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Gauge invariance in quantum mechanics: charged harmonic oscillator in an electromagnetic field†

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Abstract. The gauge-invariant formulation of quantum mechanics is applied to the charged harmonic oscillator in an electromagnetic field in the electric dipole approximation to obtain the probability that the oscillator is in a particular state at time t. This probability is compared with the corresponding 'probability' calculated from the conventional approach to the interaction of radiation with matter using the interaction $\boldsymbol{A}\cdot\boldsymbol{p}$. The probabilities do not agree with each other. From the principle of gauge invariance it is concluded that the probability calculated from the gauge-invariant formulation is correct in this case, and that the conventional approach in general is incorrect.

1. Introduction

Gauge invariance is one of the most fundamental symmetry properties of physics. However, only recently a manifestly gauge-invariant formulation of non-relativistic quantum mechanics has been developed (Yang 1976, Kobe 1978, Kobe and Smirl 1978). This formulation is based on operators that are gauge invariant (Kobe and Yang 1980). In particular, the Hamiltonian for a single charged particle in an electromagnetic field is not gauge invariant, although it describes the time evolution of the wavefunction. Energy is a gauge-invariant concept, so the Hamiltonian in this case is not the energy. The energy operator is defined as a gauge-invariant operator whose expectation value is the energy transferred to the particle by the electromagnetic field. In the gauge-invariant formulation, the wavefunction is expanded in terms of the eigenstates of the energy operator. The expansion coefficients in this basis are gauge invariant and are properly interpreted as probability amplitudes for finding the system in an energy eigenstate.

This gauge-invariant procedure is in contrast to the conventional approach to the interaction of electromagnetic radiation with a charged quantum mechanical particle (see e.g. Schiff 1968, Merzbacher 1970, pp 458–63). In the conventional approach, the quadratic term in the Hamiltonian is expanded and the resultant interaction terms are linear and quadratic in the vector potential. In addition there may also be a scalar potential. The wavefunction is expanded in terms of eigenstates of the unperturbed Hamiltonian, and the expansion coefficients are conventionally interpreted as probability amplitudes (Merzbacher 1970, pp 150–4). However, these expansion

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coefficients are gauge dependent, and therefore have no physical meaning. Thus the postulate usually made in quantum mechanics that all expansion coefficients can be interpreted as probability amplitudes is false.

This conclusion has not been accepted by some workers (Aharonov and Au 1979, Haller and Sohn 1979). They have attempted to show that the conventional approach is indeed gauge invariant (Aharonov and Au 1979). In most problems involving the interaction of electromagnetic radiation and matter, approximations, like perturbation theory and the rotating-wave approximation, are made. Thus questions of principle become intertwined with questions of approximation. However, if an exactly solvable model could be found the questions of principle could be considered separately.

In this paper a charged harmonic oscillator, initially in its ground state, which interacts with a classical electromagnetic field in the electric dipole approximation (EDA) is solved exactly (Kobe and Wen 1980, Wen 1980). It is first solved in the gauge-invariant formulation, and the probability of finding the oscillator in the unperturbed state Φ_n at time t is obtained. Then the problem is solved by the conventional approach, and the 'probability' of finding the system in the same unperturbed state Φ_n at time t is also obtained. The two probabilities are compared and found to be different in general. By gauge invariance, the correct probability is obtained from the gauge-invariant formulation. The expansion coefficients in the conventional approach are not physically meaningful probability amplitudes and are thus without physical significance. The long-held belief that all expansion coefficients can be interpreted as probability amplitudes is shown to be false in general. The model used here shows that the conventional approach is not gauge invariant, which provides a counter example to attempts to prove the contrary (Aharonov and Au 1979).

In § 2 the gauge-invariant formulation of quantum mechanics is reviewed. The one-dimensional charged harmonic oscillator in an electromagnetic field in the electric dipole approximation is solved exactly in § 3 and the probability for finding the system in the unperturbed state Φ_n is obtained as a function of time. In § 4 the conventional approach to the treatment of classical electromagnetic radiation interacting with a quantum mechanical particle is reviewed and criticised. The charged harmonic oscillator is solved by the conventional approach in § 5, and the 'probabilities' are also obtained. The conclusions are given in § 6.

2. Gauge-invariant formulation of quantum mechanics

The manifestly gauge-invariant formulation of non-relativistic quantum mechanics developed recently by Yang (1976) and by Kobe and Smirl (1978) is reviewed here. As Schwinger (1951) has pointed out 'gauge invariance difficulties naturally disappear when methods of solution are adopted that involve only gauge-invariant quantities'. After showing that the Schrödinger equation is invariant under gauge transformations, the gauge invariance of operators is discussed (Kobe and Yang 1980). Then the energy operator is obtained. The wavefunction is expanded in terms of eigenstates of the energy operator, and an equation for the gauge-invariant expansion coefficients is obtained.

2.1. Gauge invariance of the Schrödinger equation

The Hamiltonian for a single particle of mass m and charge q in an external radiation

field characterised by the vector potential $\boldsymbol{A}$ and the scalar potential A_0 is

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

where V is the external potential energy of the particle. The Schrödinger equation for the particle is

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

This equation is form invariant under gauge transformations.

A gauge transformation on the wavefunction,

$$\psi' = \exp(\mathrm{i}q\Lambda/c\hbar)\psi, \tag{2.3}$$

can be made, where Λ is a function of space and time. The usual gauge transformations on the potentials are

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

and

$$A_0' = A_0 - c^{-1}\, \partial\Lambda/\partial t. \tag{2.5}$$

When equation (2.3) is substituted into equation (2.2) and equations (2.4) and (2.5) are used, we obtain

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

which is the same form as equation (2.2). Therefore the equation is form invariant under gauge transformations, which is the meaning of gauge invariance applied to the Schrödinger equation (see e.g. Bohm 1951).

