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Gauge invariance in quantum mechanics: charged harmonic oscillator in the magnetic dipole approximation†

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Abstract. A manifestly gauge-invariant formulation of quantum mechanics is applied to a charged isotropic harmonic oscillator in a time-varying magnetic field in the magnetic dipole approximation. The energy operator for the problem is the sum of the kinetic and potential energies. The kinetic energy operator is the square of the gauge-invariant kinetic momentum operator divided by twice the mass. The energy eigenvalues and state probabilities are calculated and are shown to be the same in all gauges. In this problem there is no gauge in which the energy operator reduces to the unperturbed Hamiltonian, as there is in the electric dipole approximation. Consequently, eigenvalues of the unperturbed Hamiltonian and corresponding (gauge-dependent) state 'probabilities' are different from the gauge-invariant quantities in all gauges.

1. Introduction

One of the most fundamental principles of physics is gauge invariance. Only recently, however, has a manifestly gauge-invariant formulation of the quantum mechanics of a charged particle interacting with a time-varying classical electromagnetic field been given (Yang 1976, Kobe 1978, Kobe and Smirl 1978, Kobe and Yang 1980). In this formulation the eigenvalue problem for the gauge-invariant energy operator is solved to give the appropriate energy eigenvalues and eigenstates. The energy operator is the sum of the kinetic and potential energy operators. The kinetic energy is the kinetic or mechanical momentum operator squared divided by twice the mass. The kinetic or mechanical momentum is $\boldsymbol{p} - q\boldsymbol{A}/c$, where $\boldsymbol{p} = -i\hbar\nabla$ is the canonical momentum operator, $\boldsymbol{A}$ is the vector potential, q is the charge and c is the speed of light, which has a gauge-invariant expectation value. The kinetic momentum operator and consequently the kinetic energy operator depend on the time if the vector potential depends on time. Therefore the energy eigenvalues and eigenstates in general depend on the time as a parameter.

To illustrate the gauge-invariant approach to quantum mechanics, Kobe and Wen (1980, 1982) solved the Schrödinger equation exactly for a charged harmonic oscillator in an electromagnetic field in the electric dipole approximation. Questions of principle could thus be separated from approximations. They calculated the probabilities of finding the oscillator in excited states as a function of time, if the oscillator was initially in the ground state. These probabilities were compared with those calculated from a conventional approach (Schiff 1968 (pp 398–403), Merzbacher 1970 (pp 451–63)) using the unperturbed Hamiltonian H_0 and the conventional interaction $\boldsymbol{p} \cdot \boldsymbol{A}$ plus

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$\boldsymbol{A} \cdot \boldsymbol{p}$ plus A^2 (constants omitted). The probabilities were different as long as the electric field remained on and the principle of gauge invariance implies that the probabilities calculated in the gauge-invariant way are correct.

The gauge-invariant approach can be used in any gauge. However, in the electric dipole approximation there is a gauge, called the electric field gauge, in which the vector potential is zero and the scalar potential is $-\boldsymbol{E} \cdot \boldsymbol{r}$, where $\boldsymbol{E}$ is the electric field and $\boldsymbol{r}$ is the displacement of the electron. In this gauge the kinetic momentum reduces to the canonical momentum and the energy operator reduces to the unperturbed Hamiltonian H_0. The calculations are simplified in this gauge. Because the energy operator reduces to the unperturbed Hamiltonian in the electric field gauge, the distinction between these two operators has not been appreciated (Aharonov and Au 1981).

To avoid any misunderstanding of the gauge-invariant formulation, it is desirable to find a model in which the energy operator does not reduce to the unperturbed Hamiltonian in any gauge. Such a model is the charged isotropic harmonic oscillator in the *magnetic* dipole approximation (MDA), in which the magnetic field is varying in time. The energy eigenvalue equation for this problem can be solved exactly, although the time-dependent Schrödinger equation can be solved only approximately. The standard approaches to this problem use perturbation theory when the magnetic field is rapidly varying in time but weak or use eigenstates of the total Hamiltonian when the magnetic field is strong but slowly (adiabatically) varying in time (Schiff 1968, pp 289–90). The gauge-invariant procedure can be applied in principle when the magnetic field is both rapidly varying and strong.

