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TEST OF GAUGE INVARIANCE:
CHARGED HARMONIC OSCILLATOR IN AN
ELECTROMAGNETIC FIELD

THESIS

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The gauge-invariant formulation of quantum mechanics is compared to the conventional approach for the case of a one-dimensional charged harmonic oscillator in an electromagnetic field in the electric dipole approximation. The probability of finding the oscillator in the ground state or excited states as a function of time is calculated, and the two approaches give different results.

On the basis of gauge invariance, the gauge-invariant formulation of quantum mechanics gives the correct probability, while the conventional approach is incorrect for this problem. Therefore, expansion coefficients for a wave function cannot always be interpreted as probability amplitudes. For a physical interpretation as probability amplitudes the expansion coefficients must be gauge invariant.

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CHAPTER I

INTRODUCTION

The semiclassical treatment of the interaction between charged particles and electromagnetic radiation treats the electromagnetic field classically and the particles with which the field interacts quantum mechanically. The goal of developing a completely gauge-invariant formulation of quantum theory for a charged particle interacting with a classical electromagnetic field is of great physical significance. Since it is known that the classical laws of physics are invariant under electromagnetic gauge transformations, the quantum theory should also have the same property. The Schrödinger equation for a particle in an electromagnetic field involves the vector and scalar potentials of the field. The electromagnetic field is unchanged if the potentials undergo a gauge transformation. If the potentials undergo a gauge transformation in the Schrödinger equation, the wave function must also be multiplied by a space- and time-varying phase factor. This procedure ensures the gauge invariance of the Schrödinger equation.

A common approach^{1,2} to the problem of a particle interacting with electromagnetic radiation is to expand the Hamiltonian and treat all the terms involving the vector potential as a perturbation. I show that this approach,

although conventional, does not preserve gauge invariance. Yang³ and Kobe and Smirl⁴ recently have developed a completely gauge-invariant formulation of quantum theory. They emphasize that the description of the system is manifestly gauge invariant at all times and in all approximations because the Schrödinger equation is formally invariant under gauge transformations. In the conventional approach, the expansion coefficients for the wave function are dependent on the gauge of the potentials, and therefore cannot be interpreted as probability amplitudes. However, in the gauge-invariant formulation, the expansion coefficients are gauge invariant, and can thus be interpreted as probability amplitudes.

Quantum mechanical operators representing physical quantities which have classical analogies are constructed by requiring that the quantum and the classical equations of motion have a term-by-term correspondence. Of special importance to the interpretation of quantum mechanics is the energy operator of a particle. In the presence of a time-varying electric field, the energy operator is not the Hamiltonian. The energy operator is constructed so that it is gauge invariant, and the time derivative of its average value is the average of the power operator. Yang⁵ uses the correspondence principle to show that the energy operator is the Hamiltonian without the scalar potential of the time-dependent field. This result is also true in

classical theory, as Kobe⁶ has shown. From this fundamental point, a gauge-invariant time-dependent theory has been developed by Yang³ and Kobe and Smirl.⁴

The purpose of this paper is to use a simple model of a single spinless one-dimensional harmonic oscillator in a time-varying electromagnetic field in the electric dipole approximation (EDA) to compare the gauge-invariant formulation and the conventional approach. The Schrödinger equation can be solved exactly for this problem in the EDA, so that the results are not obscured by approximations. In this simple example the electric dipole interaction $(\vec{E} \cdot \vec{r})$ and the conventional interaction $(\vec{A} \cdot \vec{p})$ give different probabilities for finding the system in a given state. For the electric dipole interaction the expansion coefficients are shown on the basis of gauge invariance to be true probability amplitudes, while for the conventional interaction the expansion coefficients are gauge dependent. The common impression that the expansion coefficients for the wave function can always be interpreted as probability amplitudes is erroneous, since the probability that the system is in a given energy eigenstate must be gauge-invariant. Thus the correct probability is given by the gauge-invariant approach, whereas the conventional approach is incorrect in general.

The rotating-wave approximation (RMA) is also discussed for each approach in a given state and compared to the exact

solution. It remains a reasonable approximation as long as the electric field frequency is very close to the harmonic oscillator frequency.

In Chapter II the gauge-invariant formulation is given. The form invariance of the Schrödinger equation under gauge transformations is shown. The gauge invariance of expectation values for observables and their equations of motion is also discussed, leading to the gauge-invariant energy operator. The formulation of a gauge-invariant theory for the time-dependent probability amplitudes is also given. In Chapter III the conventional perturbation treatment of radiation is reviewed to point out that the expansion coefficients cannot be interpreted as the probability amplitudes. The electric dipole interaction is derived by making a multipole expansion for the multipolar gauge and neglecting magnetic and higher-order electric multipoles in Chapter IV. Then in Chapter V, solutions of the Schrödinger equation for a one-dimensional harmonic oscillator in the gauge-invariant approach are obtained for the ground state and excited states. Likewise, I obtain the solutions of the Schrödinger equation for a one-dimensional harmonic oscillator in the conventional approach for the ground state and excited states, in Chapter VI. Chapter VII compares the rotating-wave approximation in both gauge-invariant and conventional formulations. Finally, the thesis is summarized and conclusions are given in Chapter VIII.

CHAPTER II

GAUGE-INVARIANT FORMULATION OF QUANTUM MECHANICS

The form invariance of the Schrödinger equation under local gauge transformations is reviewed here. The expectation values of observables must be gauge invariant. Consequently, the distinction is made between the Hamiltonian, for which the expectation value is not gauge-invariant, and the energy operator, for which the expectation value is. The time rate of change of the average of the energy operator is shown to be equal to the average of the quantum mechanical power operator.^{5,6} The probability amplitude of finding the system in an eigenstate of the energy operator is gauge-invariant.

A. Gauge Invariance of the Schrödinger Equation

The Schrödinger equation for a particle of mass m , charge q , and momentum operator $\vec{p} = -i\hbar\nabla$ in a time-varying electromagnetic field described by the vector potential $\vec{A}$ and scalar potential A_0 , is^{1,7}

$$\frac{1}{2m} (\vec{p} - \frac{q}{c} \vec{A})^2 \psi + V \psi + q A_0 \psi = i\hbar \frac{\partial \psi}{\partial t} \quad (2.1)$$

where V is the external static potential energy. When the Hamiltonian is written as $H(\vec{A}, A_0)$, the Schrödinger equation

in Eq. (2.1) can be written as

$$H(\vec{A}, A_0)\psi = i\hbar \frac{\partial \psi}{\partial t} , \quad (2.2)$$

where the Hamiltonian is

$$H(\vec{A}, A_0) = \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + V + qA_0 . \quad (2.3)$$

I introduce the local gauge transformation on the wave function after Pauli⁸ to get a new wave function by multiplying by a phase factor

$$\psi' = \exp\left(\frac{iq}{c\hbar} \Lambda\right) \psi , \quad (2.4)$$

where $\Lambda = \Lambda(\vec{r}, t)$ is an arbitrary differentiable function.

I also introduce the usual gauge transformation on the potentials, which are⁹

$$\vec{A}' = \vec{A} + \nabla \Lambda , \quad (2.5)$$

$$A'_0 = A_0 - \frac{1}{c} \frac{\partial \Lambda}{\partial t} , \quad (2.6)$$

where $\vec{A}'$ and A'_0 are new vector and scalar potentials, respectively. If Eq. (2.4) for ψ is substituted into Eq. (2.2), the Schrödinger equation becomes (see Appendix A1)

$$\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 \psi' + V \psi' + qA'_0 \psi' = i\hbar \frac{\partial \psi'}{\partial t} , \quad (2.7)$$

where the new potentials $\vec{A}'$ and A'_0 in Eqs. (2.5) and (2.6)

are used. Equation (2.7) has the same mathematical form as Eq. (2.1). The Schrödinger equation in Eq. (2.7) can be written as

$$H(\vec{A}', A_0') \psi' = i\hbar \frac{\partial \psi'}{\partial t} \quad , \quad (2.8)$$

where $H(\vec{A}', A_0')$ is the Hamiltonian in Eq. (2.1), with the vector potential $\vec{A}'$ and scalar potential A_0' . Comparing Eq. (2.8) with Eq. (2.2), we see that the Schrödinger equation is form invariant. The Schrödinger equation is form invariant under the local gauge transformation of the wave function in Eq. (2.4) if the scalar and vector potentials transform according to the customary gauge transformations on the potentials in Eqs. (2.5) and (2.6). This form invariance of the Schrödinger equation is the meaning of the "gauge invariance" of the Schrödinger equation.

As shown in Appendix A2, the magnetic induction

$$\vec{B} = \nabla \times \vec{A} \quad , \quad (2.9)$$

is gauge invariant under Eq. (2.5). Likewise, the electric field¹⁰

$$\vec{E} = -\nabla A_0 - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \quad , \quad (2.10)$$

is also gauge invariant under Eqs. (2.5) and (2.6). Therefore it is obvious that neither the electric nor magnetic field is dependent on the choice of gauge function Λ .

B. Gauge Invariance of Expectation Values

An operator representing a physical observable must have an expectation value which is independent of the choice of gauge. Yang⁵ postulates a physical correspondence principle to select the appropriate operators to represent physical observables. According to him, an operator represents a physical quantity with a classical analogy only if the equation of motion for the expectation value of the operator is of the same form as the equation of motion for the corresponding classical Newtonian quantity.

Following Yang's postulate, the correspondence principle is used to determine the proper operators for observables. If $\alpha(\vec{A}, A_0)$ is a Hermitian operator with potentials $\vec{A}$ and A_0 which describes an observable, then the expectation value of $\alpha(\vec{A}, A_0)$ with respect to ψ must be equal to the expectation value of $\alpha(\vec{A}', A'_0)$ with respect to ψ' in the new gauge

$$\langle \psi | \alpha(\vec{A}, A_0) \psi \rangle = \langle \psi' | \alpha(\vec{A}', A'_0) \psi' \rangle \quad (2.11)$$

Here $\alpha(\vec{A}', A'_0)$ is a Hermitian operator with new potentials which are given by Eqs. (2.5) and (2.6). However, for all operators it is true that

$$\langle \psi | \alpha(\vec{A}, A_0) \psi \rangle = \langle \psi' | \alpha'(\vec{A}, A_0) \psi' \rangle \quad (2.12)$$

where the operator $\alpha'(\vec{A}, A_0)$ is defined as

$$\alpha'(\vec{A}, A_0) = \exp\left(\frac{i g \Lambda}{c \hbar}\right) \alpha(\vec{A}, A_0) \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \quad (2.13)$$

Equation (2.13) is called a gauge transformation on the operator $\alpha(\vec{A}, A_0)$. A prime on an operator denotes a gauge transformation in Eq. (2.13) on all operators except the vector potential $\vec{A}$ and the scalar potential A_0 . For the potentials a prime denotes a gauge transformation of the potentials in Eqs. (2.5) and (2.6). From the comparison of Eqs. (2.11) and (2.12), for an operator to correspond to an observable, it must satisfy

$$\alpha'(\vec{A}, A_0) = \alpha(\vec{A}', A_0') \quad (2.14)$$

If an operator has the property given in Eq. (2.14), it is said to be form invariant under gauge transformations. A necessary and sufficient condition for an operator to have a gauge-invariant expectation value is that it is form invariant under gauge transformations.¹¹

Some examples are given here to make clear the definition of the form invariance of an operator under gauge transformations. The operator $(\vec{p} - \frac{q}{c} \vec{A})$ is form invariant under gauge transformation in Eq. (2.13), since

$$(\vec{p} - \frac{q}{c} \vec{A})' = \vec{p} - \frac{q}{c} \vec{A}' \quad (2.15)$$

as shown in Appendix A3. Likewise, the operator $i\hbar \frac{\partial}{\partial t}$ is

not form invariant, but the combination $(i\hbar \frac{\partial}{\partial t} - qA_0)$ is form invariant under gauge transformation in Eq. (2.13), since as shown in Appendix A3

$$(i\hbar \frac{\partial}{\partial t} - qA_0)' = i\hbar \frac{\partial}{\partial t} - qA_0' \quad (2.16)$$

where A_0' is given in Eq. (2.6).

C. Energy Operator

An energy operator must satisfy the conditions that (1) it has a gauge-invariant expectation value, and (2) the time derivative of its expectation value is equal to the average power transferred to the particle. However, the Hamiltonian $H(\vec{A}, A_0)$ is not form invariant under gauge transformation on the wave function in Eq. (2.13), since, as shown in Appendix A4,

$$H'(\vec{A}, A_0) = H(\vec{A}', A_0) = H(\vec{A}', A_0') + \frac{q}{c} \frac{\partial \Lambda}{\partial t} \quad (2.17)$$

The Hamiltonian therefore cannot be the energy operator, since its expectation value is gauge dependent.

Although the time evolution of the system with wave function ψ is described by the Hamiltonian $H(\vec{A}, A_0)$, it is not the energy operator. In the time-dependent case qA_0 is not a potential energy, since the electric field $\vec{E}$ is not $-\nabla A_0$, but instead is given by $-\nabla A_0 - \frac{1}{c} \frac{\partial \vec{A}}{\partial t}$ from Eq. (2.10). For the electrostatic field $\vec{E}_0$ with a potential ϕ the electric

force is $q\vec{E}_0 = -\nabla\phi$; so ϕ is a true potential energy.

There is thus a fundamental difference between the time-dependent and time-independent cases.

The question thus arises as to the proper choice for the energy operator. Let us consider the operator $H(\vec{A}, 0)$, which is defined as

$$H(\vec{A}, 0) = H(\vec{A}, A_0) - \int A_0 \quad (2.18)$$

The operator $H(\vec{A}, 0)$ is form invariant under gauge transformation on the operator, since, as shown in Appendix A5

$$H'(\vec{A}, 0) = H(\vec{A}', 0) \quad (2.19)$$

By Eq. (2.12) its expectation value is independent of the gauge, so it satisfies condition (1).

The correspondence principle can be used here to show more definitely that $H(\vec{A}, 0)$ is the energy operator for the particle. If $H(\vec{A}, 0)$ is the energy operator, condition (2) shows that the time rate of change of its expectation value is^{5,11}

$$\frac{d}{dt} \langle \psi | H(\vec{A}, 0) | \psi \rangle = \langle \psi | P | \psi \rangle \quad (2.20)$$

where P is the power operator for the particle (see Appendix A6). The power operator is

$$P = -\frac{i}{\hbar} \left[i\hbar \frac{\partial}{\partial t} - \int A_0, H(\vec{A}, 0) \right] \quad (2.21)$$

Because of Eqs. (2.16) and (2.19), this operator is gauge-invariant. We show in Appendix A7 that Eq. (2.21) becomes

$$P = \frac{q}{2} (\vec{v} \cdot \vec{E} + \vec{E} \cdot \vec{v}), \quad (2.22)$$

where

$$\vec{v} = \frac{1}{m} (\vec{p} - \frac{q}{c} \vec{A}) \quad (2.23)$$

is the velocity operator. Equation (2.22) is a Hermitian operator which has the same form as the classical power.

It is thus verified that $H(\vec{A}, 0)$ is the energy operator for the particle. In order to emphasize the importance of the energy operator, it is denoted by

$$E(\vec{A}) = H(\vec{A}, 0) \quad (2.24)$$

in the following sections.

