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Gauge invariance and the space-translation method

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Abstract. The space-translation method for treating the interaction of electromagnetic radiation and matter in the electric dipole approximation is investigated from the standpoint of gauge invariance. Unless the wavefunction of the space-translation method is properly transformed, the probability of finding the system in an energy eigenstate is not in general correct. In the electric dipole approximation the probability of finding the system in an energy eigenstate is most conveniently calculated in the electric field gauge where the interaction is of the length form. The length form of the interaction is not in general equal to the velocity form or the acceleration form which comes from the space-translation method. The charged harmonic oscillator is used as an example.

1. Introduction

The space-translation method (Kramers 1950), which uses the Hertz potential, was proposed by Henneberger (1968) as a new method for treating the interaction of electromagnetic radiation and matter in the electric dipole approximation. It was proposed as a method which could be used in intense electromagnetic fields because for some problems non-perturbative solutions could be found (Choi *et al* 1974, Henneberger 1977, Brandi *et al* 1978). If the field is sufficiently weak, a Taylor series expansion of the potential can be made and the terms of first order and higher can be treated by perturbation theory (Lambropoulos *et al* 1976, Knight 1977).

In this paper the space-translation method is discussed from the standpoint of gauge invariance. In the manifestly gauge-invariant formulation of quantum mechanics given recently (Kobe and Smirl 1978, Kobe 1978, 1979a, b, Yang 1976), any gauge can be used, and the same results are guaranteed. The gauge-invariant energy operator, which is the sum of the kinetic energy operator and the potential energy operator V, determines the appropriate energy eigenstates and eigenvalues of the system. The kinetic energy operator is proportional to the square of the kinetic (i.e. mechanical) momentum $\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}/c$, not the canonical momentum $\boldsymbol{p}$, where $\boldsymbol{A}$ is the vector potential and q is the charge. In an arbitrary gauge the probability amplitude for finding the system in an energy eigenstate is the inner product between the energy eigenstate and the wavefunction which is a solution to the Schrödinger equation in the same gauge (Yang 1982). This probability amplitude is gauge invariant because under a gauge transformation both the energy eigenstate and the wavefunction change by the same phase factor.

In the electric dipole approximation (EDA), the electric field gauge (Kobe 1982) can be used in which the vector potential is zero and the scalar potential is $-\boldsymbol{E} \cdot \boldsymbol{r}$, where $\boldsymbol{E}$ is the electric field at the origin and $\boldsymbol{r}$ is the displacement of the electron.

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In this gauge the kinetic momentum $\boldsymbol{\pi}$ reduces to the canonical momentum $\boldsymbol{p}$, and the energy operator reduces to the unperturbed Hamiltonian $H_0 = p^2/2m + V$. This simplification of the energy operator in the electric field gauge to H_0 is the fundamental reason why it is convenient to use the electric field gauge with the scalar potential $-\boldsymbol{E} \cdot \boldsymbol{r}$. The reason is not that $\boldsymbol{E}$ and $\boldsymbol{r}$ are both gauge-invariant operators, which they of course are.

The space-translation method (Henneberger 1968) can be used as a technique for solving the Schrödinger equation (Choi *et al* 1974, Henneberger 1977, Brandi *et al* 1978), but care must be used in its interpretation. To obtain the time-dependent probability that the system is in an energy eigenstate it is necessary to transform the wavefunction obtained in the space-translation method to a solution of the Schrödinger equation in a definite gauge before taking the inner product with an eigenstate of the energy operator in the same gauge. This procedure is most easily done by transforming the space-translation method wavefunction to the wavefunction which is the solution to the Schrödinger equation in the electric field gauge with a zero vector potential and a scalar potential which is $-\boldsymbol{E} \cdot \boldsymbol{r}$. Then the energy eigenstates are eigenstates of the unperturbed Hamiltonian $H_0 = p^2/2m + V$. The eigenvalues E_n of the unperturbed Hamiltonian are the 'bare' energy eigenvalues, and the effect of the electric field in 'dressing' them can be calculated by perturbation theory (Kobe 1983). If expectation values of operators are to be calculated in the space-translation method, it is necessary to transform the wavefunction to the solution of the Schrödinger equation in the gauge in which the operators are given. Equivalently, the operators can be transformed to correspond with the space-translation wavefunction. By following the gauge-invariant procedure the results of a calculation are not dependent on a fortuitous choice of gauge.

