Gauge transformation of the time-evolution operator

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The time-evolution operator is in general gauge dependent. Its gauge transformation property follows from the gauge transformation of the wave function and ensures gauge-invariant matrix elements. The same transformation property is shown here to follow from the formal solution of the Schrödinger equation for the time-evolution operator, which is a time-ordered exponential of the time integral of the Hamiltonian. The gauge transformation property of the time-evolution operator in the interaction picture is also obtained. The perturbation expansion of the time-evolution operator in one gauge can be transformed to give the perturbation expansion for the time-evolution operator in another gauge. The $\mathbf{A}\cdot\mathbf{p}$ versus $\mathbf{E}\cdot\mathbf{r}$ controversy in the electric dipole approximation is resolved by specifying the correct initial and final states.

I. INTRODUCTION

The Schrödinger equation for a particle in a time-dependent external electromagnetic field can be solved formally by using the time-evolution operator which is a time-ordered exponential of the time integral of the Hamiltonian.[1] This expression can be written in the interaction picture and a perturbation expansion developed.[2] When only the states in the remote past and distant future are of interest, the S matrix is obtained from the time-evolution operator by taking the asymptotic time limits. Feynman diagrams are helpful in keeping track of the various terms in the perturbation expansion of the S matrix.[3]

The transformation property of the S matrix or more generally the time-evolution operator under a change of gauge has been of interest recently.[4–6] When it is stated that the S matrix is gauge invariant, it is assumed that the potentials are adiabatically turned on and off, so that the potentials are zero in the remote past and distant future.[7,8] This choice for the potentials is, however, a specific choice of gauge.[9] Turning the potentials on and off adiabatically, although commonly used, is not necessary.[7] In the laboratory it is only the electric and magnetic fields that are turned on and off. In general the time-evolution operator and the S matrix are gauge dependent. The gauge dependence is such that the matrix elements between the appropriate initial and final states are gauge invariant. The matrix elements are therefore interpretable as probability amplitudes.[10,11]

In this paper the properties of the time-evolution operator under gauge transformation are investigated. It is not necessary to assume that the potentials are turned on and off adiabatically. The transformation property of the time-evolution operator under a change of gauge can be immediately obtained from the gauge transformation of the wave function. On the other hand, the same gauge transformation property can also be derived directly from the formal solution for the time-evolution operator as a time-ordered exponential of the time integral of the Hamiltonian. The direct proof shows the consistency of the formal solution. The gauge transformation property of the time-evolution operator in the interaction picture is also obtained. The time-evolution operator in the interaction picture is also gauge dependent. When a perturbation expansion of the time-evolution operators in different gauges is made, and the transformation property is applied, the same perturbation expansion is obtained. A direct calculation through second order in perturbation theory illustrates this statement.

In Sec. II gauge transformations in quantum mechanics are reviewed. The time-evolution operator is defined in Sec. III and its transformation property under a gauge transformation is obtained. A factorization theorem for time-ordered exponentials is proved in Sec. IV. In Sec. V the theorem is applied to the formal solution for the time-evolution operator to obtain the gauge transformation property. The gauge transformation property for the time-evolution operator in the interaction picture is obtained in Sec. VI, and illustrated through second order of perturbation theory in Sec. VII. The $\mathbf{A}\cdot\mathbf{p}$ versus $\mathbf{E}\cdot\mathbf{r}$ interaction controversy in the electric dipole approximation is discussed and resolved in Sec. VIII. Finally, the conclusion is given in Sec. IX.

II. GAUGE TRANSFORMATIONS

The form invariance of the Schrödinger equation[12] under gauge transformations is reviewed in order to establish the notation. The gauge transformation property of the Hamiltonian is also obtained.[10,11]

The Hamiltonian for a single particle of mass m and charge q in an external classical time-dependent electromagnetic field characterized by the vector potential $\mathbf{A}(\mathbf{r},t)$ and the scalar potential $\phi(\mathbf{r},t)$ is

$$H=H(\mathbf{A},\phi)=(1/2m)(\mathbf{p}-q\mathbf{A}/c)^2+V(\mathbf{r})+q\phi\ . \tag{2.1}$$

The potential energy $V(\mathbf{r})$ of the particle is defined such that its negative gradient is a conservative force. Electrostatic fields, if present, are thus included in $V(\mathbf{r})$. The Schrödinger equation corresponding to the Hamiltonian in Eq. (2.1) is

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

The time-dependent electric field $\mathbf{E}$ and the magnetic induction field $\mathbf{B}$ are obtained from the potentials by

$$\mathbf{E} = -\nabla\phi - c^{-1}\,\partial\mathbf{A}/\partial t\ ,\quad \mathbf{B} = \nabla\times\mathbf{A}\ . \tag{2.3}$$

A gauge transformation can be made on the potential to obtain the new potentials

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda\ ,\quad \phi' = \phi - c^{-1}\,\partial\Lambda/\partial t\ , \tag{2.4}$$

where $\Lambda = \Lambda(\mathbf{r},t)$ is an arbitrary differentiable function of space and time. The electric and magnetic fields are of course unchanged if the new potentials are used in Eq. (2.3). A gauge transformation on the wave function is

$$\psi' = \exp(iq\Lambda/\hbar c)\psi\ . \tag{2.5}$$

If Eqs. (2.4) and (2.5) are used, the Schrödinger equation in the new gauge is

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

This form invariance of the Schrödinger equation under gauge transformations is called the gauge covariance of the equation.