D. Gauge Invariance of Probability Amplitudes

The energy operator $E(\vec{A})$, shown to be form invariant under gauge transformations in Eq. (2.24), satisfies the eigenvalue problem

$$E(\vec{A}) \psi_n(\vec{r}, t) = \epsilon_n(t) \psi_n(\vec{r}, t) \quad (2.25)$$

where ψ_n and ϵ_n are in general functions of time t because $\vec{A}$ is time-dependent. In terms of the complete set of

states $\{\psi_n\}$, the wave function ψ for the Schrödinger equation in Eq. (2.1) can be expanded as

$$\psi = \sum_n C_n(t) \psi_n \quad (2.26)$$

If we substitute Eq. (2.26) into Eq. (2.1) and Eq. (2.25) is used, the equation of motion for C_n is

$$i\hbar \dot{C}_n = \epsilon_n C_n + \sum_m \langle \psi_n | (fA_0 - i\hbar \frac{\partial}{\partial t}) \psi_m \rangle C_m \quad (2.27)$$

(see Appendix A8). Referring to Eq. (2.16), we see that Eq. (2.27) is gauge invariant. It should be emphasized that ψ_m in Eq. (2.27) is in general a function of time because of Eq. (2.25).

If ψ'_n is related to ψ_n by Eq. (2.4), then the gauge transformation of the eigenvalue problem in Eq. (2.25) is

$$E(\vec{A}') \psi'_n(\vec{r}, t) = \epsilon_n(t) \psi'_n(\vec{r}, t) \quad (2.28)$$

where Eqs. (2.19) and (2.24) have been used.

The eigenenergy ϵ_n is unchanged under the gauge transformation on the wave function. Since both ψ' and ψ'_n are related to ψ and ψ_n by Eq. (2.4), the expansion of ψ' in terms of ψ'_n has the same expansion coefficients as Eq. (2.26),

$$\psi' = \sum_n C_n(t) \psi'_n \quad (2.29)$$

Thus, when we substitute Eq. (2.28) into the Schrödinger equation in Eq. (2.7), the equation for the time-dependent

coefficients C_n is

$$i\hbar \dot{C}_n = E_n C_n + \sum_m \langle \psi_n' | (qA_0' - i\hbar \frac{\partial}{\partial t}) \psi_m' \rangle C_m \quad (2.30)$$

From Eqs. (2.16), (2.13), and (2.11) we can easily find that the matrix elements in Eq. (2.27) are gauge invariant. Therefore $\{C_n(t)\}$ are independent of the choice of gauge. The expansion coefficients $\{C_n\}$ of ψ in terms of $\{\psi_n\}$ can be interpreted as the probability amplitude of finding the system in energy eigenstates of $E(\vec{A})$.

CHAPTER III

CONVENTIONAL APPROACH

The term "conventional" as used here means that the quadratic part of the Hamiltonian in Eq. (2.1) is expanded and the unperturbed Hamiltonian is chosen to be the Hamiltonian without the electromagnetic field present. The main objection of the conventional theory is that it is not gauge-invariant. In particular, the expansion coefficients for the total wave function are gauge-dependent, and thus cannot be interpreted as probability amplitudes.

The quadratic term in Eq. (2.1) can be expanded to give

$$H(\vec{A}, A_0) = H_0 - \left(\frac{q}{2mc}\right)(\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) + \left(\frac{q^2}{2mc^2}\right) A^2 + qA_0. \quad (3.1)$$

The Hamiltonian $H_0 = H(0,0)$ in the absence of the time-varying electromagnetic field is

$$H_0 = \frac{\vec{p}^2}{2m} + V. \quad (3.2)$$

The unperturbed Hamiltonian H satisfies the eigenvalue problem

$$H_0 \phi_n = e_n \phi_n, \quad (3.3)$$

where ϕ_n is the eigenstate of H_0 and e_n is the eigenenergy. The wave function in the Schrödinger equation in Eq. (2.1) is expanded in terms of $\{\phi_n\}$ as

$$\psi = \sum_n a_n \phi_n, \quad (3.4)$$

in the conventional approach. If Eq. (3.4) is substituted into the Schrödinger equation in Eq. (2.1), the resulting equation for the coefficients is

$$i\hbar \dot{a}_n = e_n a_n + \sum_m \langle \phi_n | \left\{ -\frac{\hbar^2}{2mc} (\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) + \left(\frac{\hbar^2}{2mc^2}\right) A^2 + \hbar A_0 \right\} \phi_m \rangle a_m. \quad (3.5)$$

The transitions between states in Eq. (3.5) are thus induced by the gauge-dependent potentials.

The Coulomb gauge, in which

$$\nabla \cdot \vec{A} = 0 \quad (3.6)$$

and $A_0 = 0$, is often used in Eq. (3.1), so that

$$\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p} \quad (3.7)$$

(see Appendix B1). The conventional procedure uses H_0 as the unperturbed Hamiltonian, and the remainder in Eq. (3.1) as the perturbation. Equation (3.1) can be rewritten when Eq. (3.6) is used

$$H(\vec{A}, A_0) = H_0 - \frac{\hbar^2}{mc} (\vec{A} \cdot \vec{p}) + \left(\frac{\hbar^2}{2mc^2}\right) A^2. \quad (3.8)$$

However, this approach is not gauge invariant. The coefficients in the expansion of the wave function in terms of the eigenstates of H_0 are gauge dependent and can therefore not be interpreted as probability amplitudes. Even the Hamiltonian in Eq. (2.3) or Eq. (3.1) is not gauge invariant; this has been discussed in the previous section and Appendix A4.

If a gauge transformation in Eq. (2.4) is made on the wave function and Eqs. (2.5) and (2.6) are used, the new Schrödinger equation obtained is given in Eq. (2.7). The wave function ψ' can be expanded in terms of the eigenfunctions in Eq. (3.4) as

$$\psi' = \sum_n a'_n \phi_n \quad (3.9)$$

We must notice here that the coefficients a_n and a'_n are not in general the same. By substituting Eqs. (3.4) and (3.9) into Eq. (2.4) we obtain

$$a'_n = \sum_m \langle \phi_n | \exp\left(\frac{i q \Lambda}{c \hbar}\right) \phi_m \rangle a_m \quad (3.10)$$

Since $\Lambda = \Lambda(\vec{r}, t)$, the coefficients in Eq. (3.10) will in general be complex numbers not equal to δ_{nm} . When Eq. (3.9) is substituted into the Schrödinger equation in Eq. (2.7), the equation for the coefficients a'_n obtained is

$$i \hbar \dot{a}'_n = e_n a'_n + \sum_m \langle \phi_n | \left\{ -\frac{\hbar^2}{2mc} (\vec{A}' \cdot \vec{p} + \vec{p} \cdot \vec{A}') + \left(\frac{\hbar^2}{2mc^2} \right) A'^2 + q A'_0 \right\} \phi_m \rangle a'_m \quad (3.11)$$

Equation (3.10) shows that in general a_n and a'_n are not the same coefficients, so they cannot be interpreted as the probability amplitudes. There are other difficulties with the conventional perturbation theory when the case in which there is no electromagnetic field is considered. From the conventional point of view, the electric field $\vec{E} = 0$ and the magnetic induction $\vec{B} = 0$ can be described by the potentials $\vec{A} = 0$ and $A_0 = 0$. Then the perturbation in Eq. (3.1) is zero, as it should be. However, as I show in Eqs. (2.5) and (2.6), from the gauge-invariant point of view, this same situation can also be described by the vector potential $\vec{A}' = \nabla \Lambda$ and scalar potential $A'_0 = -\frac{1}{c} \frac{\partial \Lambda}{\partial t}$, where Λ is an arbitrary function of space and time. The perturbation in Eq. (3.1) is then not zero. According to Eqs. (3.5) and (3.11) it is obvious that different results will be obtained. However the gauge-invariant approach gives the same results for either gauge. We will use Eq. (3.8) as the conventional approach to solve the problem of a single charged harmonic oscillator in an electromagnetic field in the electric dipole approximation in order to compare with the gauge-invariant approach to the same problem.

CHAPTER IV

ELECTRIC DIPOLE APPROXIMATION

The electric dipole approximation (EDA) is widely used in quantum optics⁹ to treat the interaction of electromagnetic radiation with matter in the long wavelength limit. When the wavelength of the electromagnetic wave is long, compared to the size of the atomic system, we can obtain a simplified equation for the gauge-invariant probability amplitudes by making a gauge transformation under the conditions that (a) the electric field is slowly varying over the dimensions of the system and (b) the magnetic field is negligible. In this chapter I shall first discuss the multipolar gauge and obtain the multipole expansion of the potentials.

A. Multipolar Gauge

A gauge transformation can be made from an arbitrary gauge to obtain the multipolar gauge. In this gauge the vector and scalar potentials are expressed as the appropriate integrals of the magnetic and electric fields, respectively. It is a convenient gauge to use for making multipole expansions.

The gauge condition in the multipolar gauge is obtained by integrating Eq. (2.5) along a straight line from the origin 0 to the point $\vec{r}$, and setting

$$\int_0^1 du \vec{r} \cdot \vec{A}'(u\vec{r}, t) = 0 . \quad (4.1)$$

Then the gauge function Λ no longer depends on $\vec{A}'$ and is

$$\Lambda(\vec{r}, t) = \Lambda(0, t) - \int_0^1 du \vec{r} \cdot \vec{A}(u\vec{r}, t) . \quad (4.2)$$

The new vector potential can be calculated from Eq. (2.5) and is shown in Appendix C1 to be

$$\vec{A}'(\vec{r}, t) = -\vec{r} \times \int_0^1 du u \vec{B}(u\vec{r}, t) . \quad (4.3)$$

The new scalar potential can be calculated from Eq. (2.6) and is shown in Appendix C2 to be

$$A'_0(\vec{r}, t) = -\vec{r} \cdot \int_0^1 du \vec{E}(u\vec{r}, t) . \quad (4.4)$$

These are exact vector and scalar potentials from which the fields $\vec{B}$ and $\vec{E}$ can be obtained from Eqs. (2.9) and (2.10), respectively. The potentials in Eqs. (4.3) and (4.4) can be used in the Schrödinger equation to describe the interaction of the electromagnetic field with a charged particle. The Schrödinger equation is difficult to solve in general. Thus some approximations are usually made.

B. Multipole Expansion

If the wavelength of the electromagnetic wave is long compared to the size of the atomic system, the center of which is located at the origin, a multipole expansion of the

potentials in Eqs. (4.3) and (4.4) can be made. The multipole expansion of the vector potential is

$$\vec{A}'(\vec{r}, t) = -\frac{1}{2} \vec{r} \times \vec{B}(0, t) + \dots, \quad (4.5)$$

where only the magnetic dipole term is shown. The multipole expansion of the scalar potential is

$$A'(\vec{r}, t) = -\vec{r} \cdot \vec{E}(0, t) - \frac{1}{2} x_i x_j \partial_j' E_i(0, t) + \dots, \quad (4.6)$$

where the definition of the derivative is $\partial_j' E_i(0, t) \equiv \left[\partial E_i(\vec{r}', t) / \partial x_j \right] \big|_{\vec{r}'=0}$. When Eq. (4.5) is used in Eq. (2.9) for the magnetic field, we obtain

$$\vec{B}(\vec{r}, t) = \vec{B}(0, t) + \dots, \quad (4.7)$$

as shown in Appendix C3. When Eqs. (4.5) and (4.6) are used in Eq. (2.10) for the electric field, as shown in Appendix C4, we obtain

$$\vec{E}(\vec{r}, t) = \vec{E}(0, t) + (\vec{r} \cdot \nabla') \vec{E}(\vec{r}', t) \big|_{\vec{r}'=0} + \dots, \quad (4.8)$$

when Faraday's law is used.

C. Electric Dipole Approximation

If the effect of the magnetic field on the system can be neglected, the vector potential in Eq. (4.5) becomes

$$\vec{A}'(\vec{r}, t) \approx 0. \quad (4.9)$$

If the electric quadrupole and higher multipoles are omitted, the scalar potential in Eq. (4.6) becomes

$$A_0(\vec{r}, t) \simeq -\vec{r} \cdot \vec{E}(0, t) = -\vec{r} \cdot \vec{E}(t) \quad (4.10)$$

The original gauge in Eq. (2.1) can be chosen to be the Coulomb gauge in which $\nabla \cdot \vec{A} = 0$ and $A_0 = 0$. In the EDA the spatial variation of $\vec{A}$ can be neglected; so

$$\vec{A}(\vec{r}, t) \simeq \vec{A}(0, t) = \vec{A}(t) \quad (4.11)$$

This choice of gauge gives the same fields as the potentials in Eqs. (4.9) and (4.10).

In the EDA the gauge-invariant formulation is simplified by using the gauge function, which is obtained by replacing $\vec{A}(\vec{r}, t)$ in Eq. (4.2) by $\vec{A}(t)$. If we choose

$$\Lambda(0, t) = 0 \quad , \quad (4.12)$$

the gauge function in Eq. (4.2) can be written as

$$\Lambda(\vec{r}, t) = -\vec{r} \cdot \vec{A}(t) \quad (4.13)$$

D. The Gauge-Invariant Formulation in the Electric Dipole Approximation

The wave function of the Schrödinger equation can be

expanded as in Eq. (2.29), in terms of Eq. (2.28). Equation (2.28) reduces to Eq. (3.3) and the eigenfunctions ψ_n' are the time-independent eigenstates ϕ_n of H_0 in Eq. (3.3). The eigenenergies ϵ_n in Eq. (2.28) are the eigenenergies ϵ_n in Eq. (3.3). Therefore Eq. (2.30) can be written in the gauge in Eqs. (4.9) and (4.10)

$$\left(i\hbar \frac{\partial}{\partial t} - \epsilon_n\right) C_n = \sum_{m \neq n} \left[-\frac{q}{\hbar} \vec{E}(0,t) \cdot (\vec{Y})_{nm} C_m \right], \quad (4.14)$$

where the matrix element $(\vec{Y})_{nm}$ is defined as

$$(\vec{Y})_{nm} = \langle \phi_n | \vec{Y} | \phi_m \rangle \quad (4.15)$$

Instead of an arbitrary gauge, as in Eq. (2.30), we have chosen the gauges in Eqs. (4.9) and (4.10) to get Eq. (4.14), which is completely equivalent to Eq. (2.30).

The Schrodinger equation in Eq. (2.7) then becomes, in the new gauge in the EDA,

$$\left[H_0 - \frac{q}{\hbar} \vec{E}(0,t) \cdot \vec{Y} \right] \psi' = i\hbar \frac{\partial \psi'}{\partial t}, \quad (4.16)$$

with the Hamiltonian

$$H' = H_0 - \frac{q}{\hbar} \vec{E}(0,t) \cdot \vec{Y}, \quad (4.17)$$

where $H_0 = H_0(0,0)$. If (a) the magnetic field is negligible, and (b) the electric field is slowly varying, then the two Hamiltonians in Eq. (2.3) and (4.17) are equivalent. The

Hamiltonian in Eq. (4.17) is the physically meaningful Hamiltonian to use if H_0 is chosen as the unperturbed Hamiltonian. The electric dipole interaction is the correct perturbation to use in conjunction with H_0 , as Eq. (4.14) shows.

It has sometimes been thought that the Hamiltonian in Eq. (4.17) is only an approximation to Eq. (3.8), applicable in the weak field case when the A^2 term is negligible, because the electric dipole interaction is linear in the electric field. From the comparison of Eq. (3.8) and (4.17), this erroneous conclusion stems from the similarity in form between the $-q\vec{E} \cdot \vec{r}$ term and the $-(\frac{e}{mc})\vec{A} \cdot \vec{p}$ term. As I have shown above, this conclusion indeed is not correct.