The space-translation method has been criticised by Vermani and Beers (1975). They showed that the velocity form of the interaction ($\boldsymbol{A} \cdot \boldsymbol{p}$) and the space-translation method do not give the same probability for finding the system in the same state. Choi *et al* (1975a) replied that near resonance the two probabilities are almost equal, and that small oscillatory terms can be neglected. They failed to answer what happens away from resonance where there is an appreciable difference. The assumption of Vermani and Beers (1975) is that the velocity form of the interaction gives the correct probability. As has been shown previously (Kobe and Wen 1982, 1980), the velocity form of the interaction does not in general give the correct time-dependent probabilities. Therefore lack of agreement between the space-translation method and the velocity form of the interaction does not imply that the space-translation method necessarily gives incorrect probabilities. In this paper it is shown that the direct calculation of probabilities from the space-translation method is indeed incorrect because it does not agree with the gauge-invariant probabilities.

To illustrate these ideas, a charged harmonic oscillator in one dimension in an electromagnetic field in the electric dipole approximation is considered. This problem has been solved exactly (Heffner and Louisell 1965, Merzbacher 1970) and the probability that the system is in a given energy eigenstate has been calculated (Kobe and Wen 1982, 1980). The same result should be obtained from the space-translation method. It is if the wavefunction of the space-translation method is properly transformed to the wavefunction corresponding to the interaction $-qEx$. However, if the inner product of the unperturbed wavefunction and the space-translation wavefunction is taken, gauge-dependent amplitudes are obtained. Their absolute values squared do not give the same result as the gauge-invariant formulation, except in the special case of resonance between the oscillator and a harmonically varying field.

In § 2 the space-translation method is briefly reviewed. In § 3 the manifestly gauge-invariant formulation is given and compared with the space-translation method. Expectation values of operators are discussed in § 4. In § 5 a charged harmonic oscillator in one dimension in an electromagnetic field in the EDA is used to compare the gauge-invariant formulation and the space-translation method. The conclusions are given in § 6.

2. Space-translation method

The Schrödinger equation for a particle of mass m and charge q in an external electromagnetic field characterised by the vector potential $\boldsymbol{A}$ and scalar potential A_0 is

$$[(1/2m)(p-q\boldsymbol{A}/c)^2+V+qA_0]\psi=\mathrm{i}\hbar\,\partial\psi/\partial t, \tag{2.1}$$

where $V(\boldsymbol{r})$ is a potential energy. We shall consider the electric dipole approximation so the spatial dependence of the vector potential can be neglected, $\boldsymbol{A}(\boldsymbol{r},t)\simeq\boldsymbol{A}(0,t)\equiv\boldsymbol{A}(t)$ since the wavelength of the radiation is assumed to be long compared with the dimension of the atomic system, and magnetic effects on the system are neglected (Kobe 1982). The sources of the external radiation are at infinity, so the scalar potential can be chosen to be zero, $A_0=0$. Under these approximations, (2.1) can be written as

$$\left(\frac{1}{2m}p^2+V(\boldsymbol{r})-\frac{q}{2mc}\boldsymbol{A}\cdot\boldsymbol{p}+\frac{q^2}{2mc^2}A^2\right)\psi=\mathrm{i}\hbar\frac{\partial\psi}{\partial t}, \tag{2.2}$$

by expanding the quadratic term. By making a unitary transformation on (2.2), Henneberger (1968) showed that it could be expressed as

$$[(1/2m)p^2+V(\boldsymbol{r}+\boldsymbol{a})]\Psi=\mathrm{i}\hbar\,\partial\Psi/\partial t. \tag{2.3}$$