The new Hamiltonian $H(\mathbf{A}',\phi')$ in Eq. (2.6) is expressed in terms of the original Hamiltonian in Eq. (2.1) as

$$\begin{aligned} H' &= H(\mathbf{A}',\phi') \\ &= \exp(iq\Lambda/\hbar c)H(\mathbf{A},\phi)\exp(-iq\Lambda/\hbar c) - (q/c)\partial\Lambda/\partial t\ . \end{aligned} \tag{2.7}$$

Because of the last term, the Hamiltonian is a gauge-dependent operator, i.e., it has a gauge-dependent expectation value. This transformation property of the Hamiltonian is used in Sec. V to obtain the transformation property of the time-evolution operator.

III. TIME-EVOLUTION OPERATOR

The operator $U(t,t_0)$ which describes the time evolution of the wave function from an initial time t_0 to a final time t is defined as[1]

$$\psi(t) = U(t,t_0)\psi(t_0)\ . \tag{3.1}$$

Under a gauge transformation, Eq. (3.1) becomes

$$\psi'(t) = U'(t,t_0)\psi'(t_0)\ . \tag{3.2}$$

If Eq. (2.5) is used for the gauge transformation of the wave function, the time-evolution operator transforms as

$$\begin{aligned} U'(t,t_0) &= \exp[iq\Lambda(t)/\hbar c]U(t,t_0) \\ &\quad\times\exp[-iq\Lambda(t_0)/\hbar c]\ , \end{aligned} \tag{3.3}$$

where the spatial coordinates in Λ are suppressed. The time-evolution operator is thus gauge dependent, but has a definite transformation law under gauge transformations.

The S matrix is defined as $S = U(+\infty,-\infty)$, so its transformation law is

$$S' = \exp[iq\Lambda(\infty)/\hbar c]S\exp[-iq\Lambda(-\infty)/\hbar c]\ . \tag{3.4}$$

If we restrict ourselves to gauges for which the potentials are zero at $t = \pm\infty$, then $\Lambda(+\infty) = \Lambda(-\infty) = 0$ and $S' = S$, which is the basis for a commonly made statement that the S matrix is gauge invariant. The general gauge transformation property is given in Eq. (3.4), where it is not necessary to put any restrictions on $\Lambda(\pm\infty)$. Kazes *et al.*[6] assume that $\Lambda(+\infty) = \Lambda(-\infty)$, and Aharonov and Au[4] consider time-independent gauge functions.

The transformation property in Eq. (3.3) ensures that the *matrix elements* of the time-evolution operator are gauge invariant. If the initial state is $\psi(t_0)$ and the final state is $\psi(t)$ then the probability amplitude of finding the system in the state $\psi(t)$ at time t is

$$\langle\psi(t)\,|\,U(t,t_0)\psi(t_0)\rangle = \langle\psi'(t)\,|\,U'(t,t_0)\psi'(t_0)\rangle\ , \tag{3.5}$$

which is gauge invariant.

If Eq. (3.1) is substituted into the Schrödinger equation in Eq. (2.2), the operator $U(t,t_0)$ also satisfies the Schrödinger equation

$$H(t)U(t,t_0) = i\hbar\,\partial U(t,t_0)/\partial t\ , \tag{3.6}$$

where $H(t) = H(\mathbf{A},\phi)$ is the time-dependent Hamiltonian. A formal solution to the Schrödinger equation for $U(t,t_0)$ is[1]

$$U(t,t_0) = T\exp\left[-(i/\hbar)\int_{t_0}^{t} dt'\,H(t')\right]\ , \tag{3.7}$$

where T is the time-ordering operator. A similar equations holds for $U'(t,t_0)$ except that H is replaced by H' on the right-hand side. It is clear from Eq. (3.7) that the time-evolution operator is gauge dependent because the Hamiltonian is gauge dependent.

IV. FACTORIZATION THEOREM FOR TIME-ORDERED EXPONENTIALS

The formal solution to the Schrödinger equation for the time-evolution operator is the time-ordered exponential in Eq. (3.7). If the operator H is the sum of two time-dependent terms, the time-ordered exponential can be factorized into the product of two time-ordered exponentials. The factorization theorem proved here is a generalization of the well-known transformation to the interaction picture,[2] in which both parts of the Hamiltonian are time dependent.