CHAPTER V

GAUGE-INVARIANT SOLUTIONS FOR THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

In order to demonstrate the differences between the gauge-invariant approach and the conventional approach, we shall consider a one-dimensional harmonic oscillator of angular frequency ω for which $V = \frac{1}{2} m \omega^2 x^2$. It is placed in a harmonically varying electric field $E(t)$ in the x-direction in the electric dipole approximation. The problem is solved in a manifestly gauge-invariant way. The coefficients in the expansion of the wave function in terms of the unperturbed states are gauge independent, and are properly interpreted as probability amplitudes.

A. Ground State Solutions

In one dimension the Schrödinger equation in the EDA for the electric field gauge in Eqs. (4.9) and (4.10) is

$$\left\{ \frac{p_x^2}{2m} + \frac{1}{2} m \omega^2 x^2 - \int \varepsilon(t) x \right\} \psi' = i \hbar \frac{\partial \psi'}{\partial t}, \quad (5.1)$$

where the electric field is chosen in the x-direction. This equation can be solved exactly. If the system is in the ground state ϕ_0 of the unperturbed oscillator at $t = 0$, then the wave function ψ' is

$$\psi'(x,0) = \phi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left\{-\frac{m\omega}{2\hbar}x^2\right\}. \quad (5.2)$$

The solution to Eq. (5.1) is¹²

$$\begin{aligned} \psi'(x,t) = & \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left\{-\frac{i\omega t}{2} - \frac{m\omega x^2}{2\hbar}\right. \\ & + \frac{iE_0}{\hbar\omega} x \exp(-i\omega t) X(\omega t) \\ & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t)\right\}, \quad (5.3) \end{aligned}$$

which is verified in Appendix D1. The dimensionless constant $\alpha = \frac{E_0^2}{2m\hbar\omega^3}$, where E_0 is the amplitude of the electric field in the x-direction. The function $X(z)$ is defined as

$$X(z) \equiv \int_0^z ds f\left(\frac{s}{\omega}\right) \exp(is), \quad (5.4)$$

where $f(t) = \frac{E(t)}{E_0}$. The probability amplitude for the system in the ground state at time t is $C_0 = \langle \phi_0 | \psi' \rangle$ from Eq. (2.29). According to Eqs. (5.2) and (5.3) C_0 is shown in Appendix D2 to be

$$\begin{aligned} C_0 = & \exp\left\{-\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-i\omega t) X^2(\omega t)\right. \\ & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t)\right\}. \quad (5.5) \end{aligned}$$

The probability that the system is in the ground state at time t is shown in Appendix D3 to be

$$P_0(t) = |C_0(t)|^2 = \exp\{-|R(\omega t)|^2\} \quad (5.6)$$

where

$$R(\omega t) = \alpha^{1/2} X(\omega t) \quad (5.7)$$

The expression in Eq. (5.6) for $P_0(t)$ can be calculated in the electric dipole approximation for a harmonically varying electric field,

$$E(t) = E_0 \sin(\Omega t + \theta) \quad (5.8)$$

with angular frequency Ω and phase θ . If we choose $\rho = \frac{\Omega}{\omega}$, $Z = \omega t$, and substitute Eq. (5.8) into Eq. (5.6), it is shown in Appendix D4 that

$$\begin{aligned} P_0(t) &= |C_0(t)|^2 \\ &= \exp \left\{ -\alpha \left\{ \frac{\sin^2(\frac{1}{2}(1+\rho)Z)}{(1+\rho)^2} + \frac{\sin^2(\frac{1}{2}(1-\rho)Z)}{(1-\rho)^2} \right. \right. \\ &\quad \left. \left. - \frac{2 \cos(\rho Z + \theta) \sin(\frac{1}{2}(1+\rho)Z) \sin(\frac{1}{2}(1-\rho)Z)}{1-\rho^2} \right\} \right\} \end{aligned} \quad (5.9)$$

If we set $\rho = 0$ and $\theta = 0$, then $E(t) = 0$ and no transitions can take place. Thus the system remains in the ground state, so $P_0(t) = 1$ for all values of α and t . Then $P_0(t) = 1$, where α and Z can be any arbitrary real numbers. If we set $\rho = 1$, we may use L'Hôpital's rule in Eq. (5.9) to obtain

$$P_0(t)|_{t=1} = \exp \left\{ -\frac{\chi}{4} [z^2 + \sin^2 z - 2z \sin z \cos(z+20)] \right\}. \quad (5.10)$$

According to Eqs. (5.9) and (5.10), we notice that no matter what the other parameters are, $P_0(t)$ is always equal to unity when $z = \omega t = 0$. It is reassuring that the expression in Eq. (5.9) satisfies the initial condition imposed in Eq. (5.2).

The Schrödinger equation in Eq. (5.1) is gauge-equivalent to Eq. (2.1)

$$\frac{1}{2m} \left[p_x - \frac{q}{c} A(t) \right]^2 \psi + \frac{1}{2} m \omega^2 x^2 = i\hbar \frac{\partial \psi}{\partial t} \quad (5.11)$$

in EDA, where the vector potential is in the x-direction and the scalar potential is zero. The solution to Eq. (5.11), with the initial condition $\psi(x,0) = \phi_0(x)$, can also be obtained exactly by applying the gauge function in Eq. (4.13)

$$\Lambda(x,t) = -A(t)x$$

to the gauge transformation on the wave function in Eq. (2.4). This gives

$$\psi = \exp \left\{ i \frac{qA(t)}{\hbar c} x \right\} \psi' \quad (5.13)$$

where ψ' is given by Eq. (5.3) and $A(0) = 0$. Solving the energy operator eigenvalue problem in Eq. (2.25) for this gauge, we obtain $\psi_0 = \exp \left\{ i \frac{qA(t)}{\hbar c} x \right\} \phi_0$. The probability

amplitude for finding the system in the state ψ'_0 which is gauge equivalent to ϕ_0 is $\langle \psi'_0 / \psi'_0 \rangle = \langle \phi_0 / \psi'_0 \rangle = C_0$. Equation (5.6) for the probability of the system in the ground state is again obtained in this gauge.

If we change the value of the dimensionless constant α and keep the other parameters constant, we find that the probability increases as α decreases. Because the mass m and charge q are usually constants, decreasing the electric field amplitude will increase the probability of finding the system in the ground state. The probability is a rapidly varying function of phase angle θ . Figure 1 shows the curves of the probability P_0 in Eqs. (5.9) and (5.10) for $\alpha = 1$, $\theta = 0$, and for ρ equals to 0.1, 0.5, 1, 1.5, and 2. Figure 2 shows P_0 in Eq. (5.9) for $\alpha = 1$, $\rho = 0.1$ and θ equals $0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{\pi}{2}, \frac{5\pi}{8}, \frac{3\pi}{4}, \frac{7\pi}{8}$. Figure 3 shows P_0 in Eq. (5.9) for $\rho = 1$, $\theta = 0$ and α equals 0.5, 1, 1.5, 2, 5.

B. Excited State Solutions

The probability amplitude of the system in the n th excited state at time t is $C_n = \langle \phi_n / \psi' \rangle$, where ψ' is given in Eq. (5.3) and¹³

$$\phi_n(x) = 2^{-n/2} (n!)^{-1/2} \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right), \quad (5.14)$$

where $H_n(\sqrt{\frac{m\omega}{\hbar}}x)$ denotes a Hermite polynomial of degree n .

Thus, we obtain for C_n

$$C_n = 2^{-n/2} (n!)^{-1/2} \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \psi'(x,t) \quad (5.15)$$

The Hermite polynomial can be obtained from the generating function¹⁴

$$F(u, x) = \exp\left(-u^2 + 2\sqrt{\frac{m\omega}{\hbar}}ux\right) = \sum_{n=0}^{\infty} \frac{u^n}{n!} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \quad (5.16)$$

If we define a function $F(u)$ as

$$F(u) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar}x^2\right) F(u, x) \psi'(x, t) \quad (5.17)$$

and substitute Eq. (5.16) into Eq. (5.17), then it becomes

$$F(u) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \sum_{n=0}^{\infty} \frac{u^n}{n!} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \psi'(x, t) \quad (5.18)$$

Using Eq. (5.15), we can write Eq. (5.18) as

$$F(u) = \sum_{n=0}^{\infty} \frac{u^n}{n!} C_n 2^{-n/2} (n!)^{1/2} \quad (5.19)$$

so that $F(u)$ is a generating function for the probability amplitude C_n . As a consequence of Eq. (5.19), we see that

$$C_n(t) = 2^{-n/2} (n!)^{-1/2} \left(\frac{d^n F(u)}{du^n}\right) \Big|_{u=0} \quad (5.20)$$

Therefore, the probability that the system is in the n th excited state is

$$|C_n(t)|^2 = 2^{-n} (n!)^{-1} \left| \left(\frac{d^n F(u)}{du^n}\right) \Big|_{u=0} \right|^2 \quad (5.21)$$

It is shown in Appendix D5 that from Eq. (5.17) we can obtain

$$\begin{aligned}
 F(u) = & \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & + i(2\alpha)^{1/2} \exp(-i\omega t) X(\omega t) u \\
 & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} . \quad (5.22)
 \end{aligned}$$

From Eq. (5.20) for $n = 0$, the ground state the probability amplitude is

$$\begin{aligned}
 G_0(t) = & F(u)|_{u=0} \\
 = & \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} , \quad (5.23)
 \end{aligned}$$

which is exactly the same as Eq. (5.5). For $n = 1$ in the first excited state the probability amplitude is

$$C_1(t) = \frac{dF(u)}{du} \Big|_{u=0} = i\alpha^{1/2} \exp(-i\omega t) X(\omega t) C_0(t) \quad (5.24)$$

Thus, the probability is

$$|C_1(t)|^2 = |R(\omega t)|^2 P_0(t) \quad (5.25)$$

By a direct proof in Appendix D6, a general expression for the probability $|C_n(t)|^2$ in the n th excited state is obtained

$$P_n(t) = |C_n(t)|^2 = \frac{|R|^{2n}}{n!} \exp\{-|R(\omega t)|^2\} \quad (5.26)$$

where $R(\omega t)$ is defined in Eq. (5.7). The probability distribution is a Poisson distribution which is normalized to unity.

Figure 4 shows the $|C_n(t)|^2$ in Eq. (5.26) vs. ωt for $\alpha = 1$, $\theta = 0$, $\rho = 0.1$ for n from 1 to 6. The curve of $|C_0(t)|^2$ in Figure 1 for $\alpha = 1$, $\theta = 0$, $\rho = 0.1$ is quite different from those of $|C_n(t)|^2$ for excited states because of the multiplication coefficient $\frac{|R|^{2n}}{n!}$. Figure 5 shows the curves

$|C_n(t)|^2$ in Eqs. (5.9) and (5.26) vs. ωt for $\alpha = 1$, $\theta = 0$, $\rho = 0.1$ for n from 0 to 3. The sum of the probabilities for the ground state and the first three excited states is very close to unity. The contribution of the other excited states to the probability is negligible.

CHAPTER VI

CONVENTIONAL SOLUTIONS FOR THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

From the previous section we have obtained the gauge-invariant solutions for the probabilities in the ground state and excited states respectively. It is worthwhile to solve the conventional equations for the expansion coefficients. These absolute values of the expansion coefficient squared in the ground state and excited states are calculated and compared with the probabilities calculated in the previous section from the gauge-invariant formulation. The results are different, and, because of gauge invariance, the previous section gives the correct probabilities.

A. Ground State Solutions

We use a method similar to Section V to calculate the expansion coefficient a_0 in the ground state. It is obtained from Eq. (3.4) as $a_0 = \langle \phi_0 | \psi_1 \rangle$ or

$$a_0 = \langle \phi_0 | \exp \left\{ i \frac{2A(t)}{\hbar c} x \right\} | \psi' \rangle, \quad (6.1)$$

where Eq. (5.13) is used. This expression is not the same as C_0 because of the space- and time-dependent factor. Since

$E = -\frac{1}{c} \frac{\partial A}{\partial t}$, the vector potential is

$$A(t) = -c \int_0^* ds' E(s') = -\frac{cE_0}{\omega} X_0(\omega t) \quad (6.2)$$

where

$$X_0(\omega t) \equiv \int_0^Z ds f\left(\frac{s}{\omega}\right) \quad (6.3)$$

When Eq. (6.2) is substituted into Eq. (6.1) and the integral performed, the result for a_0 is shown in Appendix E1 to be

$$\begin{aligned} a_0(t) = \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X_0^2(\omega t) \right. \\ - \frac{g^2 E_0}{2mc\hbar\omega^2} \exp(-i\omega t) X(\omega t) A(t) \\ - \frac{g^2 A^2(t)}{4mc^2\hbar\omega} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ \left. + \alpha \cos \omega t \exp(-i\omega t) X_0^2(\omega t) \right\} \quad (6.4) \end{aligned}$$

The absolute value of a_0 squared as shown in Appendix E2 is

$$|a_0(\omega t)|^2 = \exp \left\{ -|D(\omega t)|^2 \right\} \quad (6.5)$$

where

$$D(\omega t) \equiv \alpha^{1/2} \left[\exp(-i\omega t) X(\omega t) - X_0(\omega t) \right] \quad (6.6)$$

and $\alpha \equiv \frac{q^2 E_0^2}{2m\hbar\omega^3}$. Equation (6.5) is obviously not the same as Eq. (5.6) for $P_0(t)$.

The expression in Eq. (6.5) for $|a_0(t)|^2$ can also be calculated for Eq. (5.7), as shown in Appendix E3, which gives

$$\begin{aligned} & |a_0(t)|^2 \\ &= \exp \left\{ -\alpha \left[\frac{2}{\rho(1+\rho)} \sin\left(\frac{1}{2}(1-\rho)Z - \theta\right) \sin\left(\frac{1}{2}(1+\rho)Z\right) (\cos\theta - \cos(\rho Z + \theta)) \right. \right. \\ &\quad \left. \left. + \frac{1}{\rho^2} (\cos\theta - \cos(\rho Z + \theta))^2 \right. \right. \\ &\quad \left. \left. - \frac{2}{\rho(1-\rho)} \sin\left(\frac{1}{2}(1+\rho)Z + \theta\right) \sin\left(\frac{1}{2}(1-\rho)Z\right) \right. \right. \\ &\quad \left. \left. \times (\cos\theta - \cos(\rho Z + \theta)) \right] \right\} P_0(t) \quad (6.7) \end{aligned}$$

If we set $\rho = 0$ and $\theta = 0$, then $|a_0(t)|^2 = 1$, where α and z can be any arbitrary numbers. It means that the system remains in the state $n = 0$ when no external electric field exists.

If we take $\rho = 1$, then we may use L'Hôpital's rule to obtain

$$\begin{aligned}
& |a_0(t)|^2_{\rho=1} \\
& = \exp\left\{-2\left[(\cos\theta - \cos(z+\theta))(\cos\theta - \cos(z+\theta))\right.\right. \\
& \quad \left.\left.- \sin\theta \sin z - z \sin(z+\theta)\right]\right\} [P_0(t)]_{\rho=1} \quad (6.8)
\end{aligned}$$

According to Eqs. (6.7) and (6.8), no matter what the other parameters are, we notice that $|a_0(t)|^2$ is always equal to unity when $z = 0$. It shows that the expression in Eq. (6.7) satisfies the initial condition imposed in Eq. (6.1).

From the comparison of Eqs. (5.9) and (6.7), we find that $|a_0(t)|^2$ has the same general exponential form, but is a different expression than $|c_0(t)|^2$. Figure 6 shows the curves of $|a_0(t)|^2$ in Eqs. (6.7) and (6.8) for $\alpha = 1$, $\theta = 0$, and ρ equals to 0.1, 0.5, 1, 1.5 and 2.