2.2. Gauge invariance of operators

In order to develop a gauge-invariant formulation of quantum mechanics, it is necessary to obtain the transformation properties of operators corresponding to observables under gauge transformations. Of the many definitions of gauge transformation of operators in the literature (Strocchi and Wightman 1974) the one used here is the form invariance of the operators under unitary transformation (Kobe and Yang 1980). If we consider a Hermitian operator $\Theta(\boldsymbol{A}, A_0)$ corresponding to some observable which can depend on the potentials of the electromagnetic field, gauge invariance of its expectation value requires that

$$\langle\psi|\Theta(\boldsymbol{A}, A_0)\psi\rangle = \langle\psi'|\Theta(\boldsymbol{A}', A_0')\psi'\rangle \tag{2.7}$$

where the wavefunction ψ' is given by equation (2.3) and the new potentials $\boldsymbol{A}'$ and A_0' are given by equations (2.4) and (2.5), respectively. The left-hand side of equation (2.7) is the expectation value calculated by someone using the old gauge, while the right-hand side is the expectation value calculated by someone using the new gauge. The two expectation values must be equal because it should make no difference which gauge is used to calculate observable quantities.

The expectation value of $\Theta(\boldsymbol{A}, A_0)$ can be written as

$$\langle\psi|\Theta(\boldsymbol{A}, A_0)\psi\rangle = \langle\psi'|\Theta'(\boldsymbol{A}, A_0)\psi'\rangle \tag{2.8}$$

where the operator $\Theta'(\boldsymbol{A}, A_0)$ is the unitarily transformed operator

$$\Theta'(\boldsymbol{A}, A_0) = \exp(iq\Lambda/\hbar c)\Theta(\boldsymbol{A}, A_0)\exp(-iq\Lambda/\hbar c). \tag{2.9}$$

The unitary transformation on the operator shall be called a 'gauge transformation on the operator'. On comparing equations (2.8) and (2.7), we see that an operator has a gauge-invariant expectation value if

$$\Theta'(\boldsymbol{A}, A_0) = \Theta(\boldsymbol{A}', A_0'). \tag{2.10}$$

In other words, an operator has a gauge-invariant expectation value if and only if a gauge transformation on the operator induces a gauge transformation on the potentials on which the operator depends.

Some examples of such gauge-invariant operators are the kinetic momentum $\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}/c$ and the operator $\pi_0 = i\hbar\,\partial/\partial t - qA_0$. The energy operator discussed in the next subsection is another example.

2.3. Energy operator

The Hamiltonian $H(\boldsymbol{A}, A_0)$ is a gauge-dependent operator, since

$$H'(\boldsymbol{A}, A_0) = H(\boldsymbol{A}', A_0) = H(\boldsymbol{A}', A_0') + \frac{q}{c}\frac{\partial\Lambda}{\partial t} \tag{2.11}$$

and so it cannot be the energy operator. On the other hand, the operator

$$\mathscr{E}(\boldsymbol{A}) \equiv H(\boldsymbol{A}, A_0) - qA_0 = H(\boldsymbol{A}, 0) \tag{2.12}$$

is gauge invariant, and is the energy operator. It satisfies the energy conservation condition in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\mathscr{E}(\boldsymbol{A})\psi\rangle = \langle\psi|P\psi\rangle. \tag{2.13}$$

The quantum mechanical power operator P is defined as (Yang 1976)

$$P = \tfrac{1}{2}q(\boldsymbol{E}\cdot\boldsymbol{v} + \boldsymbol{v}\cdot\boldsymbol{E}) \tag{2.14}$$

where $\boldsymbol{E}$ is the electric field and $\boldsymbol{v}$ is the velocity operator

$$\boldsymbol{v} = m^{-1}(\boldsymbol{p} - q\boldsymbol{A}/c). \tag{2.15}$$

Equation (2.14) reduces to the classical expression for power when $\boldsymbol{v}$ and $\boldsymbol{E}$ commute with each other. Equation (2.13) shows that the time rate of change of the average energy of the particle is equal to the average power transferred to the particle by the electromagnetic field.

2.4. Probability amplitudes

In order to have a physical interpretation for the expansion coefficients of the wavefunction, it is necessary for them to be gauge invariant. The wavefunction will be expanded in terms of the eigenstates of the energy operator $\mathscr{E}(\boldsymbol{A})$, which satisfies the eigenvalue problem

$$\mathscr{E}(\boldsymbol{A})\psi_n = \varepsilon_n\psi_n. \tag{2.16}$$

The eigenfunction ψ_n and eigenvalue ε_n depend on the time as a parameter. Since the energy operator is Hermitian, the states ψ_n are a complete orthonormal set of states for time t, and consequently the wavefunction ψ in equation (2.2) may be expanded as

$$\psi = \sum_n c_n \psi_n. \tag{2.17}$$

When this expansion is substituted into equation (2.2) we obtain the set of equations

$$i\hbar \dot{c}_n - \varepsilon_n c_n = \sum_m \langle \psi_n | (qA_0 - i\hbar\, \partial/\partial t)\psi_m \rangle c_m \tag{2.18}$$

for the expansion coefficients. The matrix element in equation (2.18) is gauge invariant. When the gauge transformation in equation (2.3) is made on the wavefunction in equation (2.17), the energy eigenstates are likewise gauge transformed. The expansion coefficients c_n are thus gauge invariant. Under a gauge transformation on equation (2.16), the energy operator $\mathscr{E}(\boldsymbol{A})$ is gauge transformed as in equation (2.9) and the energy eigenstates are transformed as in equation (2.3). Thus the energy eigenvalues ε_n are gauge invariant. Equation (2.18) is gauge invariant, and the coefficient c_n can be interpreted as the probability amplitude for the system to be in the state ψ_n at time t.

3. Gauge-invariant solution of the charged harmonic oscillator

In this section the theory given in § 2 is applied to the case of a one-dimensional charged harmonic oscillator in an electromagnetic field in the electric dipole approximation (EDA) (Kobe and Wen 1980, Wen 1980). In the EDA only the effect of the electric field on the system is considered, and magnetic effects are neglected. The wavelength of the electromagnetic radiation is taken to be long compared with the spatial dimensions of the system. Only the electric field at the origin need be considered, and the spatial variation of the field can be neglected.