The Hamiltonian $H(t)$ in Eq. (3.7) is taken to be the sum of two time-dependent terms

$$H(t) = H_1(t) + H_2(t)\ . \tag{4.1}$$

The time-evolution operator $U(t,t_0)$ in Eq. (3.7) can then be written as the product of two operators

$$U(t,t_0) = U_1(t,t_0)U_{21}(t,t_0)\ . \tag{4.2}$$

The operator $U_1(t,t_0)$ is the time-ordered exponential

$$U_1(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'H_1(t')\right]. \tag{4.3}$$

The operator $U_{21}(t,t_0)$ is

$$U_{21}(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'H_{21}(t')\right], \tag{4.4}$$

where the operator H_{21} is the operator H_2 in the interaction picture of H_1,

$$H_{21}(t)=U_1^{-1}(t,t_0)H_2(t)U_1(t,t_0). \tag{4.5}$$

In order to prove this factorization theorem, Eqs. (4.1) and (4.2) can be substituted into Eq. (3.6) which gives

$$[H_1(t)+H_2(t)]U_1U_{21} =(i\hbar\partial U_1/\partial t)U_{21}+U_1(i\hbar\partial U_{21}/\partial t). \tag{4.6}$$

The operator U_1 is chosen to satisfy

$$H_1(t)U_1(t,t_0)=i\hbar\partial U_1(t,t_0)/\partial t, \tag{4.7}$$

the formal solution of which is Eq. (4.3). When Eq. (4.7) is substituted into Eq. (4.6), the result is

$$H_{21}(t)U_{21}(t,t_0)=i\hbar\partial U_{21}(t,t_0)/\partial t, \tag{4.8}$$

where H_{21} is given in Eq. (4.5). The formal solution to Eq. (4.8) is given in Eq. (4.4), which proves the factorization theorem.

V. GAUGE TRANSFORMATION PROPERTY OF THE TIME-EVOLUTION OPERATOR FROM THE FORMAL SOLUTION

The gauge-transformation property of the time-evolution operator in Eq. (3.3) can be proved directly from the formal solution for the time-evolution operator in Eq. (3.7). The direct proof shows the consistency of the formal solution.

The time-evolution operator $U'(t,t_0)$ in the new gauge characterized by the vector potential $\mathbf{A}'$ and scalar potential ϕ' satisfies the Schrödinger equation in Eq. (3.6),

$$H'(t)U'(t,t_0)=i\hbar\partial U'(t,t_0)/\partial t, \tag{5.1}$$

where the new Hamiltonian is $H'(t)=H(\mathbf{A}',\phi')$. The formal solution to this equation is

$$U'(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'H'(t')\right]. \tag{5.2}$$

The new Hamiltonian can be written as $H'=H_1'+H_2'$.

The factorization theorem can be applied to give $U'=U_1'U_{21}'$ with

$$H_1'(t)=-(q/c)\partial\Lambda(t)/\partial t \tag{5.3}$$

and

$$H_2'(t)=\exp[iq\Lambda(t)/\hbar c]H(t)\exp[-iq\Lambda(t)/\hbar c]. \tag{5.4}$$

The new Hamiltonian H' is related to the old Hamiltonian H by Eq. (2.7). The operator U_1' is

$$U_1'(t,t_0)=T\exp\left[i(q/\hbar c)\int_{t_0}^{t}dt'\,\partial\Lambda(t')/\partial t'\right], \tag{5.5}$$

from Eq. (4.3). If the operator $\partial\Lambda/\partial t$ commutes with itself at different times, then Eq. (5.5) becomes

$$U_1'(t,t_0)=\exp\{i(q/\hbar c)[\Lambda(t)-\Lambda(t_0)]\}. \tag{5.6}$$

The operator $U_{21}'(t,t_0)$ is

$$U_{21}'(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'H_{21}'(t')\right], \tag{5.7}$$

from Eq. (4.4), where from Eq. (4.5)

$$H_{21}'(t)=\exp[iq\Lambda(t_0)/\hbar c]H(t)\exp[-iq\Lambda(t_0)/\hbar c], \tag{5.8}$$

if the operator $\Lambda(t)$ commutes with itself at different times. Equation (5.7) then becomes

$$U_{21}'(t,t_0)=\exp[iq\Lambda(t_0)/\hbar c] \times T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'H(t')\right] \times\exp[-iq\Lambda(t_0)/\hbar c], \tag{5.9}$$

which can be seen by expanding the exponential in Eq. (5.7), applying the time-ordering operator T, and substituting Eq. (5.8) into it. The exponential involving $\Lambda(t_0)$ can be factored out because it depends only on the fixed time t_0. The expansion can then be resummed to give Eq. (5.9).

When Eq. (5.9) is operated upon by Eq. (5.6), the result for the time-evolution operator U' in the new gauge is

$$U'(t,t_0)=\exp[iq\Lambda(t)/\hbar c]U(t,t_0) \times\exp[-iq\Lambda(t_0)/\hbar c], \tag{5.10}$$

when Eq. (3.7) is used. Equation (5.10) is the same transformation property as obtained in Eq. (3.3) from the transformation of the wave function. The consistency of the formal solution has therefore been established.