B. Excited States Solutions

The expansion coefficient for the system in the n th excited state at time t is $a_n = \langle \phi_n | \psi \rangle$, where ϕ_n is given by Eq. (5.14) and ψ by Eq. (5.13), with ψ' shown in Eq. (5.3). It is found that

$$a_n = 2^{-n/2} (n!)^{-1/2} \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar}x^2 + \frac{iqA(t)}{\hbar c}x\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \psi'(x,t). \quad (6.9)$$

We can construct the generating function¹⁴

$$F(v, x) = \exp(-v^2 + 2\sqrt{\frac{m\omega}{\hbar}} vx) = \sum_{n=0}^{\infty} \frac{v^n}{n!} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right), \quad (6.10)$$

which is the same as Eq. (5.16). If we define a function $G(v)$ as

$$G(v) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar} x^2 + i\frac{\mathcal{P}A(t)}{\hbar\omega} x\right) F(v, x) \psi'(x, t) \quad (6.11)$$

and substitute Eq. (6.10) into Eq. (6.11), then it becomes

$$G(v) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \sum_{n=0}^{\infty} \frac{v^n}{n!} \int_{-\infty}^{\infty} dx \exp\left(-\frac{m\omega}{2\hbar} x^2 + i\frac{\mathcal{P}A(t)}{\hbar\omega} x\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \psi'(x, t) \quad (6.12)$$

Using Eq. (6.9), we can write Eq. (6.11) as

$$G(v) = \sum_{n=0}^{\infty} \frac{v^n}{n!} a_n 2^{n/2} (n!)^{1/2} \quad (6.13)$$

so that $G(v)$ is a generating function for the expansion coefficient a_n . As a consequence of Eq. (6.13), we see that

$$a_n(t) = 2^{-n/2} (n!)^{-1/2} \left(\frac{d^n G(v)}{dv^n} \right) \Big|_{v=0} \quad (6.14)$$

Therefore, the absolute value of the expansion coefficient squared in the n th excited state is

$$|a_n(t)|^2 = 2^{-n} (n!)^{-1} \left| \left(\frac{d^n G(v)}{dv^n} \right) \Big|_{v=0} \right|^2 \quad (6.15)$$

It is shown in Appendix E4 that from Eq. (6.11) we can obtain

$$\begin{aligned}
G(r) = \exp \left\{ \frac{1}{4m\omega} \left[i \frac{\partial A(t)}{\partial \xi} + 2 \sqrt{\frac{m\omega}{\hbar}} r \right. \right. \\
\left. \left. + i \left(\frac{\partial^2 E_0}{\hbar \omega} \right) \exp(-i\omega t) X(\omega t) \right]^2 - \frac{r^2}{2} \right. \\
\left. - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \right. \\
\left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} . \quad (6.16)
\end{aligned}$$

From Eq. (6.14), for $n = 0$ in the ground state, the expansion coefficient is

$$\begin{aligned}
a_0(t) &= G(0) \\
&= \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
&\quad - \frac{\partial^2 E_0}{2m\hbar\omega^2} \exp(-i\omega t) X(\omega t) A(t) \\
&\quad - \frac{\partial^2 A^2(t)}{4m\omega^2\hbar\omega} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
&\quad \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} . \quad (6.17)
\end{aligned}$$

This expression is exactly equal to Eq. (6.4). For $n = 1$ in the first excited state, the expansion coefficient is

$$a_1(t) = \frac{dG(v)}{dv} \Big|_{v=0} = i \sqrt{\frac{\hbar}{m\omega}} \left[\frac{\partial A(t)}{\partial c} + \frac{\partial E_0}{\hbar \omega} \exp(-i\omega t) X(\omega t) \right] a_0(t). \quad (6.18)$$

From the relationship between $A(t)$ and $X_0(\omega t)$, as shown in Eq. (6.2), Eq. (6.18) can be rewritten as

$$a_1(t) = i D(\omega t) a_0(t), \quad (6.19)$$

where $D(\omega t)$ is defined in Eq. (6.6). Thus the absolute value of the expansion coefficient squared in the first excited state would be

$$|a_1(t)|^2 = |D(\omega t)|^2 |a_0(t)|^2. \quad (6.20)$$

By a direct proof, as shown in Appendix D6, a general expression for the absolute value of the expansion coefficient squared in the n th excited state can be obtained

$$|a_n(t)|^2 = \frac{|D|^2^n}{n!} \exp \{-|D|^2\}. \quad (6.21)$$

The $|a_n(t)|^2$ distribution is also a Poisson distribution and is normalized to unity. The curve of $|a_n(t)|^2$ is different from that of $|c_n(t)|^2$ for the same excited state. Figure 7 shows the curves of $|a_n|^2$ in Eqs. (6.7) and (6.21) vs. ωt for $\chi = 1$, $\theta = 0$, $\rho = 0.1$ as n varies from 0 to 6. It is obvious that Fig. 7 and Fig. 4 are not the same. We also found that the sum of $|a_n(t)|^2$ for the ground

state and the first six excited states in Fig. 7 is very close to 1. The contribution of the higher excited states is negligible until ωt is greater than 5 radians.

CHAPTER VII

ROTATING-WAVE APPROXIMATION

For frequencies such that the denominator $\omega - \Omega$ is very small, the first and third terms in Eq. (5.9) can be neglected compared to the second term. This approximation is called the rotating-wave approximation¹⁵ (RWA). The RWA is obtained if only a part of $f(t)$ shown in Eqs. (5.4) and (5.8) is used. This part gives the energy denominators $\omega - \Omega$, and is

$$f_{\text{RWA}}(t) = - \frac{e^{-i(\Omega t + \theta)}}{2i} \quad (7.1)$$

where Ω is the frequency of the electric field and θ is the phase angle.

A. Gauge-Invariant Formulation

If we use RWA when $\omega \approx \Omega$, then we should get the best results for the RWA. It is our purpose to test the RWA and see whether it is a good approximation in both the gauge-invariant and conventional approaches.

In Appendix F1 it is shown that when Eq. (7.1) is used in Eq. (5.6), it becomes

$$P_0(\text{RWA})(t) = \exp \left\{ - |R(\omega x)_{\text{RWA}}|^2 \right\}, \quad (7.2)$$

where

$$|R(\omega t)_{RWA}|^2 = \alpha \left[\frac{\sin^2(\frac{1}{2}(1-\rho)Z)}{1-\rho^2} \right] \quad (7.3)$$

If we assume $\rho = 0.9$ and 1.1 and substitute them into Eqs. (7.3) and (5.9), the differences between the two probabilities are not very great. For the case of $\rho = 1$, L'Hôpital's rule gives

$$P_0(RWA)(t)|_{\rho=1} = \exp \left\{ -|R(\omega t)_{RWA}|_{\rho=1}^2 \right\}, \quad (7.4)$$

where

$$|R(\omega t)_{RWA}|_{\rho=1}^2 = \frac{\alpha}{4} Z^2. \quad (7.5)$$

The exact result in the case where $\rho = 1$ is given in Eq. (5.10). The RWA keeps the dominant term and neglects the other terms in Eq. (5.10).

Substituting Eqs. (7.3) and (7.5) into Eq. (5.26), we find that the probability of the system in the n th state in the RWA can be obtained for both the $\rho \neq 1$ and $\rho = 1$ cases. Figure 8 shows the curves of the ground state probability in the RWA in Eq. (7.4) for $\alpha = 1$, $\rho = 1$ and the probability in Eq. (5.10) for $\alpha = 1$, $\rho = 1$, $\theta = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}$. Figure 9 shows the curves of probability in the RWA of the first excited state

B. Conventional Formulation

The rotating-wave approximation can also be used in the conventional approach. As shown previously, the values in the gauge-invariant and conventional approaches are not the same. We shall test the validity of the RWA for the conventional approach here.

It is shown in Appendix F2 that, in the RWA Eq. (6.5) can be written as

$$|J_0(RWA)(t)|^2 = \exp \{-|D_{RWA}(\omega t)|^2\} \quad (7.6)$$

where

$$|D_{RWA}(\omega t)|^2 = 2 \left[\frac{\sin^2\left(\frac{1}{2}(1-\rho)Z\right)}{(1-\rho)^2} + \frac{\sin^2\left(\frac{1}{2}\rho Z\right)}{\rho^2} - \frac{2}{\rho(1-\rho)} \cos\left(\frac{Z}{2}\right) \sin\left(\frac{(1-\rho)Z}{2}\right) \sin\left(\frac{\rho Z}{2}\right) \right] \quad (7.7)$$

When $\rho = 0.9$ and 1.1 are substituted into Eqs. (7.6) and (6.7), we find that their results are close. For the values of ρ far from unity, the RWA is not a good approximation.

For the case of $\rho = 1$, L'Hôpital's rule is used to give

$$|J_0(RWA)(t)|_{\rho=1}^2 = \exp \{-|D_{RWA}(\omega t)|_{\rho=1}^2\} \quad (7.8)$$

where

$$|D_{RWA}(Wt)|_{\rho=1}^2 = \alpha \left[\frac{z^2}{4} + \sin^2 \frac{z}{2} - \frac{z}{2} \sin z \right] \quad (7.9)$$

Even when the RWA is used in both of the two approaches, the results of the gauge-invariant approach is still different from that of the conventional approach.

If we substitute Eqs. (7.7) and (7.9) into Eq. (6.21), then we obtain the absolute value of the expansion coefficient squared $|a_n(t)|^2$ of the system in the n th state in the RWA for both the $\rho \neq 1$ and $\rho = 1$ cases. Figure 10 shows the curves of $|a_0(t)|^2$ in the RWA in Eq. (7.8) for $\alpha = 1$ and $\rho = 1$, and the curves of $|a_0(t)|^2$ in Eq. (6.8) for $\alpha = 1$, $\rho = 1$, and $\theta = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}$ in the ground state. Figure 11 shows the curves of $|a_1(t)|^2$ in the RWA in Eq. (7.6) for $\alpha = 1$, $\theta = 0$ and ρ equals to 0.5, 0.7, 0.9, 1, 1.1, 1.3, 1.5.

CHAPTER VIII

CONCLUSION

In this thesis I have studied the role of gauge transformations in the quantum theory of the interaction of the electromagnetic field and matter. The importance of gauge invariance has been emphasized. When the electric dipole approximation (EDA) can be made, the gauge-invariant equations simplify in the gauge where $\vec{A}' = 0$ and $A_0 = -\vec{E}(t) \cdot \vec{r}$.

My simple model is a single spinless one-dimensional harmonic oscillator in a time-varying electromagnetic field in the EDA. The differences between the electric dipole interaction and the $\vec{A} \cdot \vec{p}$ interaction were illustrated by calculating the absolute values of the expansion coefficient squared in a given state. The calculation using the $\vec{A} \cdot \vec{p}$ interaction gave a different result from the $\vec{E} \cdot \vec{r}$ interaction. There thus two different expressions that are usually interpreted as the probability that the system is in the same state at time t . In principle there cannot be two different values for something that is observable. On theoretical grounds, the $\vec{A} \cdot \vec{p}$ calculation can be rejected, because the expansion coefficients in the wave function are gauge-dependent and thus cannot be true probability amplitudes in general.

It is shown that the rotating-wave approximation remains a reasonable approximation compared to the exact solution when $\omega \approx \Omega$ for either the gauge-invariant or the conventional approach.

The results of this investigation show that the gauge-invariant formulation gives different results from the conventional approach. The principle of gauge invariance says that the gauge-invariant results are correct, while the conventional results are wrong. However, the ultimate test of the theory is experimental. An effort is being made to make predictions of the gauge-invariant formulation which can be confirmed experimentally. The conditions under which the gauge-invariant formulation and the conventional formulation give the same results will also be investigated.

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APPENDIX A1

Form Invariance of Schrödinger Equation

Equation (2.4) can be written as

$$\psi = \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \psi' \quad . \quad (\text{A1.1})$$

We define $\vec{\pi}$ as

$$\vec{\pi} = \left(\vec{p} - \frac{g}{c} \vec{A}\right) \quad , \quad (\text{A1.2})$$

then it is obtained that

$$\begin{aligned} \vec{\pi} \psi &= \left(\vec{p} - \frac{g}{c} \vec{A}\right) \psi \\ &= \left(-i \hbar \nabla - \frac{g}{c} \vec{A}\right) \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \psi' \\ &= \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \left(\vec{p} - \frac{g}{c} \vec{A}'\right) \psi' \quad . \end{aligned} \quad (\text{A1.3})$$

With the help of Eq. (2.5), we can also transform π^2 ,

$$\begin{aligned} \pi^2 \psi &= \left(\vec{p} - \frac{g}{c} \vec{A}\right)^2 \psi = \vec{\pi} \cdot \vec{\pi} \psi \\ &= \vec{\pi} \cdot \vec{\pi} \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \psi' \\ &= \vec{\pi} \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \cdot \left(\vec{p} - \frac{g}{c} \vec{A}'\right) \psi' \\ &= \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \left(\vec{p} - \frac{g}{c} \vec{A}'\right) \cdot \left(\vec{p} - \frac{g}{c} \vec{A}'\right) \psi' \\ &= \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \left(\vec{p} - \frac{g}{c} \vec{A}'\right)^2 \psi' \quad . \end{aligned} \quad (\text{A1.4})$$

The left-hand side of Eq. (2.1) now becomes

$$\left[\frac{1}{2m} \left(\vec{p} - \frac{g}{c} \vec{A}\right)^2 + V + g A_0 \right] \psi = \exp\left(-\frac{i g \Lambda}{c \hbar}\right) \left[\frac{1}{2m} \left(\vec{p} - \frac{g}{c} \vec{A}'\right)^2 + V + g A_0 \right] \psi' \quad , \quad (\text{A1.5})$$

the right-hand side of Eq. (2.1) is

$$\begin{aligned}
 i\hbar \frac{\partial \psi}{\partial t} &= i\hbar \frac{\partial}{\partial t} \left[\exp\left(-\frac{i q \Lambda}{c \hbar}\right) \psi' \right] \\
 &= \exp\left(-\frac{i q \Lambda}{c \hbar}\right) \left[\frac{q}{c} \frac{\partial \Lambda}{\partial t} + i\hbar \frac{\partial}{\partial t} \right] \psi' .
 \end{aligned} \tag{A1.6}$$

From the combination of Eqs. (A1.5) and Eq. (A1.6) with the cancellation of $\exp\left(-\frac{i q \Lambda}{c \hbar}\right)$, we obtain

$$\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 \psi' + V \psi' + q \left(A_0 - \frac{1}{c} \frac{\partial \Lambda}{\partial t} \right) \psi' = i\hbar \frac{\partial \psi'}{\partial t} . \tag{A1.7}$$

Now, we substitute Eq. (2.6) into Eq. (A1.7), the result is

$$\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 \psi' + V \psi' + q A_0 \psi' = i\hbar \frac{\partial \psi'}{\partial t} . \tag{2.7}$$

which is exactly the same as Eq. (2.7)

APPENDIX A2

Gauge Invariance of the Magnetic Induction and the Electric Field

The magnetic induction is

$$\vec{B} = \nabla \times \vec{A} \quad (2.9)$$

If Eq. (2.5) is substituted into Eq. (2.9), then

$$\begin{aligned} \vec{B} &= \nabla \times (\vec{A}' - \nabla \lambda) \\ &= \nabla \times \vec{A}' - \nabla \times \nabla \lambda \\ &= \nabla \times \vec{A}' \end{aligned} \quad (A2.1)$$

From the comparison of Eq. (2.9) and Eq. (A2.1),
the magnetic induction is gauge-invariant.