In most magnetic field problems a static magnetic field is applied to 'quantise' the energy levels, and a weak time-varying magnetic (or electromagnetic) field is used as a probe (Bergou and Ehlotzky 1982, Bergou and Varró 1982). When the magnetic field is both strong and time varying, the same field acts as the quantising and probe field (Anosov 1980). This magnetic field 'quantises' the energy levels and shifts them due to a dynamic or AC Zeeman effect (Gallagher and Cocker 1979). The energy eigenvalues are 'dressed' by the time-varying magnetic field. The same field 'probes' the system by inducing transitions between the 'dressed' eigenstates. The gauge-invariant procedure is thus able to deal with a new class of problems, which is illustrated here with the harmonic oscillator in the MDA. The energy eigenvalues and state probabilities calculated using the gauge-invariant energy operator are different from those calculated in any gauge using the unperturbed Hamiltonian while the magnetic field remains on.

In § 2 the gauge-invariant formulation of quantum mechanics is reviewed briefly. The gauge-invariant solution of the charged harmonic oscillator in the MDA is given in § 3. The conventional approach is reviewed in § 4 and applied to the charged harmonic oscillator in the MDA in § 5. The conclusions are given in § 6.

2. Gauge-invariant formulation

In this section the gauge-invariant formulation of quantum mechanics (Yang 1976, Kobe 1978, Kobe and Smirl 1978) is reviewed. After a brief discussion of the gauge invariance of the Schrödinger equation, the energy operator is defined and the energy eigenvalue equation is discussed. The probability amplitudes for finding the system in energy eigenstates are defined and their equation of motion is obtained.

2.1. Gauge invariance of the Schrödinger equation

The Hamiltonian for a charged particle of mass m and charge q interacting with an electromagnetic field characterised by vector potential $\boldsymbol{A}$ and scalar potential A_0 is

$$H(\boldsymbol{A}, A_0) = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A}/c)^2 + V + qA_0 \tag{2.1}$$

where $\boldsymbol{p} = -i\hbar\nabla$ is the canonical momentum operator. The potential energy V is prescribed for the problem, and is due to a static external field. Since the field is conservative, the potential energy is unique up to a constant. The scalar potential A_0 and the vector potential $\boldsymbol{A}$ are associated with a time-varying electromagnetic field and a static magnetic field, if present. Since a static electric field is a conservative field, its potential is included in V. The vector and scalar potentials are related to the magnetic induction field by $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ and the electric field by $\boldsymbol{E} = -\nabla A_0 - \partial \boldsymbol{A}/\partial(ct)$, as usual. The Schrödinger equation for the particle is

$$H(\boldsymbol{A}, A_0)\psi = i\hbar\partial\psi/\partial t. \tag{2.2}$$

Using the gauge function Λ, which is a function of space and time, we can make a gauge transformation on the wavefunction:

$$\psi' = \exp(iq\Lambda/\hbar c)\psi. \tag{2.3}$$

The corresponding gauge transformation of the potentials is

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda \tag{2.4}$$

and

$$A_0' = A_0 - \partial\Lambda/\partial(ct). \tag{2.5}$$

If equations (2.3), (2.4) and (2.5) are solved for ψ, $\boldsymbol{A}$ and A_0, respectively, and substituted into equation (2.2), we obtain the new Schrödinger equation

$$H(\boldsymbol{A}', A_0')\psi' = i\hbar\partial\psi'/\partial t. \tag{2.6}$$

The Schrödinger equation is therefore form invariant under gauge transformations.

2.2. Energy eigenvalue equation

An operator is gauge invariant if its expectation value is the same in all gauges. The Hamiltonian $H(\boldsymbol{A}, A_0)$ in equation (2.1) has a gauge-dependent expectation value, so it cannot be the energy. However, a gauge-invariant energy operator $\mathscr{E}(\boldsymbol{A})$ can be defined as (Yang 1976, Kobe 1978)

$$\mathscr{E}(\boldsymbol{A}) = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A}/c)^2 + V, \tag{2.7}$$

which is the Hamiltonian in equation (2.1) minus the scalar potential term qA_0. Equation (2.7) is the kinetic energy plus the potential energy. The kinetic energy is the square of the gauge-invariant kinetic momentum $\boldsymbol{p} - q\boldsymbol{A}/c$ divided by twice the mass. The time rate of change of the expectation value of the energy operator is the power supplied to the particle by the external time-varying electromagnetic field (Yang 1976).

The eigenvalue equation for the energy operator is

$$\mathscr{E}(\boldsymbol{A})\psi_n(t) = \varepsilon_n(t)\psi_n(t) \tag{2.8}$$

where ψ_n is an energy eigenstate and ε_n is an energy eigenvalue characterised by the quantum number n. The time t is treated as a parameter in equation (2.8). Using equations (2.7), (2.4) and (2.3), we can make a gauge transformation on equation (2.8) and obtain

$$\mathscr{E}(\boldsymbol{A}')\psi_n'(t) = \varepsilon_n(t)\psi_n'(t). \tag{2.9}$$

Equation (2.8) is thus form invariant under gauge transformations and the energy eigenvalues ε_n are gauge invariant.