In the Coulomb gauge in the EDA, the vector potential can be replaced by its value at the origin. The Schrödinger equation for a one-dimensional harmonic oscillator of angular frequency ω in the x direction is thus

$$\tfrac{1}{2}m^{-1}(p_x - qA(t)/c)^2\psi + \tfrac{1}{2}m\omega^2 x^2 \psi = i\hbar\, \partial\psi/\partial t. \tag{3.1}$$

The vector potential $A(t) = A_x(0, t)$ is in the x direction, and the scalar potential is taken as zero because the sources of this external radiation field are at infinity. The electric field E in the x direction at the origin is

$$E = -c^{-1}\, \partial A/\partial t. \tag{3.2}$$

The energy operator $\mathscr{E}(\boldsymbol{A})$ in equation (2.12) for the problem in equation (3.1) is the same as the Hamiltonian, since the scalar potential of the external field is zero. Therefore the eigenvalue problem in equation (2.16) for the energy operator is

$$[\tfrac{1}{2}(p_x - qA(t)/c)^2/m + \tfrac{1}{2}m\omega^2 x^2]\psi_n = \varepsilon_n \psi_n. \tag{3.3}$$

The wavefunction ψ in equation (3.1) is expanded in equation (2.17), where the expansion coefficients c_n satisfy equation (2.18).

Equation (3.3) can be solved exactly by making the gauge transformation in equation (2.3) on the wavefunction ψ_n with the gauge function (see e.g. Sargent *et al* 1975)

$$\Lambda(x, t) = -A(t)x. \tag{3.4}$$

The new vector potential A' in equation (2.4) is

$$A' = 0 \tag{3.5}$$

and the new scalar potential A'_0 in equation (2.5) is

$$A'_0 = -E(t)x. \tag{3.6}$$

The new wavefunction ψ' is given in terms of ψ by equation (2.3), and is related to the new expansion functions ψ'_n by

$$\psi' = \sum_n c_n \psi'_n \tag{3.7}$$

from a gauge transformation on equation (2.17). The gauge transformed energy eigenvalue problem in equation (3.3) therefore becomes

$$(\tfrac{1}{2}p_x^2/m + \tfrac{1}{2}m\omega^2 x^2)\psi'_n = \varepsilon_n \psi'_n \tag{3.8}$$

where ψ'_n is related to ψ_n by equation (2.3). This equation is the equation for a free harmonic oscillator whose solutions are $\psi'_n = \Phi_n$, the eigenstates of the free harmonic oscillator with energy eigenvalues $\varepsilon_n = \hbar\omega(n + \frac{1}{2})$, where $n = 0, 1, 2, 3, \ldots$.

Equation (2.18) for the probability amplitudes is gauge invariant, since the matrix element is gauge invariant (Kobe and Smirl 1978),

$$\langle \psi_n | (qA_0 - i\hbar\, \partial/\partial t)\psi_m \rangle = \langle \psi'_n | (qA'_0 - i\hbar\, \partial/\partial t)\psi'_m \rangle \tag{3.9}$$

from equations (2.3) and (2.5). With the new scalar potential in equation (3.6) and the time-independent eigenstates $\psi'_n = \Phi_n$, the matrix element in equation (3.9) becomes

$$\langle \psi'_n | (qA'_0 - i\hbar\, \partial/\partial t)\psi'_m \rangle = -qE(t)\langle \Phi_n | x\Phi_m \rangle. \tag{3.10}$$

Therefore equation (2.18) for the gauge invariant probability amplitudes becomes

$$i\hbar\dot{c}_n - \varepsilon_n c_n = -\sum_m qE(t)\langle \Phi_n | x\Phi_m \rangle c_m. \tag{3.11}$$

In the EDA the equations are simpler in the gauge where the potentials are given by equations (3.5) and (3.6). This choice of gauge is only valid in the EDA for the effect of the electromagnetic field on the system.

Since the harmonic oscillator Φ_n are known, the matrix elements of x are (Merzbacher 1970, p 64)

$$\langle \Phi_n | x\Phi_m \rangle = (\hbar/2m\omega)^{1/2}(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}). \tag{3.12}$$

When this matrix element is substituted into equation (3.11), the equations can be solved exactly. In appendix 1 it is shown that if the system is in the ground state Φ_0 at time zero, the solution to equation (3.11) for the probability amplitude c_n is

$$c_n(t) = e^{i\beta(t)}(n!)^{-1/2}Q(\omega t)^n \exp(-\tfrac{1}{2}|Q(\omega t)|^2). \tag{3.13}$$

The function $Q(z)$ is

$$Q(z) = i\alpha\, e^{-iz}\int_0^z ds\, e^{is} f(s/\omega) \tag{3.14}$$

where the dimensionless parameter α is

$$\alpha = qE_0(2m\hbar\omega^3)^{-1/2} \tag{3.15}$$

and the function f is

$$f(t) = E(t)/E_0. \tag{3.16}$$

The phase factor β in equation (3.13) is given in equations (A1.8) and (A1.10). Since the function f in equation (3.16) is real, the phase factor β is real. At time $t = 0$ equations (3.13) and (3.14) show that $c_n(0) = 0$ for $n = 1, 2, 3, \ldots$, and $c_0(0) = 1$. Therefore the system is in the ground state at time zero.

The probability of finding the system in the state Φ_n is the absolute value of equation (3.13) squared,

$$P_n(t) = |c_n(t)|^2 = (n!)^{-1}|Q(\omega t)|^{2n} \exp(-|Q(\omega t)|^2) \tag{3.17}$$

which is a Poisson distribution characteristic of a coherent state. The wavefunction which began in the ground state at time zero thus evolves into a coherent state at a later time. (The charged harmonic oscillator has been previously solved, see e.g. Heffner and Louisell (1965). The Feynman path integral approach to the problem has also been used (Feynman and Hibbs 1965). See also Merzbacher (1970, pp 362–9).)

