PHYSICAL REVIEW A VOLUME 20, NUMBER 4 OCTOBER 1979

Gauge invariance and pseudoperturbations

Y. Aharonov* and C. K. Au
Department of Physics and Astronomy, University of South Carolina, Columbia, South Carolina 29208

(Received 15 March 1979)

We define pseudoperturbations as the difference between two Hamiltonians that are related by a generalized gauge transformation. We state and prove the theorem that such pseudoperturbations cannot cause any real physical transitions. We also rigorously establish the generalized gauge invariance of physical transition-matrix elements in real processes. Our theorem also generates some interesting sum rules and on-shell identities which can serve as useful constraints in variational calculations.

INTRODUCTION

The large number of multiphoton experiments performed with high-power tunable lasers in recent years has revived a lot of interest in the theoretical calculation of electromagnetic (EM) transition-matrix elements in atomic and molecular systems. It is generally accepted[1] that the two forms of the EM interaction in the dipole approximation, $e\vec{E}\cdot\vec{r}$ and $(-e/m)\vec{p}\cdot\vec{A}+e^2A^2/2m$, sometimes also referred to as the EM interaction in the length gauge and velocity gauge, are equivalent. These two forms of the EM interaction are related to each other by a gauge transformation. Up to the second order, the equivalence has been demonstrated either numerically[2] or analytically.[3] However, not much has been said about higher-order transitions. In this paper we shall establish the equivalence of these two gauges to all orders in perturbation theory. A similar result has been established by Haller and Haller *et al.*[4] Moreover, we shall not limit ourselves to the dipole approximation and our discussion need not be confined to the EM interaction.

Usually in EM interactions, the gauge transformation involves a gauge function that depends only on the spatial and time coordinates. In general the gauge function may depend also on momenta and internal variables. The non-Abelian gauge transformation is an example. Unitary transformations corresponding to this class of general gauge functions will be called generalized gauge transformations. Unless specified otherwise, henceforth in this paper a gauge transformation refers to such a generalized gauge transformation. Our results extend beyond the EM interaction and are applicable to all arbitrary generalized gauges, as long as they satisfy the conditions specified below.

One can expect general gauge independence of transition-matrix elements for real physical processes on the following grounds. If two interactions that are related to each other by a gauge transformation can lead to different transition-matrix elements for a real physical process, then one can generate a perturbation that can cause real physical transition by the mere use of this gauge transformation. Obviously this cannot be ture if the gauge generation is nonsingular and vanishes at infinity,[5] since this transformation cannot affect the asymptotic scattering states. Such gauge functions and the corresponding unitary transformations will be designated as acceptable. In general, under a unitary transformation $U\equiv\exp(i\lambda\Phi)$, the Hamiltonian is transformed to $UHU^\dagger$, and this differs from the original Hamiltonians unless U is the identity transformation. However, from the argument given above, the difference $UHU^\dagger-H$ must not cause any real physical transition, provided that the gauge function Φ is acceptable. We therefore define this difference $UHU^\dagger-H$ as a "pseudoperturbation." We state and prove the theorem that such pseudoperturbations cannot cause a real physical transition to any order in perturbation theory. In real transitions the evolution operator, which is unitary, has a corresponding gauge function that is singular on the energy shell.

The scheme of the present paper is as follows. In Sec. I we establish the theorem that pseudoperturbation cannot cause any real physical transition, to any order. In Sec. II we discuss real transitions. In Sec. III we generalize our discussion to include time-dependent gauge functions. In Sec. IV we consider gauge invariance in general. In Sec. V we discuss the special case in which a system is in an external electromagnetic field. In Sec. VI we consider the equivalence of the electric dipole transition in the gauges $e\vec{r}\cdot\vec{E}$ and $(-e/m)\vec{p}\cdot\vec{A}+e^2A^2/2m$, where the field $\vec{E}$ and the vector potential $\vec{A}$ are quantized. In Sec. VII we dispute a recent erroneous claim[6] that EM transition-matrix elements are gauge dependent except in the case when energy shell condition is satisfied. We show that this discrepancy is entirely due to the incorrect use of the bare states of an isolated atom to describe the true physical states of a realistic atom that couples to the radiation field. In Appendix A we shall give a more vigorous and more lengthy proof of the invariance of the transition-matrix elements under gauge transformations that is discussed in Sec. IV. Finally, in Appendix B we demonstrate that our theorem proved in Sec. I and further extended in Sec. III leads to interesting sum rules and on-shell identities.