VI. INTERACTION PICTURE

The formal solution for the time-evolution operator in Eq. (3.7) is generally evaluated by going to the interaction picture and then using perturbation theory. In this section, the gauge transformation property of the time-evolution operator in the interaction picture is obtained.

In the interaction picture, the Hamiltonian in Eq. (2.1) is divided into two parts

$$H=H_0+\mathscr{V}, \tag{6.1}$$

where the unperturbed Hamiltonian H_0 is

$$H_0=p^2/2m+V(\mathbf{r}). \tag{6.2}$$

The perturbation $\mathscr{V}$ can be written as

$$\mathscr{V}=\mathscr{V}_1+\mathscr{V}_2, \tag{6.3}$$

where the term first order in q is

$$\mathscr{V}_1=-(q/2mc)(\mathbf{A}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{A})+q\phi, \tag{6.4}$$

and the term second order in q is

$$\mathscr{V}_2=(q^2/2mc^2)\mathbf{A}^2. \tag{6.5}$$

If the factorization theorem in Eq. (4.2) for the time-evolution operator is applied to the Hamiltonian in Eq. (6.1), with $H_1=H_0$ and $H_2=\mathscr{V}$, the result is

$$U(t,t_0)=\exp[-(i/\hbar)H_0(t-t_0)]U_I(t,t_0)\ . \tag{6.6}$$

The time-evolution operator in the interaction picture $U_I(t,t_0)$ is

$$U_I(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'\,\mathscr{V}_I(t')\right]\ , \tag{6.7}$$

from Eq. (4.4). The perturbation $\mathscr{V}$ in the interaction picture is

$$\mathscr{V}_I(t)=\exp[(i/\hbar)H_0(t-t_0)]\mathscr{V}(t)\times\exp[-(i/\hbar)H_0(t-t_0)]\ , \tag{6.8}$$

from Eq. (4.5).

In the new gauge the potentials $(\mathbf{A}',\phi')$ in Eq. (2.4) replace $(\mathbf{A},\phi)$. The new time-evolution operator $U_I'(t,t_0)$ in the interaction picture is

$$U_I'(t,t_0)=T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'\,\mathscr{V}_I'(t')\right]\ , \tag{6.9}$$

where the interaction in the new gauge $\mathscr{V}'$ is the same form as Eq. (6.3) except that the potentials are in the new gauge $(\mathbf{A}',\phi')$. Explicitly, $\mathscr{V}'$ is

$$\mathscr{V}'=\mathscr{V}_1'+\mathscr{V}_2'\ , \tag{6.10}$$

where the term first order in q is

$$\mathscr{V}_1'=-(q/2mc)(\mathbf{A}'\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{A}')+q\phi'\ , \tag{6.11}$$

and the term second order in q is

$$\mathscr{V}_2'=(q^2/2mc^2)(\mathbf{A}')^2\ . \tag{6.12}$$

From the transformation property of the time-evolution operator in Eq. (3.3), the transformation property of the time-evolution operator in the interaction picture is

$$U_I'(t,t_0)=\exp[iq\Lambda_I(t)/\hbar c]U_I(t,t_0)\times\exp[-iq\Lambda_I(t_0)/\hbar c]\ . \tag{6.13}$$

The gauge function Λ_I in the interaction picture is defined as in Eq. (6.8),

$$\Lambda_I(t)=\exp[(i/\hbar)H_0(t-t_0)]\Lambda(t)\times\exp[-(i/\hbar)H_0(t-t_0)]\ , \tag{6.14}$$

so that $\Lambda_I(t_0)=\Lambda(t_0)$. The time-evolution operator in the interaction picture can be expanded to give a perturbation series in the interaction. The perturbation series in two different gauges are related by Eq. (6.13).

A form more convenient for comparing the two perturbation series may be obtained by rewriting Eq. (6.13) as

$$U_I(t,t_0)=\exp\left[-i(q/\hbar c)\int_{t_0}^{t}dt'\,\dot{\Lambda}_I(t')-i(q/\hbar c)\Lambda_I(t_0)\right]\times U_I'(t,t_0)\exp[iq\Lambda_I(t_0)/\hbar c]\ , \tag{6.15}$$

where $\dot{\Lambda}_I=d\Lambda_I/dt$ is the total time derivation of Λ_I. The Baker-Campbell-Hausdorff theorem[13] can be used in Eq. (6.15) to give

$$U_I(t,t_0)=\exp\left[-i(q/\hbar c)\int_{t_0}^{t}dt'\,\dot{\Lambda}_I(t')\right]\exp\left[\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt'[\Lambda(t_0),\dot{\Lambda}_I(t')]\right]\times T\exp\left[-(i/\hbar)\int_{t_0}^{t}dt'\exp[-iq\Lambda(t_0)/\hbar c]\mathscr{V}_I'(t')\exp[iq\Lambda(t_0)/\hbar c]\right]\ . \tag{6.16}$$

Equation (6.16) is an exact expression relating U_I to $\mathscr{V}_I'$. A perturbation expansion can be obtained by expanding all the exponentials and grouping terms of a given order. The result of course must be the same as the expansion of Eq. (6.7).