The vector $\boldsymbol{a}$ is

$$\boldsymbol{a}=-q\boldsymbol{Z}(t)/mc, \tag{2.4}$$

where the Hertz potential $\boldsymbol{Z}(t)$ is defined so that

$$\boldsymbol{A}(t)=\partial\boldsymbol{Z}(t)/\partial t. \tag{2.5}$$

The electric field $\boldsymbol{E}$ is related to the vector potential by

$$\boldsymbol{E}=-\partial\boldsymbol{A}/\partial tc, \tag{2.6}$$

since the scalar potential is taken to be zero. The new wavefunction Ψ in (2.3) is related to the old wavefunction ψ in (2.2) by a unitary transformation

$$\Psi=\mathrm{e}^{S}\psi \tag{2.7}$$

where the operator S is

$$S=\boldsymbol{a}\cdot\boldsymbol{\nabla}+\frac{\mathrm{i}q^2}{2mc^2\hbar}\int_0^t \mathrm{d}\tau\,A(\tau)^2. \tag{2.8}$$

It is assumed that the electromagnetic field is turned on at time zero. Although (2.7) is a unitary transformation on the wavefunction, it is not a gauge transformation because of the operator term $\boldsymbol{a}\cdot\boldsymbol{\nabla}$. Under some circumstances Henneberger (1968)

says that (2.3) may be simpler to solve than (2.1) in this approximation. If the field is intense, perturbation theory may not be valid, and non-perturbative methods may be needed to solve (2.3) (Lambropoulos *et al* 1976, Knight 1977).

Equation (2.3) may be written in terms of an 'unperturbed Hamiltonian'

$$H_{01} = p^2/2m + V_1(\boldsymbol{r}), \tag{2.9}$$

as

$$[H_{01} + V(\boldsymbol{r}+\boldsymbol{a}) - V_1(\boldsymbol{r})]\Psi = \mathrm{i}\hbar\partial\Psi/\partial t. \tag{2.10}$$

Henneberger (1968) proposed that for an intense field $V_1(\boldsymbol{r})$ be chosen as the time average of $V(\boldsymbol{r}+\boldsymbol{a}(t))$, as a way to include the effect of the intense field on the energy levels. However, any criterion for choosing V_1 could be used which could make $V(\boldsymbol{r}+\boldsymbol{a}) - V_1(\boldsymbol{r})$ small in some sense. There is thus no unique physical prescription for determining V_1.

If we choose $V_1 = V$ in (2.9), the unperturbed Hamiltonian becomes

$$H_0 = p^2/2m + V(\boldsymbol{r}). \tag{2.11}$$

If a power series expansion of $V(\boldsymbol{r}+\boldsymbol{a})$ is made, (2.3) becomes

$$[H_0 + \boldsymbol{a}\cdot\nabla V(\boldsymbol{r}) + \tfrac{1}{2}(\boldsymbol{a}\cdot\nabla)^2 V(\boldsymbol{r}) + \ldots]\Psi = \mathrm{i}\hbar\,\partial\Psi/\partial t. \tag{2.12}$$

If $\boldsymbol{a}$ is sufficiently small only the first term in the expansion need be retained. It is the $\boldsymbol{a}\cdot\nabla V$ form of the interaction between matter and electromagnetic radiation which is sometimes called the 'acceleration form' (Power and Thirunamachandran 1978). This form of the interaction is valid only under very special conditions.

The unperturbed Hamiltonian H_0 satisfies the eigenvalue equation

$$H_0\phi_n = E_n\phi_n, \tag{2.13}$$

with eigenfunctions ϕ_n and eigenvalues E_n. If (2.3) or (2.10) is solved to obtain the wavefunction Ψ, the amplitude

$$b_n(t) = \langle\phi_n|\Psi(t)\rangle \tag{2.14}$$

is conventionally interpreted as the 'probability amplitude' such that $|b_n|^2$ is the 'probability' of finding the system in the state ϕ_n. However, the 'probability' calculated in this way does not agree in general with the probability calculated from the gauge-invariant formulation of quantum mechanics. The manifestly gauge-invariant formulation of quantum mechanics, discussed in § 3, guarantees that the probabilities are gauge invariant.