2.3. Probability amplitudes

The probability amplitude for finding the system in an eigenstate ψ_n of the energy operator at time t is

$$c_n(t) = \langle\psi_n(t)|\psi(t)\rangle. \tag{2.10}$$

This expression is gauge invariant, since both ψ and ψ_n transform as in equation (2.3). The probability for finding the system in the state characterised by the quantum number n is $P_n(t) = |c_n(t)|^2$.

If equation (2.10) is differentiated with respect to time and equations (2.2) and (2.9) are used, the result is

$$i\hbar\dot{c}_n - \varepsilon_n c_n = \sum_m \langle\psi_n|(qA_0 - i\hbar\partial/\partial t)\psi_m\rangle c_m. \tag{2.11}$$

As shown previously (Kobe and Smirl 1978), the matrix element in equation (2.11) is invariant under gauge transformations as are ε_n and c_n, so equation (2.11) is also gauge invariant.

3. Gauge-invariant solution to the harmonic oscillator in the magnetic dipole approximation

The formulation of § 2 is applied here to a three-dimensional isotropic harmonic oscillator interacting with a time-varying magnetic field in the magnetic dipole approximation (MDA). The potentials in the MDA in different gauges are given. Then the energy eigenvalue problem is solved exactly in the MDA. Finally, the transitions induced by the time-varying magnetic field are discussed.

3.1. Magnetic dipole approximation

The magnetic induction field $\boldsymbol{B}(t) = B(t)\hat{z}$ is assumed to be uniform in space and varying in time. The direction of the field $\hat{z}$ is taken to be the z direction which gives the system cylindrical symmetry. For a magnetic induction field $\boldsymbol{B}(t)$, a vector potential in the magnetic dipole approximation (MDA) is

$$\boldsymbol{A} = -\tfrac{1}{2}\boldsymbol{r}\times\boldsymbol{B}(t), \tag{3.1}$$

which is the first term in the multipole expansion (Kobe 1982). The scalar potential

in general has electric dipole and quadrupole terms. We assume that the time variation of the magnetic field is sufficiently slow to make the effect of the electric field negligible. In this model any transitions and energy level perturbations arising from the matrix element of the scalar potential in equation (2.11) are neglected. We thus assume in this gauge that the scalar potential $A_0 = 0$.

Equation (3.1) and $A_0 = 0$ are the potentials in the symmetric gauge in the MDA. Other gauges can also be used in the MDA. The vector potential in the mixed gauge is (Larsen 1982)

$$\boldsymbol{A}'(t) = -\xi B(t) y\hat{x} + (1-\xi)B(t)x\hat{y} \tag{3.2}$$

where the parameter ξ is any real number. The magnetic induction field $\boldsymbol{B}(t) = \boldsymbol{\nabla}\times\boldsymbol{A}'(t)$ and $\boldsymbol{\nabla}\cdot\boldsymbol{A}'(t) = 0$. Using equations (3.1) and (3.2) in equation (2.4), we can find the gauge function Λ which will produce a transformation from the symmetric gauge to the mixed gauge:

$$\Lambda = (\tfrac{1}{2} - \xi)B(t)xy. \tag{3.3}$$

Using equation (3.3) and $A_0 = 0$ in equation (2.5) the scalar potential in the mixed gauge is

$$A_0' = (\xi - \tfrac{1}{2})\dot{B}(t)xy/c. \tag{3.4}$$

There are an infinite number of different gauges in the MDA because ξ in equations (3.2) and (3.4) is arbitrary. Special cases are $\xi = \frac{1}{2}$, which yields the symmetric gauge, and $\xi = 1$ or 0, which yields the two Landau gauges.

3.2. Energy eigenvalue problem

The eigenvalue problem in equation (2.8) can be solved exactly in any gauge. However, the solution is simplest in the symmetric gauge in equation (3.1) because of cylindrical symmetry. In this gauge the energy operator happens to be the Hamiltonian since the scalar potential is zero. However, if another gauge had been chosen the Hamiltonian and the energy operator would have been different because the scalar potential in equation (3.4) is not zero. Eigenvalues of the energy operator are gauge invariant while eigenvalues of the Hamiltonian are not. It is important to make the distinction between the energy operator and the Hamiltonian in an arbitrary gauge.