VII. PERTURBATION THEORY

In this section a perturbation expansion of the time-evolution operator in the interaction picture $U_I(t,t_0)$ in Eq. (6.16) is made in terms of the interaction $\mathscr{V}'$. The result is compared with the expansion of $U_I(t,t_0)$ obtained from Eq. (6.7) in terms of the interaction $\mathscr{V}$. The two expansions must of course agree with each other in all orders of perturbation theory. An explicit calculation shows that equality does hold through second order in perturbation theory.

In order to compare the two expansions it is necessary to relate the new interaction $\mathscr{V}'$ in Eqs. (6.10)—(6.12) with the old interaction $\mathscr{V}$ in Eqs. (6.3)—(6.5). If the gauge transformations in Eq. (2.4) are used in Eq. (6.10), the new interaction $\mathscr{V}'$ is related to the old interaction by

$$\mathscr{V}'=\mathscr{V}-(q/2mc)(\mathbf{p}\cdot\nabla\Lambda+\nabla\Lambda\cdot\mathbf{p})-(q/c)\partial\Lambda/\partial t+(q^2/2mc^2)[\mathbf{A}\cdot\nabla\Lambda+\nabla\Lambda\cdot\mathbf{A}+(\nabla\Lambda)^2]\ . \tag{7.1}$$

The part of this interaction first order in q can be written as

$$\mathscr{V}_1'=\mathscr{V}_1-(q/c)\{\partial\Lambda/\partial t+(i\hbar)^{-1}[\Lambda,H_0]\}\ , \tag{7.2}$$

and the part second order in q can be written as

$$\mathscr{V}_2'=\mathscr{V}_2+(iq/\hbar c)[\Lambda,\mathscr{V}_1]+\tfrac{1}{2}(iq/\hbar c)^2[\Lambda,[\Lambda,H_0]] \tag{7.3}$$

In the interaction picture Eq. (7.2) becomes

$$\mathscr{V}_{1I}'=\mathscr{V}_{1I}-(q/c)\dot{\Lambda}_I\ , \tag{7.4}$$

where the total time derivative of Λ_I is

$$\dot{\Lambda}_I=d\Lambda_I/dt=(\partial\Lambda/\partial t)_I+(i\hbar)^{-1}[\Lambda_I,H_0]\ . \tag{7.5}$$

In the interaction picture Eq. (7.3) becomes

$$\mathscr{V}'_{2I}=\mathscr{V}_{2I}+(iq/\hbar c)[\Lambda_I,\mathscr{V}_{1I}]+\tfrac{1}{2}(i\hbar)(iq/\hbar c)^2[\Lambda_I,\dot{\Lambda}_I]\,, \tag{7.6}$$

if we assume that $[\Lambda,\partial\Lambda/\partial t]=0$.

A perturbation expansion through second order can be made in Eq. (6.16). In zeroth order the expansion gives the unit operator. In first order we obtain

$$U_I^{(1)}(t,t_0)=-i(q/\hbar c)\int_{t_0}^{t}dt'\,\dot{\Lambda}_I(t')-(i/\hbar)\int_{t_0}^{t}dt'\,\mathscr{V}'_{1I}(t')=-(i/\hbar)\int_{t_0}^{t}dt'\,\mathscr{V}_{1I}(t')\,, \tag{7.7}$$

when Eq. (7.4) is used. This result was shown in the electric dipole approximation by Schlicher *et al.*[14]

In second order of perturbation theory Eq. (6.16) gives

$$\begin{aligned}U_I^{(2)}(t,t_0)=&-(i/\hbar)\int_{t_0}^{t}dt_1\{\mathscr{V}'_{2I}(t_1)-(iq/\hbar c)[\Lambda(t_0),\mathscr{V}'_{1I}(t_1)]\}\\&+\tfrac{1}{2}(-i/\hbar)^2T\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2\,\mathscr{V}'_{1I}(t_1)\mathscr{V}'_{1I}(t_2)+\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\,\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)\\&+(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\,\dot{\Lambda}_I(t_1)\mathscr{V}'_{1I}(t_2)+\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1[\Lambda(t_0),\dot{\Lambda}_I(t_1)]\,.\end{aligned} \tag{7.8}$$

When Eq. (7.8) is simplified by substituting Eqs. (7.4) and (7.6) into it, the result is

$$U_I^{(2)}(t,t_0)=-(i/\hbar)\int_{t_0}^{t}dt_1\,\mathscr{V}_{2I}(t_1)+\tfrac{1}{2}(-i/\hbar)^2T\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2\mathscr{V}_{1I}(t_1)\mathscr{V}_{1I}(t_2)+\mathscr{I}_{\rm I}+\mathscr{I}_{\rm II}\,. \tag{7.9}$$