I. PSEUDOPERTURBATONS

Consider a time-independent Hamiltonian H under a unitary transformation $U \equiv \exp(i\lambda\Phi)$ such that the time-independent gauge function Φ is regular and vanishes at infinity. Henceforth, we shall denote such gauge functions as "acceptable." The case involving time-dependent gauge functions will be discussed in Sec. III. The transformed Hamiltonian H' is equal to $UHU^\dagger$. We shall denote the eigenstates of H by $|\psi\rangle$ and those of H' by $|\psi'\rangle$. Obviously, since H and H' are related by a unitary transformation U, we have

$$|\psi'\rangle = U|\psi\rangle . \tag{1.1}$$

It is then a trivial identity for a pair of initial and final states $|\psi_i\rangle$ and $|\psi_f\rangle$ that

$$\langle\psi_f'|H'|\psi_i'\rangle = \langle\psi_f|U^\dagger UHU^\dagger U|\psi_i\rangle = \langle\psi_f|H|\psi_i\rangle .$$

However, in general,

$$\langle\psi_f|H|\psi_i\rangle \neq \langle\psi_f|H'|\psi_i\rangle ,$$

since $H' \neq H$ unless U is the identity transformation. Thus we can regard $H' - H \equiv V$ as a perturbation that results from the unitary transformation. We call such a perturbation a pseudoperturbation, and V can be written as

$$V = \lambda V_1 + \lambda^2 V_2 + \lambda^3 V_3 + \dots , \tag{1.2}$$

where

$$\begin{aligned} V_1 &= i[\Phi, H] , \\ V_2 &= (i^2/2!)[\Phi,[\Phi,H]] , \\ V_3 &= (i^3/3!)[\Phi,[\Phi,[\Phi,H]]] , \\ &\dots , \\ V_n &= (i/n)[\Phi, V_{n-1}] . \end{aligned} \tag{1.3, 1.4}$$

In particular, if H is of the form $p^2/2m + V_0(x)$, and the gauge function is a function of x alone, then $V_n = 0$ for all $n \geqslant 3$.

According to Fermi's "golden rule," any real transition between two states ψ_i and ψ_f due to any perturbation V is subject to the energy-conservation condition: $\epsilon_i = \epsilon_f$, where ϵ_i and ϵ_f are the eigenvalues of the eigenvectors ψ_i and ψ_f of H. We shall refer to states that satisfy this energy-conservation condition as states on the energy shell. Our assertion is that on the energy shell, as long as the gauge function Φ is acceptable, the pseudoperturbation does not cause any transition to any order in λ. The proof goes as follows. From equation (1.1), the definition of V, and the Lippmann-Schwinger equation,[7] we have

$$\begin{aligned} |\psi'\rangle &= U|\psi\rangle = |\psi\rangle + GV|\psi'\rangle & (1.5\text{a}) \\ &= |\psi\rangle + GV|\psi\rangle + GVGV|\psi\rangle + \dots & (1.5\text{b}) \\ &= (1/1 - GV)|\psi\rangle . & (1.5\text{c}) \end{aligned}$$

The last relation is true provided the series converges. From equation (1.5b) we have

$$\begin{aligned} \langle\psi_f|VU|\psi_i\rangle = {} & \langle\psi_f|V|\psi_i\rangle + \langle\psi_f|VGV|\psi_i\rangle \\ & + \langle\psi_f|VGVG|\psi_i\rangle + \dots , \end{aligned} \tag{1.6}$$

and the right-hand side can be identified as the usual Lippmann-Schwinger perturbation series. Moreover, the right-hand side $\mathfrak{R}$ can be rearranged as a power series in λ. The sum of all matrix elements corresponding to nth-order transitions can be identified as

$$\langle f|M^n|i\rangle \equiv \frac{1}{n!}\frac{\partial^n}{\partial\lambda^n}\mathfrak{R}\bigg|_{\lambda=0} \tag{1.7}$$

$$= \frac{1}{n!}\frac{\partial^n}{\partial\lambda^n}\langle\psi_f|VU|\psi_i\rangle\bigg|_{\lambda=0} . \tag{1.8}$$

From the definition of V we see that

$$\begin{aligned} \langle\psi_f|VU|\psi_i\rangle &= \langle\psi_f|(UHU^\dagger - H)U|\psi_i\rangle \\ &= \langle\psi_f|UH - HU|\psi_i\rangle \\ &= \langle\psi_f|[U,H]|\psi_i\rangle & (1.9) \\ &= (\epsilon_i - \epsilon_f)\langle\psi_f|U|\psi_i\rangle , & (1.10) \end{aligned}$$

which is zero on the energy shell for any U that is acceptable. Thus our assertion is proven.