In order to evaluate equation (3.17), we assume that the electric field is harmonic with a frequency Ω

$$E(t) = E_0 \sin(\Omega t + \vartheta) \tag{3.18}$$

where ϑ is a phase factor. The function $Q(z)$ in equation (3.14) can then be evaluated, and its absolute value squared is

$$\alpha^{-2}|Q(z)|^2 = \frac{\sin^2[\frac{1}{2}(\rho+1)z]}{(\rho+1)^2} + \frac{\sin^2[\frac{1}{2}(\rho-1)z]}{(\rho-1)^2} - \frac{2}{(\rho^2-1)} \sin[\tfrac{1}{2}(\rho+1)z] \sin[\tfrac{1}{2}(\rho-1)z] \cos(\rho z + 2\vartheta) \tag{3.19}$$

where

$$\rho = \Omega/\omega \tag{3.20}$$

is the ratio of the frequency of the field to the frequency of the oscillator. The function $|Q|^2$ is plotted in figure 1 against $z = \omega t$ for $\alpha = 1$, $\vartheta = 0$, and $\rho = 1$. The probability that the system is in the ground state $P_0(t)$ in equation (3.17) is shown in figure 2 as a function of ωt for $\alpha = 1$, $\vartheta = 0$ and various values of ρ. For $n = 0$, 1, 2 and 3, $P_n(t)$ is plotted in figure 3. The contribution of other states is negligible, since the sum of the four probabilities in figure 3 is essentially one.

4. Conventional approach to the interaction of classical radiation in quantum mechanics

A critique of the conventional approach to the interaction of classical electromagnetic radiation and matter, which is found in most quantum mechanics books (see e.g. Schiff 1968, Merzbacher 1970), will be given in this section. The usual approach to the interaction of electromagnetic radiation and matter is to expand the quadratic term in

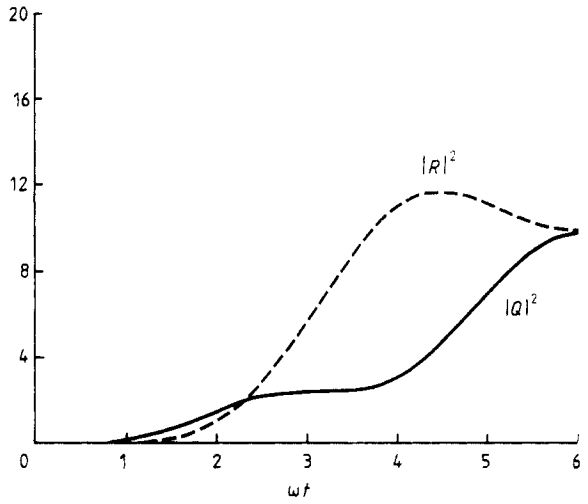

Figure 1. A plot of $|Q(\omega t)|^2$ in equation (3.19) and $|R(\omega t)|^2$ in equation (5.10) as a function of ωt for $\alpha = 1$, $\vartheta = 0$ and $\rho = 1$.

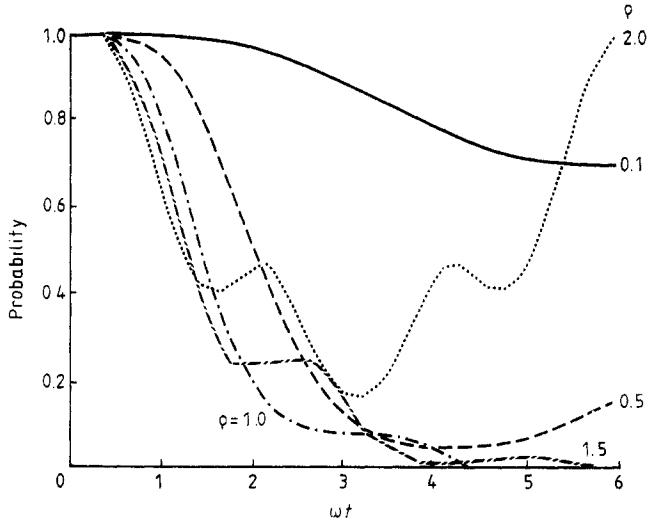

Figure 2. The probability $P_0(t)$ in equation (3.17) as a function of ωt for $\alpha = 1$, $\vartheta = 0$, and $\rho = 0.1$, 0.5, 1.0, 1.5 and 2.0.

equation (2.1). Then the Schrödinger equation in equation (2.2) becomes

$$[H_0 - q(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A})/2mc + q^2A^2/2mc^2 + qA_0]\psi = i\hbar\,\partial\psi/\partial t. \tag{4.1}$$

The unperturbed Hamiltonian H_0

$$H_0 = p^2/2m + V \tag{4.2}$$

satisfies the eigenvalue problem

$$H_0\Phi_n = e_n\Phi_n \tag{4.3}$$

with eigenfunction Φ_n and eigenvalue e_n.

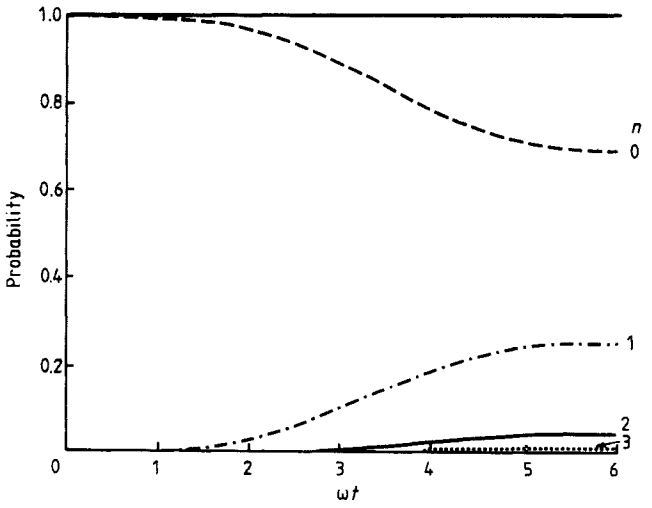

Figure 3. The probabilities $P_n(t)$ in equation (3.17) as a function of ωt for $\alpha = 1$, $\vartheta = 0$, $\rho = 0.1$ for $n = 0$, 1, 2 and 3. The full line is their sum.

The wavefunction ψ in equation (4.1) is then expanded in terms of the unperturbed eigenfunctions

$$\psi = \sum_n a_n \Phi_n \tag{4.4}$$

with expansion coefficients a_n. When equation (4.4) is substituted into equation (4.1) the equation

$$i\hbar \dot{a}_n - e_n a_n = \sum_m \langle \Phi_n | [-q(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A})/2mc + q^2A^2/2mc^2 + qA_0]\Phi_m \rangle a_m \tag{4.5}$$

is obtained for the expansion coefficients. The vector and scalar potentials are responsible for inducing a transition in contrast to equation (3.11).