For a three-dimensional isotropic harmonic oscillator of charge q, mass m and frequency ω_0, the potential energy is $V = \frac{1}{2}m\omega_0^2 r^2$. The energy operator in equation (2.2) is

$$\mathscr{E}(\boldsymbol{A}) = p^2/2m + \tfrac{1}{2}m\omega_0^2 r^2 - qB(t)L_z/2mc + q^2B^2(t)(x^2+y^2)/8mc^2. \tag{3.5}$$

By transforming to cylindrical coordinates we can take advantage of the cylindrical symmetry of the system. With the energy operator in equation (3.5), equation (2.8) becomes

$$\left\{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \tfrac{1}{2}m\omega_0^2 z^2\right) + \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + \tfrac{1}{2}m\omega^2\rho^2 - i\hbar\omega_L\frac{\partial}{\partial\phi}\right]\right\}\psi_{nl\mu}(t)$$
$$= \varepsilon_{nl\mu}(t)\psi_{nl\mu}(t). \tag{3.6}$$

In equation (3.6) ω_L is the Larmor frequency

$$\omega_L(t) = -qB(t)/2mc. \tag{3.7}$$

(for an electron $q = -e$) and

$$\omega = (\omega_0^2 + \omega_L^2)^{1/2} \tag{3.8}$$

is the 'dressed' frequency of the oscillator in the presence of the field.

The energy operator in equation (3.6) is the sum of two commuting parts. The first part is the energy operator for a one-dimensional harmonic oscillator in the z direction parallel to the field at the unperturbed frequency ω_0. The second part is the energy operator for a two-dimensional oscillator perpendicular to the field at the field-shifted frequency ω and a Zeeman term. The solution to equation (3.6) can be written as

$$\psi_{nl\mu}(t) = \psi_l(z)\psi_{n\mu}(\rho, \phi, t). \tag{3.9}$$

In equation (3.9) $\psi_l(z)$ is a one-dimensional harmonic oscillator wavefunction:

$$\psi_l(z) = 2^{-l/2}(l!)^{-1/2}(m\omega_0/\pi\hbar)^{1/4} \exp(-\tfrac{1}{2}\zeta^2)H_l(\zeta) \tag{3.10}$$

where $\zeta = (m\omega_0/\hbar)^{1/2}z$ and H_l is a Hermite polynomial. The wavefunction $\psi_{n\mu}(\rho, \phi, t)$ in equation (3.9) is the solution to a two-dimensional harmonic oscillator (Landau and Lifshitz 1977, p 459):

$$\psi_{n\mu}(\rho, \phi, t) = (m\omega/\pi\hbar)^{1/2}[n!/(n+|\mu|)!]^{1/2}\eta^{|\mu|} \exp(-\tfrac{1}{2}\eta^2)L_n^{|\mu|}(\eta^2) \exp(i\mu\phi) \tag{3.11}$$

where $\eta = (m\omega/\hbar)^{1/2}\rho$ and $L_n^{|\mu|}$ is an associated Laguerre polynomial.

The energy eigenvalues in equation (3.6) are (ter Haar 1964, pp 35 and 236)

$$\varepsilon_{nl\mu}(t) = \hbar\omega_0(l + \tfrac{1}{2}) + \hbar\omega(2n + |\mu| + 1) + \hbar\omega_L\mu \tag{3.12}$$

where the quantum numbers n, l, μ can take on the values $n, l = 0, 1, 2, \ldots$ and $\mu = 0, \pm 1, \pm 2, \ldots$. There are three contributions to the energy in equation (3.12). The first term on the right-hand side of equation (3.12) is the energy of an unperturbed one-dimensional oscillator, the second term is the energy of a perturbed two-dimensional oscillator and the last term is a Zeeman energy. Since the Larmor frequency in the Zeeman term is time dependent, this model exhibits a dynamic or AC Zeeman effect (Gallagher and Cocker 1979).

3.3. Probability amplitudes

Having solved the eigenvalue equation, we can now obtain the equation of motion for the probability amplitudes in equation (2.10). If the eigenfunctions in equation (3.9) are substituted into equation (2.11), and the matrix element is evaluated, we obtain

$$i\hbar\dot{c}_{nl\mu} - \varepsilon_{nl\mu}c_{nl\mu} = -iK(t)[(n+1)(n+|\mu|+1)]^{1/2}c_{n+1,l,\mu} + iK(t)[n(n+|\mu|)]^{1/2}c_{n-1,l,\mu} \tag{3.13}$$

where

$$K(t) = (\hbar q\omega_L(t)/4\omega^2(t)mc)\dot{B}(t). \tag{3.14}$$

Equation (3.13) shows that there are transitions from the state (n, l, μ) up to the state $(n+1, l, \mu)$ and down to the state $(n-1, l, \mu)$. The probability of transitions depends

on the function $K(t)$ which is proportional to the time derivative $\dot{B}(t)$ of the magnetic field. Thus for a static magnetic field there would be no transitions.