3. Gauge-invariant formulation

The manifestly gauge-invariant formulation of quantum mechanics developed recently (Yang 1976, Kobe and Smirl 1978, Kobe 1978, 1979a, b) guarantees that the probability of finding the system in an energy eigenstate is gauge invariant. In this formulation it is observed that the canonical momentum operator $\boldsymbol{p} = -\mathrm{i}\hbar\nabla$ has a gauge-dependent expectation value, while the kinetic momentum $\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}/c$ has a gauge-invariant expectation value. The manifestly gauge-invariant theory is based on the gauge-invariant energy operator (Yang 1976)

$$\mathscr{E}(\boldsymbol{A}) = \pi^2/2m + V(\boldsymbol{r}), \tag{3.1}$$

which satisfies the eigenvalue equation

$$\mathscr{E}(\boldsymbol{A})\psi_n = \varepsilon_n \psi_n, \tag{3.2}$$

with eigenvalue ε_n and eigenstate ψ_n. The inner product of the wavefunction ψ in (2.1) with an energy eigenstate ψ_n in (3.2) is the amplitude

$$c_n(t) = \langle \psi_n(t) | \psi(t) \rangle. \tag{3.3}$$

The amplitude c_n is manifestly gauge invariant because when the gauge is changed both ψ_n and ψ are changed by the same phase factor. It can thus be properly interpreted as a probability amplitude, and $P_n = |c_n(t)|^2$ is the probability of finding the system in the state ψ_n at time t.

In the EDA the calculations are simplified by using the electric field gauge (Goeppert–Mayer gauge) (Kobe 1982) where

$$\boldsymbol{A}' = 0, \qquad A_0' = -\boldsymbol{E}(0, t) \cdot \boldsymbol{r}, \tag{3.4}$$

since magnetic effects are neglected. These potentials are obtained from the Coulomb gauge vector potential in the EDA $\boldsymbol{A} = \boldsymbol{A}(0, t)$, $A_0 = 0$, by the gauge transformations

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla \Lambda \tag{3.5}$$

and

$$A_0' = A_0 - c^{-1}\, \partial \Lambda / \partial t, \tag{3.6}$$

where the gauge function Λ is

$$\Lambda(\boldsymbol{r}, t) = -\boldsymbol{A}(0, t) \cdot \boldsymbol{r}. \tag{3.7}$$

If a new wavefunction ψ' is defined as

$$\psi' = \exp(\mathrm{i} q \Lambda / \hbar c) \psi, \tag{3.8}$$

it satisfies the Schrödinger equation

$$[H_0 - q\boldsymbol{E}(0, t) \cdot \boldsymbol{r}]\psi' = \mathrm{i}\hbar\, \partial \psi' / \partial t, \tag{3.9}$$

which is gauge equivalent to (2.1) in the EDA. The unperturbed Hamiltonian H_0 is given in (2.11) and satisfies the eigenvalue equation in (2.13).

For the choice of potentials in (3.4), $\boldsymbol{A}' = 0$ and the kinetic momentum $\boldsymbol{\pi}' = \boldsymbol{p} - q\boldsymbol{A}'/c$ reduces to the canonical momentum $\boldsymbol{p}$. Therefore, the energy operator in (3.1) reduces to

$$\mathscr{E}(\boldsymbol{A}') = \mathscr{E}(0) = H_0, \tag{3.10}$$

the unperturbed Hamiltonian in (2.11). In this gauge (3.2) becomes

$$\mathscr{E}(\boldsymbol{A}')\psi_n' = \varepsilon_n \psi_n', \tag{3.11}$$

where the eigenstate ψ_n' transforms as in (3.8).