II. REAL SCATTERING PROCESSES

Consider a scattering potential V being introduced to a system with a Hamiltonian H. Let the eigenstates of H be denoted as $|k_{\text{free}}\rangle = |k_f\rangle$ and those of $H + V = H'$ be denoted as $|k_{\text{scattered}}\rangle = |k_{\text{sc}}\rangle$. Obviously, the transformation $\int |k_{\text{sc}}\rangle\langle k_f|\,dk \equiv U$ is unitary, and $UHU^\dagger = H'$, provided H' does not have any bound state. The scattered state $|k_{\text{sc}}\rangle$ satisfies the Lippmann-Schwinger equation,

$$|k_{\text{sc}}\rangle = |k_f\rangle + GV|k_{\text{sc}}\rangle , \tag{2.1}$$

and can be iterated as

$$|k_{\text{sc}}\rangle = [1/(1 - GV)]|k_f\rangle . \tag{2.2}$$

So, at least formally, the gauge function Φ can be written as $i\ln(1 - GV)$. However, here the gauge function is singular on the energy shell and the argument that led us to Eq. (1.10) does not apply.

This is analogous to the apparent ambiguity in the evaluation of the matrix element $\langle x'|i[p,x]|x\rangle$, where $|x\rangle$ is an eigenstate of the position operator. If we expand the commutator and apply the x operator first, the matrix element vanishes for $x = x'$; whereas, if we use the fact that the commutator is 1, the matrix element is equal to $\delta(x-x')$. The singular nature of the evolution operator U can be seen if we go to the interaction picture and turn on the scattering potential adiabatically. In this case $U = \lim_{\eta\to 0}[\exp(-i\int_{-\infty}^{T} Ve^{\eta t}\,dt)]_+$, where $[\ldots]_+$ indicates that the quantity inside the brackets is time ordered.[1] Then, to each order in the interaction V, the time integrations in the matrix element $\langle\psi_f|U|\psi_i\rangle$ give an overall energy denominator $(\epsilon_i-\epsilon_f)^{-1}$. Thus, $\langle\psi_f|[H,U]|\psi_i\rangle$, in general, does not vanish on the energy shell for real scattering processes. On the other hand, when $U = \exp(i\Phi)$ where Φ is acceptable, then $\langle\psi_f|U|\psi_i\rangle$ is always finite and is thus free from any singularity when the energy shell condition $\epsilon_i=\epsilon_f$ is met.

III. EXTENSION TO TIME DEPENDENCE

Thus far, we have limited ourselves to time-independent unitary transformation. It is well known that under a time-dependent unitary transformation U the transformed Hamiltonian is $UHU^\dagger + i\dot{U}U^\dagger$. In such cases the pseudoperturbation generated is $UHU^\dagger - H + i\dot{U}U^\dagger$, and in the usual perturbation series the energy denominator must also include the frequency of the appropriate Fourier component of the time-dependent interaction. This frequency can be interpreted as the energy of the quantum emitted or absorbed. In this section we are going to show that such explicit time dependence can still be described by a time-independent formalism with proper inclusion in the Hamiltonian a part corresponding to a clock.[8] Any system that has an isomorphism between its coordinate and time is, by definition, a clock. A particle moving in one dimension with uniform speed obviously constitutes the simplest clock. Let the average momentum of this particle be $\bar{\pi}$ and the momentum be $\bar{\pi}+\pi$. Then the kinetic energy of this particle is equal to $(1/2M)(\pi^2+2\pi\bar{\pi}+\bar{\pi}^2)$. If M is sufficiently large, the first term can be neglected, and the kinetic energy reduces to $\bar{\pi}^2/2M+\pi\bar{\pi}/M$. Since $\bar{\pi}^2/2M$ is a constant, and $\bar{\pi}/M$, which is the particle's velocity, can be arbitrarily chosen as one, the effective kinetic energy of this particle is just π. The coordinate conjugate to π, q, is then isomorphic to the time t. In this scheme we add to every Hamiltonian $H(p,x,t)$ the clock part π. Then any time-dependent unitary transformation $U(p,x,t)\equiv\exp(i\phi(p,x,t))$ may be replaced by $U(p,x,q)\equiv\exp(i\phi(p,x,q))$. When this acts on the Hamiltonian of the system and the clock, we have

$$\begin{aligned} U(p,x,q)[H(p,x,q)+\pi]U^\dagger(p,x,q) &= H(p,x,q)+\pi+i[\Phi(p,x,q),H(p,x,q)]+(i^2/2!)[\Phi,[\Phi,H]] \\ &\quad +(i^3/3!)[\Phi,[\Phi[\Phi,H]]]+\ldots+i[\Phi(p,x,q),\pi] \qquad (3.1) \\ &= U(p,x,q)H(p,x,q)U^\dagger(p,x,q)+\pi-(\partial/\partial q)\Phi(p,x,q). \qquad (3.2) \end{aligned}$$

On the other hand,

$$U(p,x,t)[H(p,x,t)+\pi]U^\dagger(p,x,t)+i\frac{\partial U}{\partial t}(p,x,t)U^\dagger(p,x,t) = U(p,x,t)H(p,x,t)U^\dagger(p,x,t)-\frac{\partial}{\partial t}\Phi(p,x,t)+\pi. \qquad (3.3)$$

This establishes our assertion.