3.4. Approximate solution

Equation (3.13) is too difficult to solve exactly, but it can be solved approximately for certain special cases. As an example, we take the case where $l = \mu = 0$, $\omega_0 \gg \omega_L$ (weak fields) and where the field is given by

$$B(t) = B_0 \sin(\omega_1 t). \tag{3.15}$$

For this case equation (3.13) becomes

$$\dot{c}_n = -i\omega_0(n + \tfrac{3}{2})c_n + \lambda\omega_1 \sin(2\omega_1 t)(n+1)c_{n+1} - \lambda\omega_1 \sin(2\omega_1 t)nc_{n-1} \tag{3.16}$$

where

$$\lambda = (qB_0/4\omega_0 mc)^2 \tag{3.17}$$

and we have set $c_n = c_{n00}$.

Equation (3.16) can be solved approximately using time-dependent perturbation theory. We assume that the system is in the ground state at time zero, so $c_n(0) = \delta_{n0}$. If second-order perturbation theory is used, the system cannot be excited above the second excited state, so the higher excited states are unoccupied. In second order the probability amplitude in the rotating wave approximation (Sargent *et al* 1974, p 18) is

$$c_0(t) = 1 + [\lambda\omega_1/2(2\omega_1 - \omega_0)]^2 (\exp[i(2\omega_1 - \omega_0)t] - 1) + \ldots \tag{3.18}$$

for the ground state,

$$c_1(t) = [\lambda\omega_1/2(2\omega_1 - \omega_0)](\exp[-i(2\omega_1 - \omega_0)t] - 1) + \ldots \tag{3.19}$$

for the first excited state and

$$c_2(t) = [\lambda\omega_1/2(2\omega_1 - \omega_0)]^2(2 - 2\exp[-i(2\omega_1 - \omega_0)t] + \exp[-2i(2\omega_1 - \omega_0)t] - 1) + \ldots . \tag{3.20}$$

for the second excited state. We have omitted 'secular' terms (Langhoff *et al* 1972) which arise from the expansion of a time-dependent phase factor $\exp\{-i[\lambda^2\omega_1^2 t/4(2\omega_1 - \omega_0)]\}$. Since a phase factor does not change the probability $|c_n|^2$, such secular terms do not contribute to the overall probability of a state being occupied.

For the values $\lambda = 0.01$, $\omega_1 = 55$ rad s^{-1} and $\omega_0 = 109$ rad s^{-1}, the probability of finding the oscillator in the states $n = 0$, 1, and 2 as a function of time is shown in figure 1. The system begins in the ground state and the excited states become populated as the ground state is depleted. The system then returns to its ground state as the excited states are depleted. Since this behaviour is periodic, it is reminiscent of Rabi flopping (Sargent *et al* 1974, pp 25–7).

Because we have only gone to second order in perturbation theory, the sum of the probabilities of the three occupied states is not exactly one (Merzbacher 1970, p 418), but $1 + g^4 F(t)$ where $g = \lambda\omega_1/2(2\omega_1 - \omega_0)$ and $F(t)$ is a function of time. For the parameters chosen the value of the sum varies in time from 1 to 1.14. Having analysed the system using the gauge-invariant formulation, we shall now consider the conventional approach.

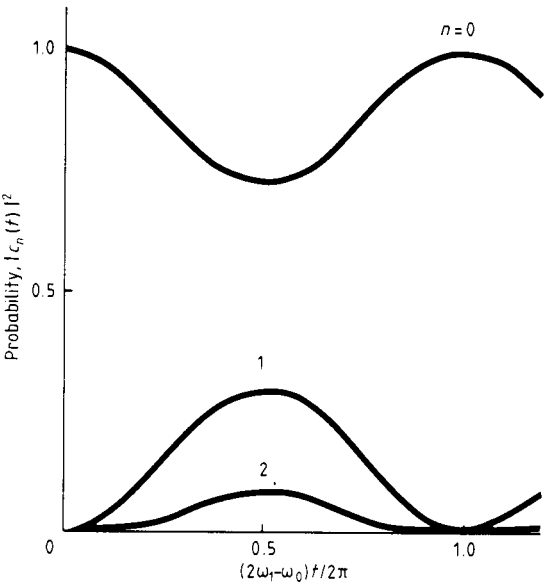

Figure 1. A plot of probability $|c_n(t)|^2$ as a function of $(2\omega_1-\omega_0)t/2\pi$ for $n=0$, 1 and 2.