Since $\boldsymbol{A}' = 0$ in (3.4), equation (3.11) reduces to the unperturbed eigenvalue problem in (2.13), with $\psi_n' = \phi_n$ and $\varepsilon_n = E_n$. The gauge-invariant probability amplitudes in (3.3) are then

$$c_n = \langle \phi_n | \psi' \rangle, \tag{3.12}$$

which are not in general the same as the amplitudes b_n in (2.14). In order to express gauge-invariant amplitudes c_n in terms of the wavefunction Ψ in (2.3), ψ' must be

written in terms of Ψ,

$$c_n = \langle \phi_n | \exp[-iq\boldsymbol{A}(t) \cdot \boldsymbol{r}/\hbar c] \exp(-S)\Psi \rangle, \tag{3.13}$$

where S is given by (2.8). This expression is quite different from $b_n = \langle \phi_n | \Psi \rangle$ in general, since both the exponentials in (3.13) involve the space and time coordinates together. However, in the limit as $t \to \infty$, $|c_n(t)|^2$ and $|b_n(t)|^2$ both approach the same limit if $\boldsymbol{A}(t)$ and $\boldsymbol{Z}(t)$ are chosen such that both approach zero. This situation occurs if the appropriate adiabatic switching hypothesis is made.

4. Expectation values

If an operator corresponds to an observable, it must have a gauge-invariant expectation value (Kobe and Yang 1980, Cohen-Tannoudji *et al* 1977). Suppose $\Theta(\boldsymbol{A}, A_0)$ is an Hermitian operator depending on the potentials $\boldsymbol{A}$ and A_0 corresponding to an observable, and the solution of the Schrödinger equation with these potentials is ψ. The operator in another gauge is $\Theta(\boldsymbol{A}', A_0')$, where the new potentials $\boldsymbol{A}'$ and A_0' are defined in general by (3.5) and (3.6) for arbitrary $\Lambda = \Lambda(\boldsymbol{r}, t)$. The solution of the Schrödinger equation with the new potentials is ψ', which is related to the solution of the Schrödinger equation with the old potentials by (3.8). The gauge invariance of the expectation values then demands that

$$\langle \psi | \Theta(\boldsymbol{A}, A_0)\psi \rangle = \langle \psi' | \Theta(\boldsymbol{A}', A_0')\psi' \rangle. \tag{4.1}$$

However, from (3.8) the matrix element on the left-hand side of (4.1) can be written as

$$\langle \psi | \Theta(\boldsymbol{A}, A_0)\psi \rangle = \langle \psi' | \Theta'(\boldsymbol{A}, A_0)\psi' \rangle, \tag{4.2}$$

where the unitarily transformed operator Θ' is

$$\Theta'(\boldsymbol{A}, A_0) = \exp(iq\Lambda/\hbar c)\Theta(\boldsymbol{A}, A_0) \exp(-iq\Lambda/\hbar c). \tag{4.3}$$

Equation (4.3) is called a gauge transformation on the operator.

For the operator Θ to be an observable it must be form invariant under gauge transformations (Kobe and Yang 1980, Cohen-Tannoudji *et al* 1977)

$$\Theta'(\boldsymbol{A}, A_0) = \Theta(\boldsymbol{A}', A_0'). \tag{4.4}$$

A gauge transformation on the operator must induce a gauge transformation on the potentials.

Because of (2.7) the expectation value in (4.1) is equal to

$$\langle \psi | \Theta(\boldsymbol{A}, A_0)\psi \rangle = \langle \Psi | \Theta_S(\boldsymbol{A}, A_0)\Psi \rangle \tag{4.5}$$

where Ψ is the solution of (2.3) and

$$\Theta_S(\boldsymbol{A}, A_0) = e^S \Theta(\boldsymbol{A}, A_0) e^{-S}. \tag{4.6}$$

The operator $\Theta_S(\boldsymbol{A}, A_0)$, although unitarily related to $\Theta(\boldsymbol{A}, A_0)$, does not in general have the same form as $\Theta(\boldsymbol{A}, A_0)$. Equation (4.6) is not a gauge transformation on the operator because (2.7) is not a gauge transformation on the wavefunction, because the operator S involves ∇.