Likewise, if we substitute Eqs. (2.5) and (2.6) into
Eq. (2.10), then

$$\begin{aligned} \vec{E} &= -\nabla \left[A_0' + \frac{1}{c} \frac{\partial \lambda}{\partial t} \right] - \frac{1}{c} \frac{\partial}{\partial t} (\vec{A}' - \nabla \lambda) \\ &= -\nabla A_0' - \frac{1}{c} \frac{\nabla \partial \lambda}{\partial t} - \frac{1}{c} \frac{\partial \vec{A}'}{\partial t} + \frac{1}{c} \frac{\partial \nabla \lambda}{\partial t} \\ &= -\nabla A_0' - \frac{1}{c} \frac{\partial \vec{A}'}{\partial t} \end{aligned} \quad (A2.2)$$

Comparing Eq. (A2.2) to Eq. (2.10), the electric field is
obviously gauge-invariant.

APPENDIX A3

Form Invariance of Kinetic Momentum and Eq. (2.16)

With the definition of Eq. (2.13), the operator

$(\vec{p} - \frac{q}{c} \vec{A})'$ becomes

$$(\vec{p} - \frac{q}{c} \vec{A})' \psi' = \exp\left(\frac{iq\Lambda}{c\hbar}\right) (\vec{p} - \frac{q}{c} \vec{A}) \exp\left(-\frac{iq\Lambda}{c\hbar}\right) \psi'. \quad (\text{A3.1})$$

If Eq. (A1.3) is substituted into Eq. (A3.1), then

$$\begin{aligned} (\vec{p} - \frac{q}{c} \vec{A})' \psi' &= \exp\left(\frac{iq\Lambda}{c\hbar}\right) \exp\left(-\frac{iq\Lambda}{c\hbar}\right) (\vec{p} - \frac{q}{c} \vec{A}') \psi' \\ &= (\vec{p} - \frac{q}{c} \vec{A}') \psi'. \end{aligned}$$

Thus, we obtain Eq. (2.15).

Likewise, with the help of Eqs. (2.13) and (2.6), the operator $(i\hbar \frac{\partial}{\partial t} - qA_0)'$ becomes

$$\begin{aligned} (i\hbar \frac{\partial}{\partial t} - qA_0)' \psi' &= \exp\left(\frac{iq\Lambda}{c\hbar}\right) (i\hbar \frac{\partial}{\partial t} - qA_0) \exp\left(-\frac{iq\Lambda}{c\hbar}\right) \psi' \\ &= \exp\left(\frac{iq\Lambda}{c\hbar}\right) \left[i\hbar \left(-\frac{iq}{c\hbar}\right) \frac{\partial \Lambda}{\partial t} - qA_0 \right] \exp\left(-\frac{iq\Lambda}{c\hbar}\right) \psi' \\ &\quad + \exp\left(\frac{iq\Lambda}{c\hbar}\right) (i\hbar) \exp\left(-\frac{iq\Lambda}{c\hbar}\right) \frac{\partial \psi'}{\partial t} \\ &= -q \left[A_0 - \frac{1}{c} \frac{\partial \Lambda}{\partial t} \right] \psi' + i\hbar \frac{\partial \psi'}{\partial t} \\ &= (i\hbar \frac{\partial}{\partial t} - qA_0') \psi'. \end{aligned} \quad (\text{A3.2})$$

Thus, we obtain Eq. (2.16).

APPENDIX A4

Gauge Transformation of the Hamiltonian

With the definition of Eq. (2.13), the gauge-transformed Hamiltonian operator $H'(\vec{A}, A_0)$ is

$$H'(\vec{A}, A_0)\psi' = \exp\left(\frac{i q \Lambda}{c \hbar}\right) H(\vec{A}, A_0) \exp\left(-\frac{i q \Lambda}{c \hbar}\right) \psi' , \quad (\text{A4.1})$$

where the Hamiltonian is given in Eq. (2.3). If we substitute Eq. (A1.4) into Eq. (A4.1), it is obtained that

$$\begin{aligned} & H'(\vec{A}, A_0)\psi' \\ &= \exp\left(\frac{i q \Lambda}{c \hbar}\right) \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + V + q A_0 \right] \exp\left(-\frac{i q \Lambda}{c \hbar}\right) \psi' \\ &= \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 + V + q A_0 \right] \psi' \\ &= H(\vec{A}', A_0) \psi' . \end{aligned} \quad (\text{A4.2})$$

If Eq. (2.6) is substituted into Eq. (A4.2), we obtain

$$\begin{aligned} H'(\vec{A}, A_0) &= H(\vec{A}', A_0) \\ &= \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}' \right)^2 + V + q \left(A_0' + \frac{1}{c} \frac{\partial \Lambda}{\partial t} \right) \\ &= H(\vec{A}', A_0') + \frac{q}{c} \frac{\partial \Lambda}{\partial t} . \end{aligned} \quad (17)$$

APPENDIX A5

Gauge Invariance of the Energy Operator

According to Eq. (2.17), when the scalar potential $A_0 \neq 0$, then

$$H'(\vec{A}, A_0) = H(\vec{A}', A_0) \quad . \quad (A5.1)$$

The operator $H(\vec{A}, A_0)$ is defined in Eq. (2.18) as

$$H(\vec{A}, A_0) = H(\vec{A}, 0) + qA_0 \quad . \quad (A5.2)$$

Thus, from Eq. (2.13) and (A5.1), it becomes

$$H'(\vec{A}, A_0) = H'(\vec{A}, 0) + qA_0 = H(\vec{A}', A_0) = H(\vec{A}', 0) + qA_0 \quad .$$

Therefore,

$$H'(\vec{A}, 0) = H(\vec{A}', 0) \quad , \quad (2.19)$$

when the scalar potential is cancelled.

APPENDIX A6

Derivation of Energy Conservation Condition

Using the Schrödinger equation in Eq. (2.2)

$$H(\vec{A}, A_0)\psi = i\hbar \frac{\partial \psi}{\partial t} \quad , \quad (2.2)$$

the time rate of change of the average value of $H(\vec{A}, 0)$ is

$$\begin{aligned} \frac{d}{dt} \langle \psi | H(\vec{A}, 0) \psi \rangle &= \langle \frac{\partial \psi}{\partial t} | H(\vec{A}, 0) \psi \rangle + \langle \psi | \frac{\partial H(\vec{A}, 0)}{\partial t} \psi \rangle \\ &\quad + \langle \psi | H(\vec{A}, 0) \frac{\partial \psi}{\partial t} \rangle \quad . \end{aligned} \quad (A6.1)$$

Thus, Eq. (A6.1) can be rewritten as

$$\begin{aligned} \frac{d}{dt} \langle \psi | H(\vec{A}, 0) \psi \rangle &= -\frac{1}{i\hbar} \langle \psi | H(\vec{A}, A_0) H(\vec{A}, 0) \psi \rangle \\ &\quad + \langle \psi | \frac{\partial H(\vec{A}, 0)}{\partial t} \psi \rangle + \frac{1}{i\hbar} \langle \psi | H(\vec{A}, 0) H(\vec{A}, A_0) \psi \rangle \\ &= \frac{1}{i\hbar} \langle \psi | [H(\vec{A}, 0) H(\vec{A}, A_0) - H(\vec{A}, A_0) H(\vec{A}, 0)] \psi \rangle \\ &\quad + \langle \psi | \frac{\partial H(\vec{A}, A_0)}{\partial t} \psi \rangle \quad . \end{aligned} \quad (A6.2)$$

where the Hermitian property of the Hamiltonian has been used. Therefore,

$$\begin{aligned} &\frac{d}{dt} \langle \psi | H(\vec{A}, 0) \psi \rangle \\ &= \frac{1}{i\hbar} \langle \psi | [H(\vec{A}, 0), H(\vec{A}, A_0)] \psi \rangle + \langle \psi | \frac{\partial H(\vec{A}, 0)}{\partial t} \psi \rangle \\ &= -\frac{i}{\hbar} \langle \psi | [H(\vec{A}, 0), \int A_0] + [i\hbar \frac{\partial}{\partial t}, H(\vec{A}, 0)] \psi \rangle \\ &= -\frac{i}{\hbar} \langle \psi | [i\hbar \frac{\partial}{\partial t} - \int A_0, H(\vec{A}, 0)] \psi \rangle \\ &= \langle \psi | P \psi \rangle \end{aligned} \quad (2.20)$$

The power operator $\mathcal{P}$ is

$$\mathcal{P} = -\frac{i}{\hbar} \left[i\hbar \frac{\partial}{\partial t} - qA_0, H(\vec{A}, 0) \right] \quad (2.21)$$

The power operator $\mathcal{P}$ is gauge invariant, as all physical observables must be, because of Eq. (2.16) and (2.19).

APPENDIX A7

Derivation of the Power Operator

Because of Eq. (2.21), we know that

$$\begin{aligned}
 P\psi &= -\frac{i}{\hbar} [i\hbar \frac{\partial}{\partial t} - qA_0, H(\vec{A}, 0)]\psi \\
 &= -\frac{i}{\hbar} [i\hbar \frac{\partial}{\partial t}, H(\vec{A}, 0)]\psi + \frac{i}{\hbar} [qA_0, H(\vec{A}, 0)]\psi \\
 &= [\frac{\partial}{\partial t}, \frac{1}{2m}(\vec{p} - \frac{q}{c}\vec{A})^2 + V]\psi + \frac{iq}{\hbar} [A_0, \frac{1}{2m}(\vec{p} - \frac{q}{c}\vec{A})^2]\psi \\
 &= \frac{1}{2m} [\frac{\partial}{\partial t}, (\vec{p} - \frac{q}{c}\vec{A})^2]\psi + \frac{iq}{2m\hbar} [A_0, (\vec{p} - \frac{q}{c}\vec{A})^2]\psi.
 \end{aligned}$$

(A7.1)

Since

$$[X, Y'] = -\{Y[Y, X] + [Y, X]Y\},$$

(A7.2)

thus

$$\begin{aligned}
 P\psi &= -\frac{1}{2m} \{(\vec{p} - \frac{q}{c}\vec{A}) \cdot [\vec{p} - \frac{q}{c}\vec{A}, \frac{\partial}{\partial t}]\psi \\
 &\quad + [\vec{p} - \frac{q}{c}\vec{A}, \frac{\partial}{\partial t}] \cdot (\vec{p} - \frac{q}{c}\vec{A})\psi\} \\
 &\quad - \frac{iq}{2m\hbar} \{(\vec{p} - \frac{q}{c}\vec{A}) \cdot [\vec{p} - \frac{q}{c}\vec{A}, A_0]\psi \\
 &\quad + [\vec{p} - \frac{q}{c}\vec{A}, A_0] \cdot (\vec{p} - \frac{q}{c}\vec{A})\psi\} \\
 &= -\frac{1}{2m} \{(\vec{p} - \frac{q}{c}\vec{A}) \cdot [-\frac{q}{c}\vec{A}; \frac{\partial}{\partial t}]\psi \\
 &\quad + [-\frac{q}{c}\vec{A}, \frac{\partial}{\partial t}] \cdot (\vec{p} - \frac{q}{c}\vec{A})\psi\} \\
 &\quad - \frac{iq}{2m\hbar} \{(\vec{p} - \frac{q}{c}\vec{A}) \cdot [\vec{p}, A_0]\psi \\
 &\quad + [\vec{p}, A_0] \cdot (\vec{p} - \frac{q}{c}\vec{A})\psi\}
 \end{aligned}$$

$$\begin{aligned}
&= -\frac{\hbar}{2m} \left\{ \left(\vec{p} - \frac{q}{c} \vec{A} \right) \cdot \frac{1}{c} \frac{\partial \vec{A}}{\partial t} + \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right) \right\} \psi \\
&\quad - \frac{i\hbar q}{2m} \left\{ \left(\vec{p} - \frac{q}{c} \vec{A} \right) \cdot (-i\hbar \nabla A_0) - i\hbar \nabla A_0 \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right) \right\} \psi \\
&= \frac{\hbar}{2} \left[\frac{1}{m} \left(\vec{p} - \frac{q}{c} \vec{A} \right) \cdot \left(-\nabla A_0 - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right) \right. \\
&\quad \left. + \frac{1}{m} \left(-\nabla A_0 - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right) \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right) \right] \psi .
\end{aligned} \tag{A7.3}$$

From Eqs. (2.10) and (2.23), Eq. (A7.3) can be written as

$$p\psi = \frac{\hbar}{2} (\vec{v} \cdot \vec{E} + \vec{E} \cdot \vec{v}) \psi , \tag{A7.4}$$

which means the power operator is

$$p = \frac{\hbar}{2} (\vec{v} \cdot \vec{E} + \vec{E} \cdot \vec{v}) . \tag{A7.5}$$

This expression is the Hermitian operator of the classical power.

APPENDIX A8

Derivation of the Equation of Motion for the Probability Amplitudes

In this Appendix, Eq. (2.27) is derived from Eqs. (2.2), (2.18), (2.26) and (2.25). If we substitute Eq. (2.26) into the right hand side of Eq. (2.2), we obtain

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= i\hbar \frac{\partial}{\partial t} \left[\sum_m C_m(t) \psi_m \right] \\ &= i\hbar \sum_m \frac{\partial C_m(t)}{\partial t} \psi_m + i\hbar \sum_m C_m(t) \frac{\partial \psi_m}{\partial t} \end{aligned} \quad (\text{A8.1})$$

If Eqs. (2.18), (2.25) and Eq. (2.26) are substituted into the left hand side of Eq. (2.2), we obtain

$$H(\vec{A}, A_0) \psi = \sum_m E_m C_m \psi_m + \sum_m g A_0 C_m \psi_m \quad (\text{A8.2})$$

If Eqs. (A8.1) and (A8.2) are equated, we obtain

$$\begin{aligned} \sum_m E_m(t) C_m(t) \psi_m + g A_0 \sum_m C_m(t) \psi_m \\ = i\hbar \sum_m \dot{C}_m(t) \psi_m + i\hbar \sum_m C_m(t) \frac{\partial \psi_m}{\partial t} \end{aligned} \quad (\text{A8.3})$$

The inner product of Eq. (A8.3) with ψ_n is

$$\begin{aligned} \langle \psi_n | \sum_m E_m(t) C_m(t) \psi_m \rangle + \langle \psi_n | \sum_m g A_0 C_m(t) \psi_m \rangle \\ = i\hbar \langle \psi_n | \sum_m \dot{C}_m(t) \psi_m \rangle + i\hbar \langle \psi_n | \sum_m C_m(t) \frac{\partial \psi_m}{\partial t} \rangle \end{aligned} \quad (\text{A8.4})$$

When the orthonormality of the $\{\psi_m\}$ is used, Eq. (A8.4) becomes

$$\begin{aligned}
& \epsilon_n(t) c_n(t) + \sum_m \langle \psi_n | \mathcal{H} A_0 \psi_m \rangle c_m \\
&= i\hbar \dot{c}_n(t) + \sum_m \langle \psi_n | i\hbar \frac{\partial \psi_m}{\partial t} \rangle c_m .
\end{aligned} \tag{A8.5}$$

Therefore, we obtain

$$i\hbar \dot{c}_n(t) = \epsilon_n(t) c_n(t) + \sum_m \langle \psi_n | (\mathcal{H} A_0 - i\hbar \frac{\partial}{\partial t}) \psi_m \rangle c_m . \tag{2.27}$$

APPENDIX B1

Proof of $\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p}$ Under Coulomb Gauge

The Coulomb gauge condition is

$$\nabla \cdot \vec{A} = 0 . \quad (3.6)$$

Since

$$\vec{p} \cdot (\vec{A}\psi) = (\vec{p} \cdot \vec{A})\psi + \vec{A} \cdot (\vec{p}\psi) . \quad (B1.1)$$