4. Conventional approach

In this section we review the conventional approach to the interaction of electromagnetic radiation and matter (Schiff 1968 (pp 398–403), Merzbacher 1970 (pp 458–63)). In the conventional approach the quadratic term in equation (2.1) is expanded and the Schrödinger equation becomes

$$(H_0+\mathcal{V}(t))\psi = i\hbar\partial\psi/\partial t. \tag{4.1}$$

The perturbation term $\mathcal{V}(t)$ contains the time-dependent potentials

$$\mathcal{V}(t) = -(q/2mc)(\boldsymbol{A}\cdot\boldsymbol{p}+\boldsymbol{p}\cdot\boldsymbol{A})+q^2A^2/2mc^2+qA_0. \tag{4.2}$$

The unperturbed Hamiltonian H_0 is

$$H_0 = p^2/2m + V \tag{4.3}$$

which satisfies the eigenvalue equation

$$H_0\phi_n = e_n\phi_n \tag{4.4}$$

with eigenfunction ϕ_n and eigenvalue e_n. Perturbation theory or other methods can be used to solve equation (4.1) for ψ. To find the probability that the system is in an energy eigenstate while the magnetic field remains on, the energy eigenvalue problem in equation (2.8) must be solved and the wavefunction ψ used in equation (2.10) for the probability amplitude. This approach is the correct one to use while the vector potential is non-zero, since then there is a difference between the energy operator and H_0 in equation (4.3).

A common misunderstanding of the conventional approach is to interpret the squared modulus of the amplitude

$$a_n = \langle\phi_n|\psi(t)\rangle \tag{4.5}$$

as the probability of finding the particle in an energy eigenstate at time t. When the magnetic field is present at time t, $|a_n(t)|^2$ is not the probability that the particle is in an energy eigenstate, because H_0 is not the appropriate energy operator for the particle. If, however, the magnetic field were switched off and a gauge in which the potential is zero were used, the energy operator in equation (2.7) would reduce to H_0 in equation (4.3). In this case equations (2.10) and (4.5) would be equal (Leubner and Zoller 1980). It is essential to use the appropriate energy eigenstate at time t. The absolute value squared of equation (2.10) gives the correct probability at all times that the particle is in an energy eigenstate.

The equation for the conventional amplitude a_n can be obtained by taking the time derivative of equation (4.5) and using equation (4.1), which gives

$$i\hbar\dot{a}_n - e_n a_n = \sum_m \langle\phi_n|\mathcal{V}(t)\phi_m\rangle a_m. \tag{4.6}$$

The matrix element in equation (4.6) is gauge dependent since it contains the gauge-dependent potentials. In general, therefore, the amplitudes a_n are gauge dependent and cannot be valid probability amplitudes for finding the system in an energy eigenstate.

5. Conventional solution to the harmonic oscillator in the magnetic dipole approximation

The conventional approach of § 4 is now applied to the charged harmonic oscillator in the magnetic dipole approximation (MDA). Calculations are first made using the symmetric gauge and compared with the gauge-invariant calculations of § 3. Then the mixed gauge is used to demonstrate the gauge dependence of the conventional approach.

5.1. Energy eigenvalue problem

The eigenvalue problem for the unperturbed Hamiltonian H_0 is the same in any gauge. For a three-dimensional isotropic harmonic oscillator of charge q, mass m and frequency ω_0, in cylindrical coordinates, equation (4.4) becomes

$$\left\{\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+\tfrac{1}{2}m\omega_0^2 z^2\right)+\left[\frac{-\hbar^2}{2m}\left(\frac{\partial}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+\tfrac{1}{2}m\omega_0^2\rho^2\right]\right\}\phi_{nl\mu}=e_{nl\mu}\phi_{nl\mu}. \tag{5.1}$$

Comparing equation (5.1) with equation (3.6) we see that the equations are similar except for the Zeeman term in equation (3.6) and the frequency ω in equation (3.6) for the two-dimensional oscillator instead of ω_0 in equation (5.1). The solutions of equation (5.1) are the product of equations (3.10) and (3.11) with ω replaced by ω_0 in equation (3.11). The energy eigenvalue $e_{nl\mu}$ in equation (5.1) is

$$e_{nl\mu}=\hbar\omega_0(l+\tfrac{1}{2})+\hbar\omega_0(2n+|\mu|+1) \tag{5.2}$$

where the quantum numbers take on the values $l, n = 0, 1, 2 \ldots$ and $\mu = 0, \pm 1, \pm 2 \ldots$. The two contributions to the energy are from the unperturbed one-dimensional

oscillator parallel to the field and the unperturbed two-dimensional oscillator perpendicular to the field. The Zeeman term in equation (3.12) is not present in equation (5.2).