The expression $\mathscr{I}_{\rm I}$ involves terms with one Λ and one $\mathscr{V}_1$, and is

$$\begin{aligned}\mathscr{I}_{\rm I}=&-(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1[\Lambda_I(t_1)-\Lambda(t_0),\mathscr{V}_{1I}(t_1)]\\&-\tfrac{1}{2}(i/\hbar)^2(q/c)T\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2[\mathscr{V}_{1I}(t_1)\dot{\Lambda}_I(t_2)+\dot{\Lambda}_I(t_1)\mathscr{V}_{1I}(t_2)]\\&+(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\dot{\Lambda}_I(t_1)\mathscr{V}_{1I}(t_2)=0\,,\end{aligned} \tag{7.10}$$

which is proved in the Appendix. The expression $\mathscr{I}_{\rm II}$ involves terms with two Λ's and is

$$\begin{aligned}\mathscr{I}_{\rm II}=&\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1[\Lambda_I(t_1)-\Lambda(t_0),\dot{\Lambda}_I(t_1)]\\&+\tfrac{1}{2}(iq/\hbar c)^2T\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2\,\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)-\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)=0\,,\end{aligned} \tag{7.11}$$

which is also proved in the Appendix. The second-order terms in Eq. (7.9) are therefore the same as obtained by expanding Eq. (6.7). The expansion could be continued to higher-order perturbation theory, but second order should suffice to illustrate that the same result is obtained from using Eq. (6.16) as from using Eq. (6.7) for $U_I(t,t_0)$.

VIII. THE A·p VERSUS E·r CONTROVERSY

In the electric dipole approximation (EDA) there has been a controversy regarding the interactions $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{E}\cdot\mathbf{r}$.[4–6] The preceding discussion of the gauge transformation property of the time-evolution operator helps to put this controversy in perspective and gives its resolution.[14]

When the wavelength of the radiation is much greater than the dimensions of the atomic system, the EDA can be made. The spatial dependence of the vector potential in the radiation gauge can be neglected so that $\mathbf{A}=\mathbf{A}(t)$, $\phi=0$. The gauge transformation in Eq. (2.4) with $\Lambda=-\mathbf{A}(t)\cdot\mathbf{r}$ can be made to a new gauge, called the electric field gauge, in which[15]

$$\mathbf{A}'=\mathbf{0}\,,\quad \phi'=-\mathbf{E}(t)\cdot\mathbf{r}\,, \tag{8.1}$$

where $\mathbf{E}(t)=-c^{-1}\partial\mathbf{A}(t)/\partial t$ is the electric field at the atom.

The time-evolution operator in the interaction picture in the radiation gauge is

$$\begin{aligned}U_I(t,t_0)=T\exp\Big[&-(i/\hbar)\int_{t_0}^{t}dt_1(-q/mc)\\&\times\mathbf{A}(t_1)\cdot\mathbf{p}_I(t_1)\Big]\\&\times\exp\Big[-(i/\hbar)(q^2/2mc^2)\int_{t_0}^{t}dt_1A(t_1)^2\Big]\,.\end{aligned} \tag{8.2}$$

The exponential involving the A^2 term is a time-dependent phase factor, which does not change probabilities. The time-evolution operator in the interaction picture in the electric field gauge is

$$U'_I(t,t_0)=T\exp\Big[-(i/\hbar)\int_{t_0}^{t}dt_1(-q)\mathbf{E}(t_1)\cdot\mathbf{r}_I(t_1)\Big]\,. \tag{8.3}$$

Obviously, Eqs. (8.2) and (8.3) are not generally equal to each other, so the time-evolution operator is generally gauge dependent. The two operators are related to each other by Eq. (6.13), which is

$$\begin{aligned}U'_I(t,t_0)=&\exp[-iq\,\mathbf{A}(t)\cdot\mathbf{r}_I(t)/\hbar c]U_I(t,t_0)\\&\times\exp[iq\,\mathbf{A}(t_0)\cdot\mathbf{r}_I(t_0)/\hbar c]\,.\end{aligned} \tag{8.4}$$

In the case that $\mathbf{A}(t)=\mathbf{0}$, $\mathbf{A}(t_0)=\mathbf{0}$ then $U'_I=U_I$ in Eq. (8.4). If the potentials are turned on and off adiabatically, then in the limit that $t\to+\infty$, $t_0\to-\infty$, we have $U'_I(+\infty,-\infty)=U_I(+\infty,-\infty)$, since $\mathbf{A}(+\infty)=\mathbf{A}(-\infty)=0$. The same S matrix in the two gauges is obtained in this case.