The first term on the right-hand side of Eq. (B1.1) is

$$(\vec{p} \cdot \vec{A})\psi = i\hbar(\nabla \cdot \vec{A})\psi = 0 . \quad (B1.2)$$

Thus,

$$\vec{p} \cdot (\vec{A}\psi) = \vec{A} \cdot (\vec{p}\psi) , \quad (B1.3)$$

which means

$$\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p} . \quad (3.7)$$

result is $\vec{A}(\vec{r}, t)$, which cancels the $\vec{A}(\vec{r}, t)$ on the right hand side of Eq. (C1.2). We are left with

$$\vec{A}'(\vec{r}, t) = -\vec{r} \times \int_0^1 du [\nabla \times \vec{A}(u\vec{r}, t)] \quad (C1.4)$$

Since

$$\nabla \times \vec{A}(u\vec{r}, t) = u\vec{B}(u\vec{r}, t) \quad (C1.5)$$

from Eq. (C1.4) it can be written as Eq. (4.3)

APPENDIX C1

The New Vector Potential in the Multipolar Gauge

When the gauge function of Eq. (4.2) is substituted into Eq. (2.5) for the new vector potential, we get

$$\vec{A}'(\vec{r}, t) = \vec{A}(\vec{r}, t) - \int_0^1 du \nabla [\vec{r} \cdot \vec{A}(u\vec{r}, t)] \quad (C1.1)$$

When the vector identity for the gradient of a dot product is used, Eq. (C1.1) becomes

$$\begin{aligned} \vec{A}'(\vec{r}, t) = \vec{A}(\vec{r}, t) - \int_0^1 du \{ & [\vec{r} \cdot \nabla] \vec{A}(u\vec{r}, t) + [\vec{A}(u\vec{r}, t) \cdot \nabla] \vec{r} \\ & + \vec{r} \times [\nabla \times \vec{A}(u\vec{r}, t)] + \vec{A}(u\vec{r}, t) \times (\nabla \times \vec{r}) \} \quad (C1.2) \end{aligned}$$

The last term vanishes and the first two terms in the integrand combine to give

$$\begin{aligned} & (\vec{r} \cdot \nabla) \vec{A}(u\vec{r}, t) + (\vec{A}(u\vec{r}, t) \cdot \nabla) \vec{r} \\ & = \left(u \frac{\partial u\vec{r}}{\partial u} \frac{\partial}{\partial(u\vec{r})} \right) \vec{A}(u\vec{r}, t) + \vec{A}(u\vec{r}, t) \\ & = u \frac{\partial \vec{A}(u\vec{r}, t)}{\partial u} + \vec{A}(u\vec{r}, t) \\ & = \frac{d}{du} [u \vec{A}(u\vec{r}, t)] \quad (C1.3) \end{aligned}$$

When Eq. (C1.3) is integrated on u from 0 to 1, the

APPENDIX C2

The New Scalar Potential in the Multipolar Gauge

When the gauge function of Eq. (4.2) is substituted into Eq. (2.6) for the new scalar potential, we get

$$A_0'(\vec{r}, t) = A_0(\vec{r}, t) - \frac{1}{c} \frac{\partial \Lambda(0, t)}{\partial t} + \frac{1}{c} \int_0^1 du \vec{r} \cdot \frac{\partial \vec{A}(u\vec{r}, t)}{\partial t} \quad (C2.1)$$

Since by the chain rule,

$$\frac{dA_0(u\vec{r}, t)}{du} = \left[\frac{\partial A_0(u\vec{r}, t)}{\partial (u\vec{r})} \right] \cdot \left[\frac{\partial (u\vec{r})}{\partial u} \right], \quad (C2.2)$$

the old scalar potential $A_0(\vec{r}, t)$ can be written as

$$A_0(\vec{r}, t) = \int_0^1 du \vec{r} \cdot \frac{\partial A_0(u\vec{r}, t)}{\partial (u\vec{r})} + A_0(0, t) \quad (C2.3)$$

Therefore, Eq. (C2.1) becomes

$$\begin{aligned} A_0'(\vec{r}, t) = & \int_0^1 du \vec{r} \cdot \left[\frac{\partial A_0(u\vec{r}, t)}{\partial (u\vec{r})} + \frac{1}{c} \frac{\partial \vec{A}(u\vec{r}, t)}{\partial t} \right] \\ & + A_0(0, t) - \frac{1}{c} \frac{\partial \Lambda(0, t)}{\partial t} \end{aligned} \quad (C2.4)$$

If we choose the gauge so that the last two terms cancel, and use Eq. (2.10), we obtain

$$A_0'(\vec{r}, t) = - \int_0^1 du \vec{r} \cdot \vec{E}(u\vec{r}, t) \quad (4.4)$$

APPENDIX C3

Derivation of the Magnetic Field From the Multipole Expansion for the Potentials in the Multipolar Gauge

When Eq. (4.5) is used in Eq. (2.9) for the magnetic field, since the magnetic induction is gauge-invariant,

$$\vec{B} = \nabla \times \vec{A} = \nabla \times \vec{A}' \quad (2.9)$$

Thus, from Eqs. (2.9) and (4.5), the magnetic induction becomes

$$\nabla \times \vec{A}' = -\frac{1}{2} \nabla \times [\vec{r} \times \vec{B}(0,t) + \dots] \quad (C3.1)$$

If we use the vector identity¹⁶

$$\begin{aligned} \nabla \times (\vec{F} \times \vec{G}) &= (\vec{G} \cdot \nabla) \vec{F} - \vec{G} (\nabla \cdot \vec{F}) \\ &\quad - (\vec{F} \cdot \nabla) \vec{G} + \vec{F} (\nabla \cdot \vec{G}) \end{aligned} \quad (C3.2)$$

in Eq. (C3.1), it becomes

$$\begin{aligned} \vec{B}(\vec{r}, t) &= -\frac{1}{2} \left\{ \vec{B}(0,t) \cdot \nabla \vec{r} - \vec{B}(0,t) \nabla \cdot \vec{r} \right. \\ &\quad \left. - (\vec{r} \cdot \nabla) \vec{B}(0,t) + \vec{r} [\nabla \cdot \vec{B}(0,t)] + \dots \right\} \end{aligned} \quad (C3.3)$$

Because $\vec{B}(0,t)$ is space independent, the third term and fourth term on the right hand side in Equation (C3.3) both vanish therefore Eq. (4.7) is obtained

$$\begin{aligned} \vec{B}(\vec{r}, t) &= -\frac{1}{2} \left\{ \vec{B}(0,t) - 3\vec{B}(0,t) + \dots \right\} \\ &= \vec{B}(0,t) + \dots \end{aligned}$$

APPENDIX C4

Derivation of the Electric Field From the Multipole Expansion for the Potentials in the Multipolar Gauge

When Eqs. (4.5) and (4.6) are used in Eq. (2.10) for the electric field, since the electric field is gauge-invariant,

$$\vec{E} = -\nabla A_0' - \frac{1}{c} \frac{\partial \vec{A}'}{\partial t} \quad (2.10)$$

The gradient of A_0' in Eq. (4.6) is

$$\begin{aligned} \nabla A_0' &= \nabla \left\{ -\vec{r} \cdot \vec{E}(0, t) - \frac{1}{2} x_i x_j \partial_j' E_i(\vec{r}', t) + \dots \right\} \Big|_{\vec{r}'=0} \\ &= \partial_k \hat{x}_k \left\{ -x_i E_i(0, t) - \frac{1}{2} x_i x_j \partial_j' E_i(0, t) + \dots \right\} \\ &= -\delta_{ik} E_i(0, t) \hat{x}_k - \frac{1}{2} \hat{x}_k \left\{ \delta_{ik} x_j \partial_j' E_i(0, t) \right. \\ &\quad \left. + \delta_{jk} x_i \partial_j' E_i(0, t) \right\} + \dots \\ &= -E_k(0, t) \hat{x}_k - \frac{1}{2} \hat{x}_k x_j \partial_j' E_k(0, t) \\ &\quad - \frac{1}{2} \hat{x}_k x_i \partial_k' E_i(0, t) + \dots \\ &= -E(0, t) - \frac{1}{2} (\vec{r}' \cdot \nabla') \vec{E}(0, t) - \frac{1}{2} \nabla' (\vec{r}' \cdot \vec{E}(0, t)) \\ &\quad + \dots \end{aligned} \quad (C4.1)$$

where the definition of the derivative is

$$\partial_j' E_i(0, t) = \left\{ \partial E_i(\vec{r}', t) / \partial x_j' \right\} \Big|_{\vec{r}'=0}$$

If we use the vector identity¹⁶

$$\nabla(\vec{F} \cdot \vec{G}) = (\vec{G} \cdot \nabla)\vec{F} + (\vec{F} \cdot \nabla)\vec{G} + \vec{G} \times (\nabla \times \vec{F}) + \vec{F} \times (\nabla \times \vec{G}) \quad , \quad (C4.2)$$

the last term on the right hand side in Eq. (C4.1) becomes

$$\begin{aligned} \nabla'(\vec{r} \cdot \vec{E}(0,t)) &= (\vec{E}(0,t) \cdot \nabla')\vec{r} + (\vec{r} \cdot \nabla')\vec{E}(0,t) \\ &\quad + \vec{E}(0,t) \times (\nabla' \times \vec{r}) \\ &\quad + \vec{r} \times (\nabla' \times \vec{E}(0,t)) \quad , \end{aligned} \quad (C4.3)$$

The first and third term vanish in Eq. (C4.3) because $\vec{r}$ is independent of the prime del operator. By Faraday's law we obtain that

$$\nabla' \times \vec{E}(\vec{r}',t) = -\frac{1}{c} \frac{\partial \vec{B}(\vec{r}',t)}{\partial t} \quad , \quad (C4.4)$$

which also satisfies

$$\nabla' \times \vec{E}(\vec{r}',t) \Big|_{\vec{r}'=0} = -\frac{1}{c} \frac{\partial \vec{B}(\vec{r}',t)}{\partial t} \Big|_{\vec{r}'=0} \quad . \quad (C4.5)$$

Therefore, we get

$$\begin{aligned} \nabla A_0' &= -\vec{E}(0,t) - \frac{1}{2}(\vec{r} \cdot \nabla')\vec{E}(\vec{r}',t) \Big|_{\vec{r}'=0} \\ &\quad - \frac{1}{2}(\vec{r} \cdot \nabla')\vec{E}(\vec{r}',t) \Big|_{\vec{r}'=0} \\ &\quad - \frac{1}{2}\vec{r} \times \left(-\frac{\partial \vec{B}(\vec{r}',t)}{\partial t}\right) \Big|_{\vec{r}'=0} + \dots \\ &= -\vec{E}(0,t) - (\vec{r} \cdot \nabla')\vec{E}(\vec{r}',t) \Big|_{\vec{r}'=0} \\ &\quad + \frac{1}{2}\vec{r} \times \frac{1}{c} \frac{\partial \vec{B}(\vec{r}',t)}{\partial t} \Big|_{\vec{r}'=0} + \dots \quad . \end{aligned} \quad (C4.6)$$

If we substitute Eqs. (4.5) and (C4.6) into Eq. (2.10), we obtain

$$\begin{aligned}
 \vec{E}(\vec{r}, t) &= \vec{E}(0, t) + (\vec{r} \cdot \nabla') \vec{E}(\vec{r}', t) \Big|_{\vec{r}'=0} \\
 &\quad - \frac{1}{2} \vec{r} \times \frac{1}{c} \frac{\partial \vec{B}(\vec{r}', t)}{\partial t} \Big|_{\vec{r}'=0} \\
 &\quad + \frac{1}{2} \vec{r} \times \frac{1}{c} \frac{\partial \vec{B}(\vec{r}', t)}{\partial t} \Big|_{\vec{r}'=0} + \dots \\
 &= \vec{E}(0, t) + (\vec{r} \cdot \nabla') \vec{E}(\vec{r}', t) \Big|_{\vec{r}'=0} + \dots
 \end{aligned} \tag{4.8}$$

APPENDIX D1

Proof That Eq. (5.3) is
A Solution of Eq. (5.1)

Using Eq. (5.1) with momentum operator $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ and $E(t) = E_0 f(t)$, we obtain

$$\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 - q E_0 f(t) x \right\} \psi' = i\hbar \frac{\partial \psi'}{\partial t} \quad (D1.1)$$

Now, let the new wave function $\psi'(x, t)$ in Eq. (5.3) be substituted into Eq. (D1.1). If both sides are equal to each other, then we know that Eq. (5.3) is an exact solution of Eq. (5.1). Here we recall

$$\begin{aligned} \psi'(x, t) = & \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} \exp \left\{ -\frac{i\omega t}{2} - \frac{m\omega x^2}{2\hbar} + \frac{i q E_0}{\hbar\omega} x \exp(-i\omega t) X(\omega t) \right. \\ & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} \end{aligned} \quad (5.3)$$

Thus,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi'}{\partial x^2} = - \left\{ \frac{m\omega x}{\hbar} + \left[-\frac{m\omega x}{\hbar} + \frac{i q E_0}{\hbar\omega} \exp(-i\omega t) X(\omega t) \right]^2 \right\} \psi'$$

so the left hand side (LHS) of Eq. (D1.1) becomes

$$\begin{aligned} L.H.S. = & \left\{ \frac{\hbar\omega}{2} + i q E_0 x \exp(-i\omega t) X(\omega t) \right. \\ & + \frac{q^2 E_0^2}{2m\omega^2} \exp(-2i\omega t) X^2(\omega t) \\ & \left. - q E_0 f(t) x \right\} \psi' \end{aligned} \quad (D1.2)$$

Likewise, the right hand side (RHS) of Eq. (D1.1) is

$$\begin{aligned}
 \text{R.H.S.} = & i\hbar \left\{ -\frac{i\omega}{2} + \frac{qE_0\chi}{\hbar} \exp(-i\omega t) X(\omega t) \right. \\
 & + \frac{iqE_0}{\hbar\omega} \chi \exp(-i\omega t) \dot{X}(\omega t) \\
 & - 2\alpha \frac{d}{dt} \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & - \omega\alpha \sin \omega t \exp(-i\omega t) X^2(\omega t) \\
 & - i\omega\alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \\
 & \left. + 2\alpha\omega \cos \omega t \exp(-i\omega t) X(\omega t) \dot{X}(\omega t) \right\} \psi' ,
 \end{aligned}
 \tag{D1.3}$$

where $\alpha \equiv \frac{q^2 E_0^2}{2m\hbar\omega^3}$. The function $X(\omega t)$ is defined as

$$X(\omega t) = \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \exp(i s) , \tag{5.4}$$

According to Leibnitz's rule for differentiation of integrals, we know that

$$\dot{X}(\omega t) = \omega f(t) \exp(i\omega t) , \tag{D1.4}$$

and

$$\frac{d}{dt} \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) = \omega f(t) \cos \omega t X(\omega t) . \tag{D1.5}$$

If Eqs. (D1.4) and (D1.5) are substituted into Eq. (D1.3)

we obtain

$$\begin{aligned}
 \text{R.H.S.} = & \left\{ \frac{\hbar\omega}{2} + iqE_0\chi \exp(-i\omega t) X(\omega t) \right. \\
 & + \frac{q^2 E_0^2}{2m\omega^2} \exp(-2i\omega t) X^2(\omega t) \\
 & \left. - qE_0 f(t) \chi \right\} \psi' .
 \end{aligned}
 \tag{D1.6}$$

From the comparison of Eqs. (D1.2) and (D1.6), both sides of Eq. (D1.1) are equal. Thus, Eq. (5.3) is an exact solution of Eq. (5.1).