5.2. Amplitudes in the symmetric gauge

We now turn to the solution of equation (4.6) for the conventional amplitudes. The vector potential in the symmetric gauge in equation (3.1) is

$$\boldsymbol{A} = \tfrac{1}{2}\rho B(t)\hat{\boldsymbol{\phi}} \tag{5.3}$$

in cylindrical coordinates. The scalar potential A_0 is zero. When these potentials are used in equation (4.2), the perturbation $\mathcal{V}(t)$ in the symmetric gauge is

$$\mathcal{V}(t) = \tfrac{1}{2}m\omega_L^2\rho^2 - i\hbar\omega_L\partial/\partial\phi. \tag{5.4}$$

With the unperturbed wavefunction $\phi_{nl\mu}$ and equation (5.4) the matrix elements in equation (4.6) can be evaluated. The resulting equation for the conventional amplitudes $a_{nl\mu}$ is

$$i\hbar\dot{a}_{nl\mu} - e_{nl\mu}a_{nl\mu} = a_{nl\mu}[\mu\hbar\omega_L + (2n + |\mu| + 1)\hbar\omega_L^2/2\omega_0]. \tag{5.5}$$

If a 'dressed' eigenvalue $\tilde{e}_{nl\mu}(t)$ is defined as

$$\tilde{e}_{nl\mu}(t) = \hbar\omega_0(l + \tfrac{1}{2}) + (2n + |\mu| + 1)\hbar\omega_0(1 + \omega_L^2/2\omega_0^2) + \mu\hbar\omega_L \tag{5.6}$$

we can write equation (5.5) as

$$i\hbar\dot{a}_{nl\mu} - \tilde{e}_{nl\mu}(t)a_{nl\mu} = 0. \tag{5.7}$$

Equation (5.7) can be easily solved to give

$$a_{nl\mu}(t) = a_{nl\mu}(0)\exp\left(-(i/\hbar)\int_0^t dt'\,\tilde{e}_{nl\mu}(t')\right), \tag{5.8}$$

the squared modulus of which is time independent. If we interpret the conventional amplitude as a probability amplitude, equation (5.8) predicts no transitions. This behaviour is quite different from the solution for the gauge-invariant probability amplitude in equation (3.13).

The eigenvalue $\varepsilon_{nl\mu}(t)$ in equation (3.12) from the gauge-invariant formulation is not the same as $\tilde{e}_{nl\mu}(t)$ in equation (5.6). The frequency ω in equation (3.8) can be written as $\omega_0(1 + \omega_L^2/\omega_0^2)^{1/2}$. For the weak-field case the square root can be expanded and the first two terms give $\omega_0(1 + \omega_L^2/2\omega_0^2)$, which is what occurs in equation (5.6).

In order to compare the gauge-invariant energy $\varepsilon_{nl\mu}$ and the dressed energy $\tilde{e}_{nl\mu}$, their time average was calculated numerically for $l = \mu = n = 1$. In figure 2 the time-averaged energies are plotted against the magnetic field magnitude B_0 in units of $(e/2mc\omega_0)^{-1}$, where e is the magnitude of the charge on the electron. For weak fields ($\omega_L \ll \omega_0$), the two energies are the same because the square root in equation (3.8) may be expanded to give the next to the last term in equation (5.6). At high fields, however, they differ significantly. The instantaneous energy can be measured if the duration of the measurement is small compared with the period of the field. A comparison of the instantaneous energies $\varepsilon_{nl\mu}(t)$ and $\tilde{e}_{nl\mu}(t)$ yields a figure similar to figure 2.

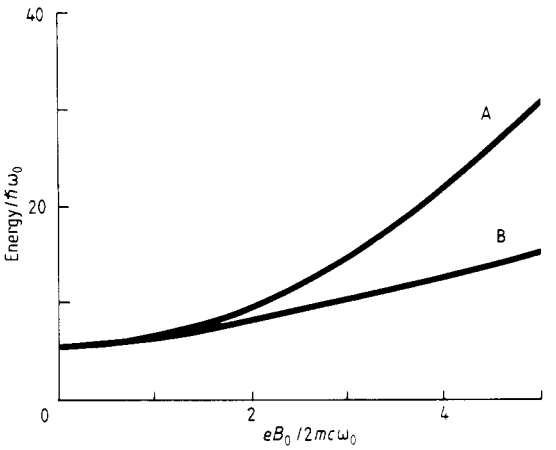

Figure 2. A plot of the time-averaged energies $\langle\tilde{\epsilon}_{111}\rangle$ (A) and $\langle\epsilon_{111}\rangle$(B) for $n = l = \mu = 1$ as a function of $eB_0/2mc\omega_0$, where B_0 is the amplitude of the sinusoidal magnetic field. The intercept at $B_0 = 0$ is $\frac{11}{2}\hbar\omega_0$.

