} = \phi_n, \tag{6.9}$$

from (4.3) and (6.4). Thus in the Coulomb gauge the conventional expansion coefficient in (6.7) becomes

$$a_n^{c}(t) = \langle \psi_n^{c} | \psi^{c}(t) \rangle = c_n(t), \tag{6.10}$$

which is equal to the gauge-invariant probability amplitude in (4.9) for all times.

Even though the probability amplitudes are the same for the conventional procedure in the Coulomb gauge and the gauge-invariant procedure, the unperturbed energy in (6.5) does not depend on the flux. The equation of motion for the expansion coefficients $a_n^{c}(t)$ in the Coulomb gauge is obtained from (6.8) by using $g^{c} = 1$, which gives

$$\mathrm{i}\hbar \dot{a}_n^{c} - e_n a_n^{c} = \sum_k [(\mathrm{i}\hbar^2/I)\alpha(t)\langle \phi_n | (\partial/\partial\theta)\phi_k \rangle + (\hbar^2/2I)\alpha(t)^2 \langle \phi_n | \phi_k \rangle] a_k^{c}. \tag{6.11}$$

When (6.4) is substituted into (6.11) and the orthonormality of the eigenstates is used, we obtain

$$\mathrm{i}\hbar \dot{a}_n^{c} - \varepsilon_n(t) a_n^{c} = 0, \tag{6.12}$$

where $\varepsilon_n(t)$ is given in (4.5). The energy e_n in (6.11) becomes 'dressed' by the terms in the sum for which $k = n$ to give $\varepsilon_n(t)$. Equation (6.12) is the same as (4.12), and the solution is also (4.13) since $a_n^{c} = c_n$ by (6.10). In the Coulomb gauge ($g^{c} = 1$), and in this gauge only, the conventional procedure agrees with the gauge-invariant procedure.

7. Conclusion

The problem of a quantum mechanical plane rotor with time-dependent magnetic flux on the axis is solved exactly. The energy eigenvalues, probabilities, and expectation values of observables are all manifestly gauge invariant. The time-varying magnetic flux on the axis induces an electric field on the electron by Faraday's law. The induced electric field exerts a torque and does work on the electron. Consequently, the kinetic angular momentum and energy, respectively, of the electron are changed in agreement with generalised Ehrenfest theorems.

The plane rotor with time-dependent magnetic flux on its axis is an excellent model to use to illustrate the manifestly gauge-invariant formulation of quantum mechanics (Yang 1976, Kobe and Smirl 1978). The problem is solved exactly, and the results of the manifestly gauge-invariant formulation are compared with a conventional approach using eigenstates of the unperturbed Hamiltonian. A comparison with the adiabatic approximation, which uses eigenstates of the total Hamiltonian, can also be made. Only in the Coulomb gauge do the results of the different methods for the rotor agree, because in this gauge the Hamiltonian reduces to the energy operator. Since the Coulomb gauge is often used in practice, the gauge dependence of the conventional approach and the adiabatic approximation has not been fully appreciated (Aharonov and Au 1981).

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Appendix. Verification of Ehrenfest theorems

The three Ehrenfest theorems in equations (5.1), (5.4), and (5.7) are verified here using the wavefunction in (4.8).

A1. Angular displacement

Using equation (4.8) we find that the expectation value of $\exp(\mathrm{i}\theta)$ is

$$\langle\psi\,|\,\exp(\mathrm{i}\theta)\psi\rangle=\sum_n c_n^*(t)c_{n-1}(t), \qquad \text{(A1)}$$

if use is made of the orthonormality of the energy eigenstates in (4.3). The time rate of change of (A1) is

$$\mathrm{d}\langle\psi\,|\,\exp(\mathrm{i}\theta)\psi\rangle/\mathrm{d}t=\sum_n [\dot{c}_n^*(t)c_{n-1}(t)+c_n^*(t)\dot{c}_{n-1}(t)]. \qquad \text{(A2)}$$

When (4.13) and (4.5) are substituted into (A2) we obtain

$$\mathrm{d}\langle\psi\,|\,\exp(\mathrm{i}\theta)\psi\rangle/\mathrm{d}t=\mathrm{i}\sum_n \hbar(n-\alpha-\tfrac{1}{2})I^{-1}c_n^*(t)c_{n-1}(t). \qquad \text{(A3)}$$

The right-hand side of (A3) is the same as the right-hand side of (5.1) when (4.7) and (4.8) are used in it. Therefore we have verified (5.1) for the wavefunction in (4.8).

A2. Kinetic angular momentum

The expectation value of the z component of the kinetic angular momentum with respect to $\psi(t)$ in (4.8) at time t is

$$\langle\psi(t)|L_z\psi(t)\rangle=\sum_n \hbar[n-\alpha(t)]|c_n(0)|^2, \tag{A4}$$

from (4.7) and (4.13). The time derivative of (A4) gives

$$\mathrm{d}\langle\psi|L_z\psi\rangle/\mathrm{d}t=-\hbar\dot{\alpha}(t), \tag{A5}$$

which is the same as (5.4) when (5.5) is used.

A3. Energy

The expectation value of the energy operator $\mathscr{E}$ in (4.1) with respect to ψ in (4.8) is

$$\langle\psi(t)|\mathscr{E}\psi(t)\rangle=\sum_n \varepsilon_n(t)|c_n(0)|^2, \tag{A6}$$

from (4.2) and (4.13). When the time derivative of (A6) is taken and the energy eigenvalues in (4.5) are used, we obtain

$$\mathrm{d}\langle\psi(t)|\mathscr{E}\psi(t)\rangle/\mathrm{d}t=-\sum_n \hbar\dot{\alpha}(t)[\hbar(n-\alpha(t))/I]|c_n(0)|^2. \tag{A7}$$

Equations (5.5) and (A4) show that the right-hand side of (A7) is the same as the right-hand side of (5.7) with the power operator given by (5.8).

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