APPENDIX D2

Derivation of the Probability Amplitude in the Ground State

Referring to Eq. (2.29), the probability amplitude that the system is in the ground state at time t is $C_0 = \langle \phi_0 | \psi' \rangle$. Thus, from Eqs. (5.2) and (5.3), we obtain that

$$C_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{m\omega x^2}{\hbar} + \frac{i\hbar\epsilon_0}{\hbar\omega} x \exp(-i\omega t) X(\omega t) \right. \\ \left. - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \zeta(s) X(s) \right. \\ \left. + \alpha \zeta(\omega t) \exp(-i\omega t) X^2(\omega t) \right\} \quad (D2.1)$$

If we choose

$$A = \frac{m\omega}{\hbar} \quad , \quad (D2.2a)$$

$$B = -\frac{i\hbar\epsilon_0}{\hbar\omega} \exp(-i\omega t) X(\omega t) \quad , \quad (D2.2b)$$

$$C = \frac{i\omega t}{2} + 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \zeta(s) X(s) \\ - \alpha \zeta(\omega t) \exp(-i\omega t) X^2(\omega t) \quad , \quad (D2.2c)$$

then Eq. (D2.1) can be written as

$$\begin{aligned}
 G_0 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx \exp(-Ax^2 - Bx - C) \\
 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \sqrt{\frac{\pi}{A}} \exp\left(\frac{B^2}{4A} - C\right) \quad . \quad (D2.3)
 \end{aligned}$$

Now, if Eqs. (D2.2a), (D2.2b) and (D2.2c) are substituted into Eq. (D2.3), we get

$$\begin{aligned}
 G_0 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \left(\frac{\hbar\pi}{m\omega}\right)^{1/2} \exp\left\{-\frac{q^2 E_0^2}{4m\hbar\omega^3} \exp(-2i\omega t) X^2(\omega t) \right. \\
 &\quad \left. - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \right. \\
 &\quad \left. + \alpha \cos\omega t \exp(-i\omega t) X^2(\omega t) \right\} \\
 &= \exp\left\{-\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 &\quad \left. - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \right. \\
 &\quad \left. + \alpha \cos\omega t \exp(-i\omega t) X^2(\omega t) \right\} \quad . \quad (5.5)
 \end{aligned}$$

APPENDIX D3

Derivation of the Probability in Ground State

According to Equation (5.5), the probability amplitude that the system is in the ground state at time t is

$$C_0 = \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \omega(s) X(s) + \alpha \omega t \exp(-i\omega t) X^2(\omega t) \right\} \quad (5.5)$$

The argument of the exponential in Eq. (5.5) is defined to be

$$\beta = -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \omega(s) X(s) + \alpha \omega t \exp(-i\omega t) X^2(\omega t), \quad (D3.1)$$

and its complex conjugate is

$$\beta^* = \frac{i\omega t}{2} - \frac{\alpha}{2} \exp(2i\omega t) (X^2(\omega t))^* - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \omega(s) X^*(s) + \alpha \omega t \exp(i\omega t) (X^2(\omega t))^*. \quad (D3.2)$$

Therefore the absolute value of Eq. (5.5) squared is

$$\begin{aligned}
 |C_0(t)|^2 &= C_0(t) C_0^*(t) = \exp\{\beta + \beta^*\} \\
 &= \exp\left\{-\frac{\alpha}{2}\left[\exp(-2i\omega t)X^2(\omega t) + \exp(2i\omega t)(X^2(\omega t))^*\right] \right. \\
 &\quad \left. - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) (X(s) + X^*(s)) \right. \\
 &\quad \left. + \alpha \cos \omega t \left[\exp(-i\omega t)X^2(\omega t) + \exp(i\omega t)(X^2(\omega t))^*\right] \right\}.
 \end{aligned}
 \tag{D3.3}$$

The first term in Eq. (D3.3) is

$$\begin{aligned}
 &-\frac{\alpha}{2}\left[\exp(-2i\omega t)X^2(\omega t) + \exp(2i\omega t)(X^2(\omega t))^*\right] \\
 &= -\frac{\alpha}{2}\left[2\cos 2\omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s)\right)^2 - 2\cos 2\omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s)\right)^2 \right. \\
 &\quad \left. + 4\sin 2\omega t \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^{\omega t} d\tau f\left(\frac{\tau}{\omega}\right) \cos \tau \right] \\
 &= -2\alpha \cos^2 \omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s)\right)^2 + \alpha \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s)\right)^2 \\
 &\quad + 2\alpha \cos^2 \omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s)\right)^2 - \alpha \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s)\right)^2 \\
 &\quad - 2\alpha \sin 2\omega t \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^{\omega t} d\tau f\left(\frac{\tau}{\omega}\right) \sin \tau.
 \end{aligned}
 \tag{D3.4}$$

The third term in Eq. (D3.3) is

$$\begin{aligned}
 &\alpha \cos \omega t \left[\exp(-i\omega t)X^2(\omega t) + \exp(i\omega t)(X^2(\omega t))^*\right] \\
 &= 2\alpha \cos^2 \omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s)\right)^2 - 2\alpha \cos^2 \omega t \left(\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s)\right)^2 \\
 &\quad + 2\alpha \sin 2\omega t \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^{\omega t} d\tau f\left(\frac{\tau}{\omega}\right) \sin \tau.
 \end{aligned}
 \tag{D3.5}$$

If we define a function for which

$$\theta(y) = \begin{cases} 1 & , y \geq 0 \\ 0 & , y < 0 \end{cases} , \quad (D3.6)$$

then the integral for the second term in Eq. (D3.3) can be written as

$$\begin{aligned} & \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^s du f\left(\frac{u}{\omega}\right) \cos(u) \\ &= \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^{\omega t} du f\left(\frac{u}{\omega}\right) \cos(u) \theta(s - u) \\ &= \int_0^{\omega t} ds \int_0^{\omega t} du f\left(\frac{u}{\omega}\right) \cos(u) f\left(\frac{s}{\omega}\right) \cos(s) \theta(u - s) \\ &= \frac{1}{2} \int_0^{\omega t} ds \int_0^{\omega t} du f\left(\frac{s}{\omega}\right) f\left(\frac{u}{\omega}\right) \cos(s) \cos(u) \left[\theta(s - u) + \theta(u - s) \right] . \end{aligned} \quad (D3.7)$$

We know that

$$\theta(s - u) + \theta(u - s) = 1 , \quad (D3.8)$$

so we obtain

$$\begin{aligned} & -2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) (X(s) + X^*(s)) \\ &= -4\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \int_0^s du f\left(\frac{u}{\omega}\right) \cos(u) \\ &= -2\alpha \left[\int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \right]^2 . \end{aligned} \quad (D3.9)$$

If we substitute Eqs. (D3.4), (D3.5) and (D3.9) into Eq. (D3.3) and simplify it, then Eq. (D3.3) becomes

$$P_0(t) = |C_0(t)|^2 = \exp \{-|R(\omega t)|^2\} , \quad (5.6)$$

where

$$R(\omega t) = \alpha^{1/2} X(\omega t) . \quad (5.7)$$

APPENDIX D4

Calculation of the Probability in the Ground State

The probability for the system in the ground state at time t is given by Eq. (5.6). According to Eqs. (5.4) and (5.7), the function $R(z)$ is defined as

$$R(z) = \alpha^{1/2} \int_0^z ds f\left(\frac{s}{\omega}\right) \exp(i s) \quad (5.4)$$

If we choose $f(t) = E(t)/E_0 = \sin(\Omega t + \theta)$, the function $R(z)$ is

$$\begin{aligned} R(z) &= \alpha^{1/2} \int_0^z ds \sin(\rho s + \theta) e^{is} \\ &= \alpha^{1/2} \left\{ \frac{1}{2(1+\rho)} [e^{i\theta} (1 - e^{i(1+\rho)z})] - \frac{1}{2(1-\rho)} [e^{-i\theta} (1 - e^{i(1-\rho)z})] \right\}, \end{aligned} \quad (D4.1)$$

where $\rho = \frac{\Omega}{\omega}$. The complex conjugate of Eq. (D4.1) is

$$R^*(z) = \alpha^{1/2} \left\{ \frac{1}{2(1+\rho)} [e^{-i\theta} (1 - e^{-i(1+\rho)z})] - \frac{1}{2(1-\rho)} [e^{i\theta} (1 - e^{-i(1-\rho)z})] \right\}, \quad (D4.2)$$

The absolute value squared of $R(z)$ is

$$\begin{aligned} |R(z)|^2 &= \alpha \left\{ \frac{\sin^2 \frac{1}{2}(1+\rho)z}{(1+\rho)^2} + \frac{\sin^2 \frac{1}{2}(1-\rho)z}{(1-\rho)^2} \right. \\ &\quad \left. - \frac{2 \cos(\rho z + 2\theta) \sin(\frac{1}{2}(1+\rho)z) \sin(\frac{1}{2}(1-\rho)z)}{1-\rho^2} \right\}. \end{aligned} \quad (D4.3)$$

If we substitute Eq. (D4.3) into Eq. (5.6), we obtain Eq. (5.9)

$$\begin{aligned} P_0(t) = |C_0|^2 &= \exp \left\{ -\alpha \left[\frac{\sin^2 \frac{1}{2}(1+\rho)z}{(1+\rho)^2} + \frac{\sin^2 \frac{1}{2}(1-\rho)z}{(1-\rho)^2} \right. \right. \\ &\quad \left. \left. - \frac{2 \cos(\rho z + 2\theta) \sin \frac{1}{2}(1+\rho)z \sin \frac{1}{2}(1-\rho)z}{1-\rho^2} \right] \right\}. \end{aligned}$$

APPENDIX D5

Derivation of Equation (5.22)

If we substitute Eqs. (5.3) and (5.14) into Eq. (5.17), it is found that

$$\begin{aligned}
 F(u) &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx \exp\left\{-\frac{m\omega}{\hbar}x^2\right. \\
 &\quad + \left[2\sqrt{\frac{m\omega}{\hbar}}u + i\left(\frac{\hbar E_0}{\hbar\omega}\right)\exp(-i\omega t)X(\omega t)\right]x \\
 &\quad - u^2 - i\frac{\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right)\cos(s)X(s) \\
 &\quad \left. + \alpha \cos\omega t \exp(-i\omega t)X^2(\omega t)\right\} \\
 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx \exp(-Ax^2 - Bx - C) \\
 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \sqrt{\frac{\pi}{A}} \exp\left(\frac{B^2}{4A} - C\right)
 \end{aligned} \tag{D5.1}$$

where

$$A = \frac{m\omega}{\hbar} \tag{D5.2a}$$

$$B = -2\sqrt{\frac{m\omega}{\hbar}}u - i\left(\frac{\hbar E_0}{\hbar\omega}\right)\exp(-i\omega t)X(\omega t) \tag{D5.2b}$$

$$\begin{aligned}
 C &= u^2 + i\frac{\omega t}{2} + 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right)\cos(s)X(s) \\
 &\quad - \alpha \cos\omega t \exp(-i\omega t)X^2(\omega t)
 \end{aligned} \tag{D5.2c}$$

Therefore, Eq. (D5.1) can be written as Eq. (5.22)

$$\begin{aligned}
 F(u) = & \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & + i(2\alpha)^{1/2} u \exp(-i\omega t) X(\omega t) \\
 & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} .
 \end{aligned}$$

APPENDIX D6

General Expression for the Probability in Eq. (5.26)

According to Eq. (5.22), we see that

$$\begin{aligned}
 F(u) = & \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & + i(2\alpha)^{1/2} \exp(-i\omega t) X(\omega t) \\
 & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\}
 \end{aligned} \quad (5.22)$$

The probability amplitude C_n can be written as

$$C_n(t) = 2^{-n/2} (n!)^{-1/2} \left[\frac{d^n F(u)}{du^n} \right] \Big|_{u=0} \quad (5.20)$$

If we substitute Eq. (5.22) into Eq. (5.20), we can obtain

$$C_n(t) = 2^{-n/2} (n!)^{-1/2} [i(2\alpha)^{1/2} \exp(-i\omega t) X(\omega t)]^n F(u) \Big|_{u=0} \quad (D6.1)$$

with the help of Eq. (5.23), Eq. (D6.1) becomes

$$C_n(t) = i^n (n!)^{-1/2} [\alpha^{1/2} \exp(-i\omega t) X(\omega t)]^n C_0(t), \quad (D6.2)$$

thus, the probability would be

$$\begin{aligned}
 |C_n(t)|^2 &= \frac{|R|^{2n}}{n!} |C_0(t)|^2 \\
 &= \frac{|R|^{2n}}{n!} \exp \{ -|R|^2 \}
 \end{aligned} \quad (5.26)$$

is the general expression for the probability in each state.

APPENDIX E1

Derivation of the Expansion Coefficient in the Ground State

Referring to Eq. (3.4), the expansion coefficient a_n in the ground state is $a_0 = \langle \phi_0 | \psi \rangle$ or

$$a_0 = \langle \phi_0 | \exp \left\{ i \frac{\mathcal{E} A(t)}{\hbar c} x \right\} \psi \rangle \quad (6.1)$$

From Eqs. (5.2) and (5.3), we know that

$$\begin{aligned} a_0 = & \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{m\omega x^2}{\hbar} + i \left[\frac{\mathcal{E} E_0}{\hbar\omega} \exp(-i\omega t) X(\omega t) + \frac{\mathcal{E} A(t)}{\hbar c} \right] \right. \\ & - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ & \left. - \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} \quad (E1.1) \end{aligned}$$

If we choose A and C the same as Eqs. (D2.2a) and (D2.2c), but

$$B = -i \left[\frac{\mathcal{E} E_0}{\hbar\omega} \exp(-i\omega t) X(\omega t) + \frac{\mathcal{E} A(t)}{\hbar c} \right], \quad (E1.2)$$

then Eq. (E1.1) can be written as

$$\begin{aligned} a_0 &= \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} \int_{-\infty}^{\infty} dx \exp(-Ax^2 - Bx - C) \\ &= \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} \sqrt{\frac{\pi}{A}} \exp\left(\frac{B^2}{4A} - C\right) \quad (E1.3) \end{aligned}$$

Now, if Eqs. (D2.2a), (E1.2) and (D2.2c) are substituted into Eq. (E1.3), we get

$$\begin{aligned}
 a_0 = & \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \left(\frac{\hbar\pi}{m\omega}\right)^{1/2} \exp \left\{ -\frac{\beta^2 E_0^2}{4m\hbar\omega^3} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & - \frac{\beta^2 E_0 A(t)}{4m\hbar\omega^3} \exp(-i\omega t) X(\omega t) - \frac{\beta^2 A^2(t)}{4m\hbar\omega^3} \\
 & - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. + \alpha \cos\omega t \exp(-i\omega t) X^2(\omega t) \right\} \\
 = & \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 & - \frac{\beta^2 E_0 A(t)}{2m\hbar\omega^3} \exp(-i\omega t) X(\omega t) - \frac{\beta^2 A^2(t)}{4m\hbar\omega^3} \\
 & - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 & \left. - \cos\omega t \exp(-i\omega t) X^2(\omega t) \right\} .
 \end{aligned} \tag{6.1}$$

APPENDIX E2

Derivation of the Absolute Value of the Expansion Coefficient Squared in Ground State