To illustrate the transformation of operators, consider the kinetic momentum $\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}(\boldsymbol{r}, t)/c$, and the operator $\pi_0 = i\hbar\,\partial/\partial t - qA_0(\boldsymbol{r}, t)$. In the Coulomb gauge and the EDA these operators are $\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}(0, t)/c$ and $\pi_0 = i\hbar\,\partial/\partial t$. Under the

transformation in (4.6) $\boldsymbol{\pi}$ is unchanged,

$$\boldsymbol{\pi}_S = \boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}(0, t)/c, \tag{4.7}$$

and π_0 becomes

$$(\pi_0)_S = \mathrm{i}\hbar\, \partial/\partial t - (q/mc)\boldsymbol{A}(0, t) \cdot \boldsymbol{p} + (q^2/2mc^2)\boldsymbol{A}(0, t)^2, \tag{4.8}$$

which has a quite different form from π_0. For a function $F(\boldsymbol{r})$ the new operator is

$$F_S(\boldsymbol{r}) = F(\boldsymbol{r} + \boldsymbol{a}). \tag{4.9}$$

Therefore it is necessary to transform the operators also when using the solution Ψ in (2.3) of the space-translation method.

The energy operator $\mathscr{E}(\boldsymbol{A})$ in (3.1) in the EDA upon the unitary transformation in (4.6) becomes

$$\mathscr{E}_S(\boldsymbol{A}) = (2m)^{-1}[\boldsymbol{p} - q\boldsymbol{A}(0, t)/c]^2 + V(\boldsymbol{r} + \boldsymbol{a}), \tag{4.10}$$

from (4.7) and (4.9). Eigenstates Ψ_n of this operator are

$$\Psi_n = \mathrm{e}^S \psi_n, \tag{4.11}$$

with eigenenergies ε_n from (3.2). In the space-translation method, the proper gauge-invariant probability amplitudes c_n can thus be written as

$$c_n(t) = \langle \Psi_n | \Psi \rangle, \tag{4.12}$$

which is equal to (3.13).

5. Charged harmonic oscillator

In order to illustrate the differences between the amplitudes c_n and b_n, a charged harmonic oscillator in one dimension in an electromagnetic field in the EDA is considered as an example. The exact solutions of (2.2) and (3.9) in one dimension with the potential $V = \frac{1}{2}m\omega^2 x^2$ have previously been given (Kobe and Wen 1982, 1980). The exact solution of (2.3) can likewise be found.

For a harmonic oscillator in one dimension (2.3) becomes

$$[(2m)^{-1}p^2 + \tfrac{1}{2}m\omega^2(x + a)^2]\Psi = \mathrm{i}\hbar\, \partial\Psi/\partial t. \tag{5.1}$$

If the quadratic term in (5.1) is expanded, it can be written as

$$(H_0 + m\omega^2 ax + \tfrac{1}{2}m\omega^2 a^2)\Psi = \mathrm{i}\hbar\, \partial\Psi/\partial t. \tag{5.2}$$

The term $\frac{1}{2}m\omega^2 a^2$ contributes only a time-dependent phase factor to Ψ. The interaction term

$$m\omega^2 ax = -q\omega^2 Z(t)x/c \tag{5.3}$$

should be compared with the interaction $-qE(t)x$ in (3.9) for one dimension. In general the two interactions are not equal.