The expansion coefficients a_n are not gauge invariant (Kobe and Smirl 1978). If a gauge transformation is made on the problem as in equation (2.6), then the wavefunction and potentials in equation (4.1) are replaced by ψ', $\boldsymbol{A}'$ and A_0', respectively. To follow the conventional procedure in the new gauge, the wavefunction ψ' in equation (2.3) is expanded in terms of the eigenfunctions Φ_n of H_0 in equation (4.3) as

$$\psi' = \sum_n a_n' \Phi_n \tag{4.6}$$

where new expansion coefficients a_n' are needed. The new expansion coefficients satisfy equation (4.5) with a_n, $\boldsymbol{A}$ and A_0 replaced with a_n', $\boldsymbol{A}'$ and A_0', respectively. A relationship between the new expansion coefficients and the old expansion coefficients can be obtained by substituting equations (4.4) and (4.6) into equation (2.3), multiplying by Φ_n^* and integrating. The result is

$$a_n' = \sum_m \langle \Phi_n | \exp(iq\Lambda/\hbar c) \Phi_m \rangle a_m. \tag{4.7}$$

Since Λ is an arbitrary function of space and time the matrix elements in equation (4.7) are not the Kronecker delta. In general $|a_n'|^2 \neq |a_n|^2$ and the expansion coefficients are

not gauge invariant. Therefore they cannot properly be interpreted as probability amplitudes.

In an effort to circumvent this problem it has been suggested that the proper expansion in equation (4.6) should be

$$\psi' = \sum_n a_n \Phi'_n \tag{4.8}$$

where

$$\Phi'_n = \exp(iq\Lambda/\hbar c)\Phi_n. \tag{4.9}$$

The functions Φ'_n satisfy the eigenvalue problem

$$[\tfrac{1}{2}(\boldsymbol{p}')^2/m + V]\Phi'_n = e_n \Phi'_n \tag{4.10}$$

where the momentum operator $\boldsymbol{p}'$ is

$$\boldsymbol{p}' = \boldsymbol{p} - q\nabla\Lambda/c. \tag{4.11}$$

The momentum operator $\boldsymbol{p}'$ also satisfies the canonical commutation relations.

In the new gauge, the equation for the expansion coefficients a_n in equation (4.5) becomes

$$i\hbar\dot{a}_n - e_n a_n = \sum_m \langle \Phi'_n | [-q(\boldsymbol{A}\cdot\boldsymbol{p}' + \boldsymbol{p}'\cdot\boldsymbol{A})/2mc + q^2A^2/2mc^2 + qA_0]\Phi'_m \rangle a_m. \tag{4.12}$$

The matrix element in equation (4.12) is the same as the matrix element in equation (4.5) so the two equations are the same.

By following this procedure we have guaranteed that once we have chosen a gauge, all the calculations performed in other gauges give the same result. The question arises then as to how to choose the original gauge. The conventional answer to this problem is to choose the radiation gauge in which the vector potential $\boldsymbol{A}^{(r)}$ satisfies

$$\nabla\cdot\boldsymbol{A}^{(r)} = 0 \tag{4.13}$$

and the scalar potential $A_0^{(r)}$ satisfies

$$A_0^{(r)} = 0 \tag{4.14}$$

because the sources are at infinity. Equation (4.5) simplifies in this gauge to

$$i\hbar\dot{a}_n^{(r)} - e_n a_n^{(r)} = \sum_m \langle \Phi_n | (-q\boldsymbol{A}^{(r)}\cdot\boldsymbol{p}/mc + q^2A^{(r)2}/2mc^2)\Phi_m \rangle a_m^{(r)} \tag{4.15}$$

where $a_n^{(r)}$ denotes the expansion coefficient in the radiation gauge. The choice of the radiation gauge is, however, only a convention. It is then a postulate that the absolute value squared of the expansion coefficients $|a_n^{(r)}|^2$ have a physical interpretation as the probability of finding the system in the state Φ_n.

The justification which is sometimes given for using the radiation gauge is that the gauge transformation in equation (2.4) on the vector potential changes only the longitudinal part of the vector potential (Barut 1964). The transverse part of the vector potential is unchanged by a gauge transformation. The vector potential can be written in terms of its transverse part $\boldsymbol{A}_T$ and its longitudinal part $\boldsymbol{A}_L$ as

$$\boldsymbol{A} = \boldsymbol{A}_T + \boldsymbol{A}_L \tag{4.16}$$

where $\nabla\cdot\boldsymbol{A}_T = 0$ and $\nabla\times\boldsymbol{A}_L = 0$. Under the gauge transformation in equation (2.4) the

vector potential $\boldsymbol{A}'$ is

$$\boldsymbol{A}' = \boldsymbol{A}_{\mathrm{T}} + \boldsymbol{A}'_{\mathrm{L}} \tag{4.17}$$

where

$$\boldsymbol{A}'_{\mathrm{L}} = \boldsymbol{A}_{\mathrm{L}} + \nabla\Lambda. \tag{4.18}$$

Therefore the transverse part of the vector potential appears unchanged by a gauge transformation. If the gauge function is also independent of the time, the scalar potential in equation (4.14) is likewise unchanged. In the radiation gauge only the transverse part of the vector potential is used. Thus by this procedure it appears that the choice of the radiation gauge has been justified.

On the other hand if the gauge function Λ satisfies Laplace's equation

$$\nabla^2\Lambda = 0 \tag{4.19}$$

then the gauge transformation in equation (2.4) can equally well be written as

$$\boldsymbol{A}' = \boldsymbol{A}'_{\mathrm{T}} + \boldsymbol{A}_{\mathrm{L}} \tag{4.20}$$

where

$$\boldsymbol{A}'_{\mathrm{T}} = \boldsymbol{A}_{\mathrm{T}} + \nabla\Lambda \tag{4.21}$$

since $\nabla \cdot \boldsymbol{A}'_{\mathrm{T}} = 0$. Although the potential $\boldsymbol{A}'_{\mathrm{T}}$ would not satisfy the same boundary conditions as $\boldsymbol{A}_{\mathrm{T}}$, the electric and magnetic fields would be unchanged. Thus the radiation gauge is not unique and unique values for the expansion coefficients $a_n^{(r)}$ are not guaranteed.