In order to calculate the probability amplitude that the particle is in a given state, the states must be specified in the two gauges. If the initial state $\psi_i(t_0)$ and final state $\psi_f(t)$ are specified in the radiation gauge, then the initial state in the electric field gauge is

$$\psi_i'(t_0)=\exp[-iq\,\mathbf{A}(t_0)\cdot\mathbf{r}/\hbar c]\psi_i(t_0)\ , \tag{8.5}$$

and the final state in the electric field gauge is

$$\psi_f'(t)=\exp[-iq\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar c]\psi_f(t)\ . \tag{8.6}$$

From Eqs. (3.5) and (6.6) the probability amplitudes

$$\langle\psi_f(t)\,|\,\exp[-(i/\hbar)H_0(t-t_0)]U_I(t,t_0)\psi_i(t_0)\rangle = \langle\psi_f'(t)\,|\,\exp[-(i/\hbar)H_0(t-t_0)]U_I'(t,t_0)\psi_i'(t_0)\rangle \tag{8.7}$$

are equal.

The initial state i is determined by the preparation of the system and the final state f is determined by the type of measurement performed. If the system is prepared in an energy eigenstate and an energy measurement is made, then i and f must be energy eigenstates. The energy operator is[10,11]

$$\mathscr{E}=(1/2m)(\mathbf{p}-q\,\mathbf{A}/c)^2+V(\mathbf{r})\ . \tag{8.8}$$

In the radiation gauge ($\phi=0$) the energy operator coincides with the Hamiltonian. The energy eigenvalue equation is

$$\mathscr{E}\psi_n=\epsilon_n\psi_n\ . \tag{8.9}$$

The energy eigenstate n is an equivalence class of wave functions $\{\psi_n\}=\{\psi_n'\,|\,\psi_n'=\exp(iq\Lambda/\hbar c)\psi_n\}$. The initial state i and final state f are such equivalence classes. Which phase factor to use depends on the gauge chosen.

In the electric field gauge in the EDA the energy operator $\mathscr{E}'$ reduces to the unperturbed Hamiltonian H_0, since in this gauge the vector potential $\mathbf{A}'=0$. The energy eigenvalue equation in Eq. (8.9) in this gauge becomes the eigenvalue problem for the unperturbed Hamiltonian

$$H_0\Phi_n=E_n\Phi_n\ , \tag{8.10}$$

so that $\epsilon_n=E_n$ and $\psi_n'=\Phi_n$ in the EDA.

In the Coulomb gauge in the EDA where $\mathbf{A}=\mathbf{A}(t)$, the solution to the energy eigenvalue problem in Eq. (8.9) is

$$\psi_n=\exp[iq\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar c]\Phi_n\ . \tag{8.11}$$

In this gauge the initial state i is

$$\psi_i(t_0)=\exp[iq\,\mathbf{A}(t_0)\cdot\mathbf{r}/\hbar c]\Phi_i\ , \tag{8.12}$$

where the initial state in the electric field gauge is $\psi_i'(t_0)=\Phi_i$. The final state f in this gauge is likewise

$$\psi_f(t)=\exp[iq\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar c]\Phi_f\ , \tag{8.13}$$

where the final state in the electric field gauge is $\psi_f'(t)=\Phi_f$. From Eq. (8.7) the probability amplitude calculated in this gauge is equal to the one calculated from the electric field gauge.

When an energy measurement is made and eigenstates of H_0 are used to specify the initial and final states, the time-evolution operator calculated using the $\mathbf{E}\cdot\mathbf{r}$ interaction should be used to calculate the probability amplitude in Eq. (8.7). On the other hand, the Coulomb gauge with the vector potential $\mathbf{A}(t)$ and the interaction $\mathbf{A}\cdot\mathbf{p}$ can also be used to calculate the time-evolution operator. The appropriate initial and final states in this case are Eqs. (8.12) and (8.13) which are the eigenstates of the energy operator in this gauge. Equation (8.7) then guarantees that the amplitude calculated in this gauge agrees with the one calculated in the electric field gauge. If $\mathbf{A}(t)\neq\mathbf{0}$ or $\mathbf{A}(t_0)\neq\mathbf{0}$, then an incorrect amplitude would be obtained using the $\mathbf{A}\cdot\mathbf{p}$ interaction with eigenstates of H_0. Thus the relationship between the two interactions $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{E}\cdot\mathbf{r}$ is clearly seen by using the time-evolution operator in the interaction picture.

IX. CONCLUSION

The gauge transformation on the wave function implies the gauge transformation property of the time-evolution operator $U(t,t_0)$. A formal solution of the Schrödinger equation for the time-evolution operator can be given in terms of a time-ordered exponential of the time integral of the Hamiltonian. The gauge transformation property of the time-evolution operator can also be obtained directly from the formal solution. The consistency of the formal solution is thereby established.