For a harmonically varying electric field

$$E(t) = E_0 \sin(\Omega t + \theta), \tag{5.4}$$

with frequency Ω and phase θ, the Hertz vector in (2.5) is

$$Z(t) = (cE_0/\Omega^2)\sin(\Omega t + \theta) + [A(0) - (cE_0/\Omega)\cos\theta]t + [Z(0) - (cE_0/\Omega^2)\sin\theta]. \tag{5.5}$$

This expression involves the arbitrary initial values of the vector potential $A(0)$ and the Hertz potential $Z(0)$. Thus the interaction in (5.3) is not well defined because the initial values of A and Z must still be specified. Different results are obtained if different values of $A(0)$ and $Z(0)$ are used. For simplicity the choice $A(0) = (cE_0/\Omega)\cos\theta$ and $Z(0) = (cE_0/\Omega^2)\sin\theta$ is made here, but this choice represents a *specific choice of gauge* for the potential. Then the quantities in the square brackets in (5.5) vanish. The interaction in (5.3) can then be written as

$$-q\omega^2 Z(t)x/c = -\rho^{-2}qE(t)x, \tag{5.6}$$

where $\rho = \Omega/\omega$ is the ratio of the frequency of the field to the frequency of the oscillator. Thus the space-translation method gives an interaction that is different from the $-qEx$ interaction by a factor of ρ^{-2}. When the field is resonant with the oscillator ($\rho = 1$), the interactions are the same. In general the field and the oscillator are not in resonance, so the interactions and the corresponding state probabilities are different.

If the harmonic oscillator is initially in its ground state at time zero and the field is applied, it develops into a coherent state at a later time (Heffner and Louisell 1965, Merzbacher 1970). For the interaction $-qE(t)x$, the probability $P_n = |c_n|^2$ that the oscillator is in the state ϕ_n if it is initially in the ground state, is

$$P_n(t) = (1/n!)|Q(\omega t)|^{2n}\exp[-|Q(\omega t)|^2]. \tag{5.7}$$

The function Q is (Kobe and Wen 1982, 1980)

$$Q(z) = i\alpha\, e^{-iz}\int_0^z ds\, e^{is} f(s/\omega), \tag{5.8}$$

where the dimensionless parameter α is

$$\alpha = qE_0(2m\hbar\omega^3)^{-1/2}, \tag{5.9}$$

and the function f is

$$f(t) = E(t)/E_0, \tag{5.10}$$

where $E(t)$ is given in (5.4).

For the space-translation method, (5.2) can also be solved exactly. The amplitude $b_n = \langle\phi_n|\Psi\rangle$ in (2.14) has an absolute value which is

$$|b_n(t)|^2 = (1/n!)|T(\omega t)|^{2n}\exp[-|T(\omega t)|^2]. \tag{5.11}$$

The function T in this case where the values of $A(0)$ and $Z(0)$ have been chosen to simplify (5.5) is

$$T(z) = \rho^{-2}Q(z), \tag{5.12}$$

where $Q(z)$ is defined in (5.8). For non-resonant situations ($\rho \neq 1$) equation (5.11) is different from (5.7). There cannot be two different values for the same physical quantity. The principle of gauge invariance determines that the correct probability for finding the particle in the state ϕ_n at time t is given by (5.7) which is calculated from the gauge-invariant formulation, and not by (5.11) or by the velocity form of the interaction.

A similar discussion holds for the velocity form of the interaction in (2.2). In the EDA the A^2 term contributes only a time-dependent phase factor, and so it is not relevant for calculating probabilities. The velocity form of the interaction is $-(q/mc)A(t)p_x$. The vector potential $A(t)$ for the harmonically varying electric field

in (5.4) is obtained by integrating (2.5) to give

$$A(t) = (cE_0/\Omega)\cos(\Omega t + \theta) + [A(0) - (cE_0/\Omega)\cos\theta]. \tag{5.13}$$