5.3. Amplitudes in the mixed gauge

The amplitude in the mixed gauge is

$$a'_{nl\mu} = \langle\phi_{nl\mu}|\psi'(t)\rangle \tag{5.9}$$

where the mixed gauge wavefunction ψ' is given in equation (2.3) in terms of the symmetric gauge wavefunction ψ and the gauge function Λ given in equation (3.3). The amplitude $a'_{nl\mu}$ is thus

$$a'_{nl\mu} = \langle\phi_{nl\mu}|\exp[iq(\tfrac{1}{2}-\xi)B(t)xy/\hbar c]\psi(t)\rangle, \tag{5.10}$$

which reduces to the amplitude $a_{nl\mu} = \langle\phi_{nl\mu}|\psi(t)\rangle$ only when $\xi = \frac{1}{2}$. These conventional amplitudes and the corresponding 'probabilities' are thus gauge dependent.

The equation satisfied by the amplitudes in equation (5.9) is obtained by using the vector and scalar potentials in the mixed gauge in equations (3.2) and (3.4), respectively, in equation (4.6). In general transitions are predicted between unperturbed states unless $\xi = \frac{1}{2}$. The 'probability' of transitions using eigenstates of the unperturbed Hamiltonian is not only gauge dependent, but different in all gauges from the correct gauge-invariant probability using energy eigenstates. Use of the conventional amplitude as a probability amplitude for an energy eigenstate is, in this case, incorrect in all gauges and can lead to incorrect conclusions.

6. Conclusions

The three-dimensional charged isotropic harmonic oscillator in a time-varying magnetic field in the magnetic dipole approximation (MDA) is solved using a manifestly gauge-invariant formulation of quantum mechanics. The gauge-invariant formulation is based on the gauge-invariant energy operator which corresponds to the physically observable energy. It yields instantaneous eigenvalues which are 'dressed' by the field and state probabilities which are gauge invariant.

The conventional approach to this problem uses eigenstates of the unperturbed Hamiltonian. When these eigenstates are used to calculate amplitudes, the corresponding 'state probabilities' are gauge dependent and different in all gauges from the correct gauge-invariant energy eigenstate probabilities. Since the magnetic field remains on, these 'state probabilities' are not physically meaningful.

In the adiabatic approximation the eigenvalue problem for the total Hamiltonian is solved (Schiff 1968, pp 289–90). In an arbitrary gauge, the eigenvalues of the total Hamiltonian depend on the gauge. The amplitudes calculated from the eigenstates of the total Hamiltonian are also gauge dependent and give gauge-dependent 'state probabilities'. These eigenvalues and amplitudes are in general meaningless since the total Hamiltonian is not in general the energy operator. For a gauge, like the symmetric gauge in the MDA, in which the scalar potential is zero, the Hamiltonian reduces to the energy operator and correct eigenvalues and amplitudes are obtained. In the case of the harmonic oscillator in § 3, equation (3.5) is also the total Hamiltonian because the symmetric gauge is used. In general the gauge-invariant approach is different from the adiabatic approximation and the assumption that the field is slowly varying does not have to be made.

For problems in which a time-varying electromagnetic field is present, there is a distinction between the energy operator and the Hamiltonian. A quantum-mechanical operator which corresponds to a classical observable must be gauge invariant in addition to being Hermitian. A gauge-invariant operator is one with a gauge-invariant expectation value. The expectation values of the Hamiltonian and the unperturbed Hamiltonian are gauge dependent (Kobe and Yang 1980). The energy operator in equation (2.7) is Hermitian, gauge invariant and has the same form as the classical energy (Kobe 1981). It also satisfies the condition that the time rate of change of its expectation value is equal to the power which the electromagnetic field supplies to the particle. There are indeed some gauges in which the energy operator is equal to the Hamiltonian (or the unperturbed Hamiltonian). For example, in a gauge in which the scalar potential is zero the Hamiltonian reduces to the energy operator. However, an experiment designed to measure energy differences measures differences in the eigenvalues of the energy operator. Transitions between energy eigenstates must also be calculated using eigenstates of the energy operator. Eigenstates of the Hamiltonian (or unperturbed Hamiltonian) should not be used in general to calculate the probability that the particle is in an energy eigenstate.

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