From Equation (6.4), the expansion coefficient for the system in the ground state at time t is

$$\begin{aligned}
 a_0(t) = \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 - \frac{g^2 E_0}{2mc\hbar\omega} \exp(-i\omega t) X(\omega t) A(t) \\
 - \frac{g^2 A^2(t)}{4mc^2\hbar\omega} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} \quad , \quad (6.4)
 \end{aligned}$$

where $A(t)$ is defined by Eq. (6.2). If we substitute Eq. (6.2) into Eq. (6.4), it becomes

$$\begin{aligned}
 a_0(t) = \exp \left\{ -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \right. \\
 + \alpha \exp(-i\omega t) X(\omega t) X_0(\omega t) \\
 - \frac{\alpha}{2} X_0^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} \quad . \quad (E2.1)
 \end{aligned}$$

where $X_0(\omega t)$ is given in Eq. (6.3). The argument of the exponential in Eq. (6.4) is defined as

$$\begin{aligned} \delta = & -\frac{i\omega t}{2} - \frac{\alpha}{2} \exp(-2i\omega t) X^2(\omega t) \\ & + \alpha \exp(-i\omega t) X(\omega t) X_0(\omega t) \\ & - \frac{\alpha}{2} X_0^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\ & + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \end{aligned} \quad (E2.2)$$

and its complex conjugate is

$$\begin{aligned} \delta^* = & \frac{i\omega t}{2} - \frac{\alpha}{2} \exp(2i\omega t) (X^2(\omega t))^* \\ & + \alpha \exp(i\omega t) X^*(\omega t) X_0(\omega t) \\ & - \frac{\alpha}{2} X_0^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X^*(s) \\ & + \alpha \cos \omega t \exp(i\omega t) (X^2(\omega t))^* \end{aligned} \quad (E2.3)$$

Thus, the absolute value squared of a_0 is

$$\begin{aligned} |a_0(t)|^2 = & a_0(t) a_0^*(t) = \exp \{ \delta + \delta^* \} \\ = & \exp \left\{ -\frac{\alpha}{2} \left[\exp(-2i\omega t) X^2(\omega t) + \exp(2i\omega t) (X^2(\omega t))^* \right] \right. \\ & + \alpha \left[\exp(-i\omega t) X(\omega t) X_0(\omega t) + \exp(i\omega t) X^*(\omega t) X_0(\omega t) \right. \\ & - X_0^2(\omega t) - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) (X(s) + X^*(s)) \\ & \left. \left. + \alpha \cos \omega t \left[\exp(-i\omega t) X^2(\omega t) + \exp(i\omega t) (X^2(\omega t))^* \right] \right] \right\} \end{aligned} \quad (E2.4)$$

The second term in Eq. (E2.4) is

$$\begin{aligned} & \alpha \left[\exp(-i\omega t) X(\omega t) X_0(\omega t) + \exp(i\omega t) X^*(\omega t) X_0(\omega t) \right] \\ &= 2\alpha \left[\cos \omega t X_0(\omega t) \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \right. \\ & \quad \left. + \sin \omega t X_0(\omega t) \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s) \right] \quad . \quad (E2.5) \end{aligned}$$

The combination of the first term, fourth term and fifth term in Eq. (E2.4) has been shown in the argument of Eq. (5.6).

Now we substitute Eqs. (E2.5) and (5.6) into Eq. (E2.4) to give

$$\begin{aligned} |a_0(t)|^2 &= \exp \left\{ -\alpha |X(\omega t)|^2 + 2\alpha \cos \omega t X_0(\omega t) \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) \right. \\ & \quad \left. + 2\alpha \sin \omega t X_0(\omega t) \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \sin(s) - \alpha X_0^2(\omega t) \right\} \\ &= \exp \left\{ -\alpha \left| \exp(-i\omega t) X(\omega t) - X_0(\omega t) \right|^2 \right\} \\ &= \exp \left\{ -|D(\omega t)|^2 \right\} \quad , \quad (6.5) \end{aligned}$$

where

$$D(\omega t) = \alpha^{1/2} \left\{ \exp(-i\omega t) X(\omega t) - X_0(\omega t) \right\} \quad . \quad (6.6)$$

APPENDIX E3

Calculation of the Absolute Value of Expansion Coefficient Squared in the Ground State

The absolute value of the expansion coefficient squared for the system in the ground state at time t is given in Eq. (6.4).

From Eq. (6.3) the function $X_0(z)$ is defined as

$$\begin{aligned} X_0(z) &\equiv \int_0^z ds f\left(\frac{s}{\omega}\right) \\ &= \int_0^z ds \sin(\rho s + \theta) \\ &= -\frac{\cos(\rho z + \theta)}{\rho} + \frac{\cos \theta}{\rho} \end{aligned} \quad (E3.1)$$

where $f(t) = \frac{E(t)}{E_0}$. The absolute value of $D(z)$ in Eq. (6.6) squared is

$$|D(z)|^2 = \alpha \left\{ |X(z)|^2 X(z) X_0(z) e^{-iz} - X_0(z) X^*(z) e^{iz} + X_0^2(z) \right\} \quad (E3.2)$$

With the help of Eq. (5.7), if we substitute Eqs. (D4.1), (D4.2), (D4.3) and (E3.1) into Eq. (E3.2). It becomes

$$\begin{aligned}
|D(z)|^2 = & \alpha \left\{ |X(z)|^2 - \frac{2}{\rho(1-\rho)} \sin\left(\frac{1}{2}(1+\rho)z + \theta\right) \sin\left(\frac{1}{2}(1-\rho)z\right) (\cos\theta - \cos(\rho z + \theta)) \right. \\
& + \frac{2}{\rho(1+\rho)} \sin\left(\frac{1}{2}(1-\rho)z - \theta\right) \sin\left(\frac{1}{2}(1+\rho)z\right) (\cos\theta - \cos(\rho z + \theta)) \\
& \left. + \frac{1}{\rho^2} (\cos\theta - \cos(\rho z + \theta))^2 \right\} \quad (E3.3)
\end{aligned}$$

According to Eq. (6.5), we know that

$$\begin{aligned}
|a_0(t)|^2 &= \exp \{-|D(z)|^2\} \\
&= \exp \{-\alpha |X(z)|^2\} \cdot \\
&\quad \exp \left\{ -\alpha \left[\frac{2}{\rho(1+\rho)} \sin\left(\frac{1}{2}(1-\rho)z - \theta\right) \sin\left(\frac{1}{2}(1+\rho)z\right) (\cos\theta - \cos(\rho z + \theta)) \right. \right. \\
&\quad \left. \left. + \frac{1}{\rho^2} (\cos\theta - \cos(\rho z + \theta))^2 \right. \right. \\
&\quad \left. \left. - \frac{2}{\rho(1-\rho)} \sin\left(\frac{1}{2}(1+\rho)z + \theta\right) \sin\left(\frac{1}{2}(1-\rho)z\right) (\cos\theta - \cos(\rho z + \theta)) \right] \right\} \quad (E3.4)
\end{aligned}$$

Since $P_0(t) = \exp \{-\alpha |X(z)|^2\}$, as shown in Eqs. (5.6) and (5.7), we get Eq. (6.5).

APPENDIX E4

Derivation of Equation (6.16)

When Eqs. (6.10) and (5.3) are substituted into Eq. (6.11), it is found that

$$\begin{aligned}
 G(v) &= 2^{-n/2} (n!)^{-1/2} \left(\frac{m\omega}{\hbar\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{m\omega}{\hbar} x^2 \right. \\
 &\quad + \left[i \frac{\mathcal{F}A(t)}{\hbar\zeta} + 2\sqrt{\frac{m\omega}{\hbar}} v + \frac{i\mathcal{F}E_0}{\hbar\omega} \exp(-i\omega t) X(\omega t) \right] x \\
 &\quad - v^2 - \frac{i\omega t}{2} - 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 &\quad \left. + \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \right\} \\
 &= 2^{-n/2} (n!)^{-1/2} \left(\frac{m\omega}{\hbar\pi} \right)^{1/2} \sqrt{\frac{\pi}{A}} \exp\left(\frac{B^2}{4A} - C\right) \quad , \quad (E4.1)
 \end{aligned}$$

where

$$A = \sqrt{\frac{m\omega}{\hbar}} \quad , \quad (E4.2a)$$

$$B = -i \frac{\mathcal{F}A(t)}{\hbar\zeta} - 2\sqrt{\frac{m\omega}{\hbar}} v - i \left(\frac{\mathcal{F}E_0}{\hbar\omega} \right) \exp(-i\omega t) X(\omega t) \quad , \quad (E4.2b)$$

$$\begin{aligned}
 C &= v^2 + i \frac{\omega t}{2} + 2\alpha \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \cos(s) X(s) \\
 &\quad - \alpha \cos \omega t \exp(-i\omega t) X^2(\omega t) \quad . \quad (E4.2c)
 \end{aligned}$$

If we substitute Eqs. (E4.2a), (E.2b) and (E4.2c) into Eq. (E4.1) then we can obtain Eq. (6.16).

APPENDIX F1

Calculation of the Probability in the Ground State in the RWA

Referring to Eqs. (5.4), (7.1), we obtain

$$\begin{aligned} X_{RWA}(\omega t) &= \int_0^{\omega t} ds f\left(\frac{s}{\omega}\right) \exp(i s) \\ &= -\frac{1}{2\lambda} \int_0^{\omega t} ds e^{-i[(p-1)z + \theta]} \\ &= -\frac{1}{2(p-1)} e^{-i\theta} [e^{-i(p-1)z} - 1] \end{aligned} \quad (F1.1)$$

and its complex conjugate is

$$X_{RWA}^*(\omega t) = -\frac{1}{2(p-1)} e^{i\theta} [e^{i(p-1)z} - 1] \quad (F1.2)$$

Thus, the absolute value of X_{RWA} squared is

$$\begin{aligned} |X_{RWA}(\omega t)|^2 &= \frac{1}{(p-1)^2} \left\{ \frac{e^{i\frac{1}{2}(p-1)z} - e^{-i\frac{1}{2}(p-1)z}}{2i} \right\}^2 \\ &= \frac{\sin^2 \frac{1}{2}(1-p)z}{(1-p)^2} \end{aligned} \quad (F1.3)$$

If Eq. (F1.3) is substituted into Eq. (7.2), we obtain Eq.

(7.3)

$$P_{0(RWA)}(t) = \exp \left\{ -\alpha \left[\frac{\sin^2 \frac{1}{2}(1-p)z}{(1-p)^2} \right] \right\}.$$

APPENDIX F2

Calculation of the Absolute Value of Expansion Coefficient Squared in the Ground State in the RWA

Referring to Eq. (F1.1), we obtain

$$X_{RWA}(z) = -\frac{1}{2(\rho-1)} e^{-i\theta} \left\{ e^{-i(\rho-1)z} - 1 \right\}, \quad (F1.1)$$

substituting Eq. (7.1) into Eq. (6.3), then Eq. (6.3) becomes

$$\begin{aligned} X_{0(RWA)}(z) &= \int_0^z ds f\left(\frac{s}{\omega}\right) \\ &= -\frac{1}{2\tau} \int_0^z ds e^{-i(\rho s + \theta)} \\ &= -\frac{1}{2\rho} e^{-i\theta} \left\{ e^{-i\rho z} - 1 \right\}. \end{aligned} \quad (F2.1)$$

If Eq. (6.6) is in the rotating-wave approximation, then

$$\begin{aligned} D_{RWA}(z) &= \alpha^{1/2} \left\{ e^{-iz} X(z) - X_0(z) \right\} \\ &= \alpha^{1/2} \left\{ -\frac{1}{2(\rho-1)} e^{-i\theta} \left\{ e^{-i\rho z} - e^{-iz} \right\} \right. \\ &\quad \left. + \frac{1}{2\rho} e^{-i\theta} \left\{ e^{-i\rho z} - 1 \right\} \right\} \end{aligned} \quad (F2.2)$$

The complex conjugate of Eq. (F2.2) is

$$D_{RWA}^*(z) = \alpha^{1/2} \left\{ -\frac{1}{2(\rho-1)} e^{i\theta} [e^{i\rho z} - e^{iz}] + \frac{1}{2\rho} e^{i\theta} [e^{i\rho z} - 1] \right\}, \quad (F2.3)$$

thus,

$$|D_{RWA}(z)|^2 = \alpha \left\{ \frac{\sin^2(\frac{1}{2}(\rho-1)z)}{(\rho-1)^2} + \frac{\sin^2(\frac{1}{2}\rho z)}{\rho^2} - \frac{2}{\rho(\rho-1)} \cos(\frac{z}{2}) \sin(\frac{(\rho-1)z}{2}) \sin(\frac{\rho z}{2}) \right\}. \quad (F2.4)$$

If Eq. (F2.4) is substituted into Eq. (6.5), we obtain Eq. (6.7)

$$|Q_0(RWA)(t)|^2 = \exp \left\{ -\alpha \left[\frac{\sin^2 \frac{1}{2}(1-\rho)z}{(1-\rho)^2} + \frac{\sin^2(\frac{1}{2}\rho z)}{\rho^2} - \frac{2}{\rho(1-\rho)} \cos(\frac{z}{2}) \sin(\frac{(\rho-1)z}{2}) \sin(\frac{\rho z}{2}) \right] \right\}.$$

Fig. 1--The curves of the probability $P_0(t)$ for $\alpha = 1$, $\theta = 0$ and $\rho = 0.1, 0.5, 1, 1.5, 2$.

Fig. 2--The curves of the probability $P_0(t)$ for $\alpha = 1$, $\rho = 0.1$ and $\theta = 0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{\pi}{2}, \frac{5\pi}{8}, \frac{3\pi}{4}, \frac{7\pi}{8}$.

Fig. 3--The curves of the probability $P_0(t)$ for $\theta = 0$, $\rho = 0.1$ and $\alpha = 0.1, 0.5, 1, 1.5, 2, 5, 50$.

$$\alpha=1 \quad \theta=0 \quad \rho=1$$

$$\text{---} \quad n=1$$

$$\text{---} \quad n=2$$

$$\text{---} \quad n=3$$

$$\text{---} \quad n=4$$

$$\text{---} \quad n=5$$

$$\text{---} \quad n=6$$

Fig. 4--The curves of $|C_n(t)|^2$ for $\alpha=1, \theta=0, \rho=1$ for the first six excited states.

Fig. 5--The curves of the probability $|C_n(t)|^2$ for $\alpha = 1$, $\theta = 0$, $\rho = 0.1$, n varies from 0 to 3 and the curves of the sum for the four probabilities.

Fig. 6--The curves of $|a_0(t)|^2$ for $\alpha = 1$, $\theta = 0$ and $\rho = 0.1, 0.5, 1, 1.5$ and 2 .

Fig. 7--The curves of $|a_n(t)|^2$ for $\alpha = 1$, $\theta = 0$, $\rho = 0.1$, n varies from 0 to 6 and the curve of their sum.

Fig. 8--The curves of the probability $P_0(t)$ in the RWA for $\alpha = 1$, $\rho = 1$ and the curves of the probability for $\alpha = 1$, $\rho = 1$, $\theta = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}$.

$\alpha = 1 \quad \theta = 0$

— $\rho = 0.5$

- - - $\rho = 0.7$

- · - $\rho = 0.9$

o o o o $\rho = 1.0$

- - - $\rho = 1.1$

· · · · · $\rho = 1.3$

· · · · · $\rho = 1.5$

Fig. 9--The curves of probability $|C_1(t)|^2$ in the RWA for $\alpha = 1$, $\theta = 0$, $\rho = 0.5, 0.7, 0.9, 1, 1.1, 1.3, 1.5$.

Fig. 10--The curves of $|a_0(t)|^2$ in the RWA for $\alpha=1, \rho=1$; and the curves of $|a_0(t)|^2$ for $\alpha=1, \rho=1, \theta=0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}$.

Fig. 11--The curves of $|a_1(t)|^2$ in the RWA for $\alpha = 1$, $\theta = 0$, $\rho = 0.5$, 0.7, 0.9, 1, 1.1, 1.3, 1.5.

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