The velocity form of the interaction is not well defined because of the arbitrary initial value $A(0)$ of the vector potential. Different results are obtained for different values of $A(0)$. A vector potential $A'(t)$ that differs from $A(t)$ by a different initial value $A'(0)$ differs from $A(t)$ by a gauge transformation with $\Lambda = [A'(0) - A(0)]x$ in (3.5). For simplicity the value $A(0) = (cE_0/\Omega)\cos\theta$ can be used. Vermani and Beers (1975) have shown for the one-dimensional harmonic oscillator that the velocity and acceleration forms of the interaction do not give the same state probabilities, and imply that the velocity form is correct. The relationship between the length form and the velocity form of the interaction for the one-dimensional harmonic oscillator has been discussed elsewhere (Kobe and Wen 1982, 1980), where the choice $A(0) = 0$ was made. For non-resonance the two methods do not give the same probabilities for finding the system in an eigenstate ϕ_n of the unperturbed Hamiltonian H_0, and the length form must be used to obtain the correct gauge-invariant probability (Yang 1976, Kobe and Smirl 1978, Kobe 1979a, b, 1978). That there is a difference between state probabilities calculated from the velocity form and the acceleration form of the interaction does not necessarily imply that the acceleration form is incorrect, since the velocity form itself is in general incorrect. The acceleration form is indeed incorrect except on resonance because it does not agree with the length form, which arises from the gauge-invariant formulation of quantum mechanics.

6. Conclusion

The conclusion of this paper is not that the space-translation method is invalid in general, but only that extreme care must be exercised in its interpretation. For some problems, like the scattering of electrons in a laser beam, it leads to known results in a simple way (Choi *et al* 1975b). However, time-dependent state probability amplitudes cannot be obtained correctly by merely taking the inner product of the unperturbed eigenfunction with the wavefunction of the space-translation method. If eigenstates of the unperturbed Hamiltonian H_0 are to be used, the manifestly gauge-invariant formulation specifies that the interaction $-q\boldsymbol{E}(0, t) \cdot \boldsymbol{r}$ must be used in the EDA. It is necessary to transform from the space-translation wavefunction Ψ to the wavefunction ψ' obtained from the length form of the interaction before taking the inner product with an eigenstate ϕ_n of the unperturbed Hamiltonian H_0 to obtain the probability amplitude that the system is in the state ϕ_n. Failure to do so leads in general to incorrect results. Only when $\boldsymbol{Z}(t)$ and $\boldsymbol{A}(t)$ are both zero will equation (2.14) be equal to (3.13) times a time-dependent phase factor which does not affect the probability.

In the EDA it is common to think that with the unperturbed Hamiltonian H_0 the interactions in the length form $(-q\boldsymbol{E} \cdot \boldsymbol{r})$, the velocity form $(-q\boldsymbol{A} \cdot \boldsymbol{p}/mc)$, and the acceleration form $(-q\boldsymbol{Z} \cdot \nabla V/mc)$ are all equivalent interactions (Power and Thirunamachandran 1978). In this paper we show that for a charged harmonic oscillator in a harmonically varying electric field the usual application of the acceleration form does not give the same result for the probability of finding the system in an unperturbed state ϕ_n as the length form. In previous papers (Kobe and Wen 1982, 1980) we showed that for the same problem the velocity form does not in general

give the same probability as the length form. There cannot be more than one *correct* probability for finding the system in the same state. Gauge invariance specifies that when the unperturbed Hamiltonian H_0 is used, the length form of the interaction must be used (Yang 1976, Kobe and Smirl 1978, Kobe 1979a, b, 1978). In general, any gauge can be used in the manifestly gauge-invariant formulation. However, it is only when the vector potential can be chosen to be zero, as it is when the EDA is made and the scalar potential is taken as the length form, that the energy operator reduces to H_0, the unperturbed Hamiltonian.

In a recent paper (Ferrante and Leone 1982) it was shown that the space-translation method gives essentially the same results as the conventional treatment using the velocity form of the interaction in atomic collision problems. Only the matrix elements of the S-matrix were examined in that paper. If it is assumed that the interaction is switched on and off adiabatically so that at infinite time the $\boldsymbol{A}(t)$ and $\boldsymbol{Z}(t)$ in (3.13) are zero, equation (3.13) reduces to b_n in (2.14) times a phase factor. The considerations of the present paper are for all times including the time during which the electromagnetic field remains on.

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