The S matrix is $S=U(+\infty,-\infty)$ and also satisfies a gauge-transformation property. The S matrix in two different gauges need not be the same because the gauge function $\Lambda(+\infty)$ and $\Lambda(-\infty)$ at times $t=+\infty$ and $t=-\infty$, respectively, need not be zero[4] or equal to each other.[6] The matrix elements of the S matrix between the appropriate initial and final states are gauge invariant, and are hence interpretable as probability amplitudes. If the potentials are turned on and off adiabatically, then $\Lambda(+\infty)$ and $\Lambda(-\infty)$ are indeed zero which is a specific choice of gauge. Only the electromagnetic field can be turned on and off in the laboratory, so the adiabatic turning on and off the potentials is artificial.[7] As shown here a specific choice of gauge is not necessary. The manifestly gauge-invariant formulation of quantum mechanics[10,11] allows an arbitrary gauge for the potentials at all times, including the asymptotic times ($t=\pm\infty$).

The gauge transformation property of the time-evolution operator can be transformed to the interaction picture. In the interaction picture perturbation expansions are easily made. It is shown explicitly through second order of perturbation theory that the perturbation expansion of $U_I(t,t_0)$ in terms of the perturbation $\mathscr{V}'$ is the same as for $\mathscr{V}$. Indeed, the equality must hold in all orders of perturbation theory.

The $\mathbf{A}\cdot\mathbf{p}$ versus $\mathbf{E}\cdot\mathbf{r}$ controversy in the electric dipole approximation is reviewed here.[4–6,14,16,17] Either interaction may be used to calculate the time-evolution operator. Nevertheless, when an energy measurement is made, the probability amplitude must be calculated with the correct energy eigenstates. The energy operator reduces to the unperturbed Hamiltonian when the interaction $\mathbf{E}\cdot\mathbf{r}$ is used. If the unperturbed eigenstates are used to calculate the probability amplitude at an arbitrary time, the time-evolution operator calculated from the interaction $\mathbf{E}\cdot\mathbf{r}$ should be used.[10] If the asymptotic time limits $t\to+\infty$,

$t_0 \to -\infty$ are taken and the potentials are turned on and off adiabatically, then the unperturbed states may be used with the S matrix calculated from either interaction. This result has previously been shown in first and second orders of perturbation theory for the general case.[18]

APPENDIX: VANISHING OF EQS. (7.10) AND (7.11)

The expressions $\mathscr{I}_{\rm I}$ and $\mathscr{I}_{\rm II}$ given in Eqs. (7.10) and (7.11), respectively, are shown in this appendix to vanish. The expression $\mathscr{I}_{\rm I}$ in Eq. (7.10) can be rewritten as

$$\begin{aligned}\mathscr{I}_{\rm I}=&-(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2[\dot{\Lambda}_I(t_2),\mathscr{V}_{1I}(t_1)]\\&-(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\,\mathscr{V}_{1I}(t_1)\dot{\Lambda}_I(t_2)\\&+(i/\hbar)^2(q/c)\int_{t_0}^{t}dt_1\int_{t_1}^{t}dt_2\,\dot{\Lambda}_I(t_1)\mathscr{V}_{1I}(t_2)\,,\end{aligned}\tag{A1}$$

when the time-ordering operator is allowed to act. Two of the integrals cancel, and the remaining two may be rewritten in terms of the unit step function $\Theta(x)=0$, $x<0$ and $\Theta(x)=1$, $x>0$, as

$$\begin{aligned}\mathscr{I}_{\rm I}=&(i/\hbar)^2(q/c)\\&\times\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2[-\dot{\Lambda}_I(t_2)\mathscr{V}_{1I}(t_1)\Theta(t_1-t_2)\\&+\dot{\Lambda}_I(t_1)\mathscr{V}_{1I}(t_2)\Theta(t_2-t_1)]=0\,.\end{aligned}\tag{A2}$$

Equation (A2) is zero because the dummy variables of integration t_1 and t_2 in the second term can be interchanged, so that it cancels with the first term.

The expression $\mathscr{I}_{\rm II}$ in Eq. (7.11) can be rewritten as

$$\begin{aligned}\mathscr{I}_{\rm II}=&\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2[\dot{\Lambda}_I(t_2),\dot{\Lambda}_I(t_1)]\\&+\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\,\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)\\&-\tfrac{1}{2}(iq/\hbar c)^2\int_{t_0}^{t}dt_1\int_{t_1}^{t}dt_2\,\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)\end{aligned}\tag{A3}$$

when the time-ordering operator is allowed to act. Two integrals cancel, and the remaining two integrals can be written in terms of the unit step function to give

$$\begin{aligned}\mathscr{I}_{\rm I}=&\tfrac{1}{2}(iq/\hbar c)^2\\&\times\int_{t_0}^{t}\int_{t_0}^{t}dt_1\,dt_2[\dot{\Lambda}_I(t_2)\dot{\Lambda}_I(t_1)\Theta(t_1-t_2)\\&-\dot{\Lambda}_I(t_1)\dot{\Lambda}_I(t_2)\Theta(t_2-t_1)]=0\,.\end{aligned}\tag{A4}$$

Equation (A4) is zero because the dummy variables of integration t_1 and t_2 in the second term can be interchanged, so that it cancels the first term.

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