A deeper criticism of this approach can be made. The approach is not manifestly gauge invariant in the sense that the equations are not *form invariant* under gauge transformations. The equations of § 2 are all form invariant under gauge transformations, so that two physicists using different gauges will automatically obtain the same results. In the radiation gauge paradigm, it is necessary for the two physicists to transform to the same common gauge, namely, the radiation gauge, before making their calculations. Even if the radiation gauge were unique, this procedure is obviously not manifestly gauge invariant. It is only a convention which is agreed upon by all workers. But gauge invariance is not a matter of choosing a particular gauge by convention, any more than Lorentz invariance is a matter of choosing a particular coordinate system. Lorentz invariance, of course, means form invariance under all Lorentz transformations. Likewise, gauge invariance means form invariance under all gauge transformations. In the next section we shall see that for the harmonic oscillator the conventional approach does not agree with the gauge-invariant approach of § 3.

5. Conventional solution of the charged harmonic oscillator

In this section we show that in the case of a charged harmonic oscillator the conventional approach gives a probability that the system is in an eigenstate of the harmonic oscillator Φ_n which is in general different from the probability of the gauge-invariant formulation of § 3. There cannot be two different results for something that is in principle observable. (Power (1978, p 12) derives two different expressions for the probability of finding the system in the ground state, and does not have a criterion for choosing between them.) The principle of gauge invariance tells us that the results

of § 3 are correct and the results of the conventional approach are incorrect. (Geltman (1977) gauge transforms to the proper wavefunction before calculating the probability, without giving a reason for this procedure.)

In the conventional approach, equation (3.1) for the one-dimensional harmonic oscillator in the EDA is expanded, which gives

$$(H_0 - qA(t)p_x/mc + q^2A(t)^2/2mc^2)\psi = i\hbar\,\partial\psi/\partial t. \tag{5.1}$$

In this case the unperturbed Hamiltonian H_0 is given in equation (4.2), where V is the one-dimensional harmonic oscillator potential. The eigenvalue problem for this H_0 is given in equation (4.3), where Φ_n are the harmonic oscillator eigenfunctions and $e_n = \hbar\omega(n+\frac{1}{2})$ for $n = 0, 1, 2, 3, \ldots$. In this case equation (4.3) is the same as equation (3.8). The wavefunction ψ in equation (5.1) is expanded in equation (4.4) in terms of the eigenstates Φ_n. When equation (4.4) is substituted into equation (5.1) the equation for the expansion coefficients a_n is obtained

$$i\hbar\dot{a}_n - \tilde{\varepsilon}_n a_n = -\sum_m \frac{q}{mc} A(t)\langle\Phi_n|p_x\Phi_m\rangle a_m \tag{5.2}$$

where the energy $\tilde{\varepsilon}_n$ is

$$\tilde{\varepsilon}_n = \hbar\omega(n+\tfrac{1}{2}) + q^2A^2/2mc^2. \tag{5.3}$$

For the harmonic oscillator the matrix elements of the momentum operator p_x are (Merzbacher 1970, p 64)

$$\langle\Phi_n|p_x\Phi_m\rangle = i(\tfrac{1}{2}\hbar m\omega)^{1/2}(\sqrt{n}\,\delta_{m,n-1} - \sqrt{n+1}\,\delta_{m,n+1}). \tag{5.4}$$

When equation (5.4) is substituted into equation (5.2), it can be solved exactly as shown in appendix 2. If the system is originally in the ground state it develops into a coherent state at a later time (Heffner and Louisell 1965, Feynman and Hibbs 1965, Merzbacher 1970, pp 362–9). The solution of equation (5.2) with equation (5.4) substituted into it is

$$a_n(t) = e^{i\gamma(t)}\frac{R(\omega t)^n}{\sqrt{n!}}\exp(-\tfrac{1}{2}|R(\omega t)|^2). \tag{5.5}$$

The function R is

$$R(z) = Q(z) - i\alpha g(z/\omega) \tag{5.6}$$

where $Q(z)$ is given in equation (3.14). The function g is defined as

$$g(t) = \int_0^{\omega t} ds\, f(s/\omega) \tag{5.7}$$

where f is defined in equation (3.16). If $g(t) = 0$, then the conventional and gauge-invariant approaches agree with each other. If the field $E(t)$ is zero for times $t > \tau$ and $g(t) = 0$ (i.e. $A(t) = 0$) for $t > \tau$, the same probabilities are obtained. The phase angle $\gamma(t)$ is given in equations (A2.3) and (A2.4). If the function g is real, as it would be for a realistic electric field, then the imaginary part in equation (A2.3) vanishes. The state ψ in equation (4.4) is thus a coherent state, but it is different from the coherent state ψ' in equation (3.7).

The absolute value squared of the expansion coefficient in equation (5.5) is

$$|a_n(t)|^2 = (n!)^{-1}|R(\omega t)|^{2n}\exp(-|R(\omega t)|^2). \tag{5.8}$$

This expression is also a Poisson distribution, but it is different from the one for $|c_n|^2$ in equation (3.17). Since this conventional approach is not gauge invariant, it is equation (3.17) for $|c_n|^2$ which should be interpreted as the gauge-invariant probability $P_n(t)$ of finding the system in the state Φ_n at time t if the system is in the ground state at time zero.

If we choose the harmonically varying electric field in equation (3.18), the function $g(z/\omega)$ in equation (5.7) is

$$g(z/\omega) = \rho^{-1}[\cos\vartheta - \cos(\rho z + \vartheta)]. \tag{5.9}$$

The absolute value squared of the function R in equation (5.6) is thus

$$\begin{aligned}\alpha^{-2}|R(z)|^2 = \alpha^{-2}|Q(z)|^2 + [g(z/\omega)]^2 \\ - 2g(z/\omega)\{(\rho+1)^{-1}\sin[\tfrac{1}{2}(\rho+1)z]\sin[\tfrac{1}{2}(\rho-1)z+\vartheta] \\ + (1-\rho)^{-1}\sin[\tfrac{1}{2}(1-\rho)z]\sin[\tfrac{1}{2}(\rho+1)z+\vartheta]\}.\end{aligned} \tag{5.10}$$

The function $|R|^2$ is plotted against $z = \omega t$ in figure 1 for $\alpha = 1$, $\vartheta = 0$ and $\rho = 1$. A comparison with the function $|Q|^2$ shows that the functions are not the same, so that the probabilities calculated by the conventional approach and the gauge-invariant formulation are not the same. The function $|a_0|^2$ is plotted in figure 4 against ωt for the same values of α, ϑ, and ρ as in figure 2. Since these curves are different from the gauge-invariant probability in figure 2, they cannot properly be called 'probabilities'. However the values of $|a_n|^2$ do add to unity, as shown in figure 5. These quantities $|a_n|^2$ are not the same as $P_n(t)$ in figure 3 for the same values of α, ϑ and ρ. Therefore, regardless of being normalised to unity they cannot be interpreted as probabilities.

5. Conclusion

The charged harmonic oscillator in an electromagnetic field in the electric dipole approximation (EDA) is solved using both the manifestly gauge-invariant formulation of quantum mechanics and the conventional approach. The results for the probability of finding the system in the unperturbed state Φ_n at time t differ in general. Since there cannot be two different expressions for the same physical quantity, we must conclude that the gauge-invariant formulation gives the correct answer. In this problem the conventional approach is incorrect. This problem is a counter example to the proofs that the conventional approach is gauge invariant. Although in some cases the conventional approach does give the same result as the gauge-invariant formulation, it is not true in general (Leubner and Zoller 1980). To be certain that a gauge-invariant result is obtained it is necessary to use the gauge-invariant formulation of quantum mechanics.

This paper shows that the long-held view that all expansion coefficients have a physical interpretation as probability amplitudes is false. The probability amplitudes must be gauge invariant to have such an interpretation. Gauge invariance is ensured by using the gauge-invariant formulation. The conventional treatment of the interaction of classical electromagnetic radiation with a charged quantum mechanical particle leads to gauge-dependent expansion coefficients.

The gauge-invariant formulation of quantum mechanics can be used with an arbitrary gauge. However, in the EDA the equations become simpler when a gauge transformation is made to the gauge in which the vector potential is zero and the scalar

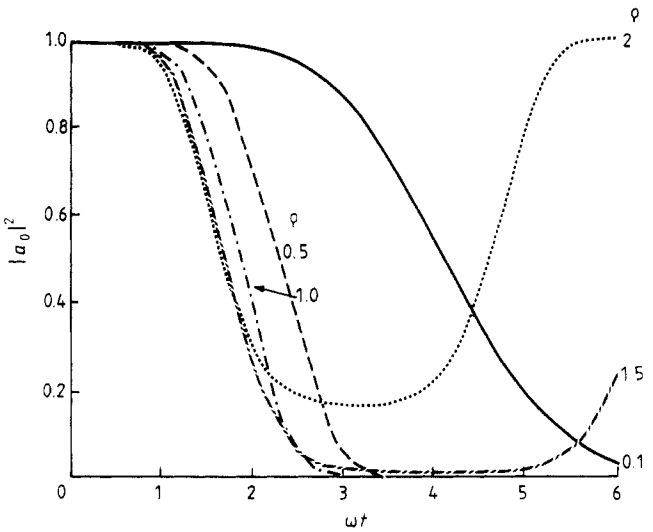

Figure 4. The function $|a_0(t)|^2$ in equation (5.8) as a function of ωt for $\alpha = 1$, $\vartheta = 0$ and $\rho = 0.1$, 0.5, 1.0, 1.5 and 2.0.

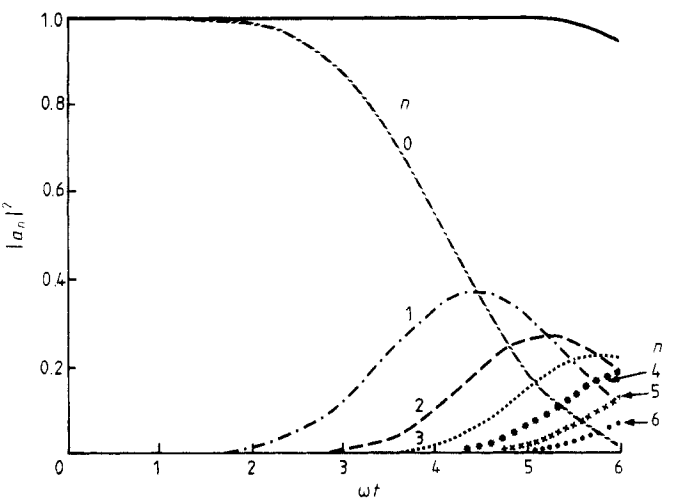

Figure 5. The functions $|a_n(t)|^2$ in equation (5.8) as a function of ωt for $\alpha = 1$, $\vartheta = 0$, $\rho = 0.1$ and $n = 0$, 1, 2, 3, 4, 5 and 6. The full curve is their sum.

potential is $-\boldsymbol{E}(0, t)\cdot\boldsymbol{r}$. In fact, the gauge transformation to this gauge can be regarded as a technique for solving the problem. Even though this particular gauge simplifies the gauge-invariant formulation, the problem can be expressed in an arbitrary gauge.

The charged harmonic oscillator in the EDA can be solved exactly, so that approximations do not obscure questions of principle. The case of a classical electromagnetic field is of interest since many practical problems can be formulated in terms of classical fields. The quantisation of the electromagnetic field is guided by the structure of the classical theory. However for the quantised electromagnetic field the electromagnetic field itself becomes part of the dynamical system. The treatment of a charged harmonic

oscillator interacting with a quantised electromagnetic field involves considerations other than those dealt with in this paper.

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Appendix 1. Solution for probability amplitudes

Equation (3.11) for c_n can be solved exactly when the matrix element in equation (3.12) is used. If equation (3.12) is substituted into equation (3.11) the equation becomes

$$i\hbar\dot{c}_n - \varepsilon_n c_n = -\alpha\hbar\omega f(t)(\sqrt{n}c_{n-1} + \sqrt{n+1}c_{n+1}) \tag{A1.1}$$

where $\varepsilon_n = \hbar\omega(n+\frac{1}{2})$, α is given in equation (3.15), and $f(t)$ is given in equation (3.16). If the system is in the ground state at time $t = 0$, then it has been shown that the system develops into a coherent state at a later time (Heffner and Louisell 1965, Feynman and Hibbs 1965). Thus we shall assume that c_n is given by equation (3.13), where the functions Q and β are to be determined. When equation (3.13) is substituted into equation (A1.1) we obtain

$$(i\dot{Q} + \alpha\omega f(t) - \omega Q)Q^{-1}nc_n = (\tfrac{1}{2}\omega + \dot{\beta} + i\tfrac{1}{2}d|Q|^2/dt - \alpha\omega f(t)Q)c_n. \tag{A1.2}$$

For this equation to be valid for all values of n it is necessary that the left-hand side vanish identically,

$$i\dot{Q} + \alpha\omega f(t) - \omega Q = 0. \tag{A1.3}$$

This equation has the solution

$$Q(\omega t) = i\alpha\, e^{-i\omega t}\int_0^{\omega t} ds\, e^{is} f(s/\omega) \tag{A1.4}$$

so we have obtained the function Q in equation (3.14).

If the left-hand side of equation (A1.2) is zero, the right-hand side of the equation must also be zero. Therefore, the function β must satisfy

$$\dot{\beta} + \tfrac{1}{2}\omega + i\tfrac{1}{2}\, d|Q|^2/dt - \alpha\omega f(t)Q = 0. \tag{A1.5}$$

This equation is a complex equation, so that both the real and imaginary parts must be separately equal to zero. The imaginary part of this equation is

$$\operatorname{Im}\dot{\beta} + \tfrac{1}{2}\, d|Q|^2/dt - \operatorname{Im}\alpha\omega f(t)Q = 0. \tag{A1.6}$$

When equation (A1.3) is substituted into equation (A1.6), the result is

$$\operatorname{Im}\dot{\beta}(t) = 2\alpha\omega\ \operatorname{Re} Q(\omega t)\operatorname{Im} f(t). \tag{A1.7}$$

This equation can be integrated to give

$$\operatorname{Im}\beta(t) = 2\alpha\int_0^{\omega t} ds\ \operatorname{Re} Q(s)\operatorname{Im} f(s/\omega). \tag{A1.8}$$

The constant of integration is zero because $\operatorname{Im}\beta(0)=0$. If $f(t)$ is a real function, as it should be for the Hamiltonian to be Hermitian, then the right-hand side of equation (A1.8) is zero. However, in the rotating-wave approximation, it is convenient to take f to be complex.

The real part of equation (A1.5) gives the equation

$$\operatorname{Re}\dot{\beta}(t)=-\tfrac{1}{2}\omega+\alpha\omega\operatorname{Re}f(t)Q(\omega t). \tag{A1.9}$$

When this equation is integrated and equation (A1.4) is used, the result is

$$\operatorname{Re}\beta(t)=-\tfrac{1}{2}\omega t-\alpha^2\operatorname{Im}\int_0^{\omega t}\mathrm{d}s\int_0^{s}\mathrm{d}\tau f(s/\omega)f(\tau/\omega)\exp[\mathrm{i}(\tau-s)] \tag{A1.10}$$

since $\operatorname{Re}\beta(0)=0$. Therefore, the phase angle β in equation (3.13) is real, and does not contribute when the absolute value of equation (3.13) is taken.

Appendix 2. Solution for the conventional expansion coefficients

When equation (5.4) is substituted into equation (5.2) for the expansion coefficients a_n, the result is

$$\mathrm{i}\hbar\dot{a}_n-\tilde{\varepsilon}_n a_n=\hbar\omega\alpha g(t)\mathrm{i}(\sqrt{n}\,a_{n-1}-\sqrt{n+1}\,a_{n+1}) \tag{A2.1}$$

where the energy $\tilde{\varepsilon}_n$ is given in equation (5.3). The function $g(t)$ is defined in equation (5.7), and is proportional to the vector potential since $E=-\partial A/\partial(ct)$. Equation (A2.1) has a structure similar to equation (A1.1), and can be solved in a manner similar to that used in appendix 1.

When equation (5.5) is substituted into equation (A2.1), an equation for the function R is obtained. The solution to this equation is

$$R(z)=\alpha\,\mathrm{e}^{-\mathrm{i}z}\int_0^{z}\mathrm{d}s\,\mathrm{e}^{\mathrm{i}s}g(s/\omega) \tag{A2.2}$$

which is the same as equation (A1.4) with f replaced by $-\mathrm{i}g$. The complex equation for $\gamma(t)$ gives the imaginary part and the real part. The imaginary part of $\gamma(t)$ is

$$\operatorname{Im}\gamma(t)=-2\alpha\int_0^{\omega t}\mathrm{d}s\operatorname{Im}R(s)\operatorname{Im}g(s/\omega)-2\alpha^2\int_0^{\omega t}\mathrm{d}s\operatorname{Re}g(s/\omega)\operatorname{Im}g(s/\omega) \tag{A2.3}$$

since $\operatorname{Im}\gamma(0)=0$, which vanishes when g is a real function. The real part of $\gamma(t)$ is

$$\operatorname{Re}\gamma(t)=-\frac{\omega t}{2}-\alpha^2\int_0^{\omega t}\mathrm{d}s\operatorname{Re}[g(s/\omega)]^2-\alpha^2\operatorname{Im}\int_0^{\omega t}\mathrm{d}s\int_0^{s}\mathrm{d}\tau\,g(s/\omega)g(\tau/\omega)\exp[\mathrm{i}(\tau-s)] \tag{A2.4}$$

since $\operatorname{Re}\gamma(0)=0$.

The function $R(z)$ can be rewritten by substituting equation (5.7) into equation (A2.2) to give

$$R(z)=-\mathrm{i}\alpha\,\mathrm{e}^{-\mathrm{i}z}\int_0^{z}\mathrm{d}s\,(\mathrm{d}\mathrm{e}^{\mathrm{i}s}/\mathrm{d}s)\int_0^{s}\mathrm{d}\tau f(\tau/\omega). \tag{A2.5}$$

After an integration by parts this equation becomes equation (5.6).

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