Another role of this clock Hamiltonian can be seen as follows. Let ϵ and ω denote the eigenvalues of H and π. The energy-shell condition $E_i = E_f$ now becomes $\epsilon_i+\omega_i=\epsilon_f-\omega_f$ or $\epsilon_f-\epsilon_i=\omega_i-\omega_f$. Hence, the change in π is equivalent to the change in the energy of the free field that causes a transition in the system described by H. This will be further discussed in Sec. VI.

IV. GAUGE INVARIANCE[4]

In Sec. I we showed that the pseudoperturbation that arises from a regular gauge transformation cannot lead to any real transitions. In this section we show that if an interaction V that causes a real transition is related to another interaction V' by a regular gauge transformation, then the transition rate calculated with either of the interactions V and V' will be the same to all orders in perturbation theory. By assumption there exists an acceptable gauge function Φ such that $U = \exp(i\Phi)$ and

$$U(H_0+V)U^\dagger = H_0+V'. \qquad (4.1)$$

We denote the eigenstate of H_0 by $|\Phi\rangle$, those of $H = H_0+V$ by $|\psi\rangle$, and those of $H' = H_0+V'$ by $|\psi'\rangle$.

From the relation expressed in Eq. (4.1) we have

$$|\psi'\rangle = U|\psi\rangle \, . \tag{4.2}$$

Then, according to the theorem we proved in Sec. I,

$$\langle\psi_f|(UHU^\dagger - H)U|\psi_i\rangle = \langle\psi_f|(H' - H)|\psi'_i\rangle = 0 \, , \tag{4.3}$$

where the states i and f are on the same energy shell. In particular, we can rewrite Eq. (4.3) as[9]

$$\langle\psi_{f-}|H' - H|\psi'_{i+}\rangle = 0 \, , \tag{4.4}$$

since $H'|\psi'_{i+}\rangle = E_i|\psi'_{i+}\rangle$ and $\langle\psi_{f-}|H = E_f\langle\psi_{f-}|$. According to the Lippmann-Schwinger equation,[9]

$$|\psi'_{i+}\rangle = \lim_{\eta\to 0} \frac{i\eta}{E_f - H' + i\eta} |\phi_i\rangle \, , \tag{4.5}$$

and

$$\langle\psi_{f-}| = \lim_{\eta\to 0} \left\langle \frac{-i\eta}{E_f - H - i\eta} \phi_f \right| \, , \tag{4.6}$$

$$= \lim_{\eta\to 0} \left\langle \Phi_f \left| \frac{+i\eta}{E_f - H + i\eta} \right. \right. . \tag{4.7}$$

Hereafter the limiting processes $\eta \to 0$ are assumed understood, and the notation will be dropped. From Eq. (4.4) we then have

$$\eta^2 \left\langle \phi_f \left| \frac{1}{E_i - H + i\eta} (H' - H) \frac{1}{E_i - H' + i\eta} \right| \phi_i \right\rangle = 0 \tag{4.8}$$

upon using the on-shell condition $E_i = E_f$. From the identity

$$1/A - 1/B = (1/B)(B - A)(1/A) \, , \tag{4.9}$$

Eq. (4.8) becomes

$$-i\eta \left\langle \phi_f \left| \frac{i\eta}{E_i - H + i\eta} - \frac{i\eta}{E_i - H' + i\eta} \right| \phi_i \right\rangle = 0 \tag{4.10}$$

or

$$-i\eta[\langle\phi_f|\psi_{i+}\rangle - \langle\phi_f|\psi'_{i+}\rangle] = 0 \, , \tag{4.11}$$

where $\langle\Phi_f|\psi_{i+}\rangle$ and $\langle\Phi_f|\psi'_{i+}\rangle$, respectively, are the Møller scattering matrix elements calculated in the gauges V and V'. Equation (4.11) implies that the difference between the scattering matrix elements calculated in the two gauges is not proportional to a δ function. This implies that the part in the S matrix that is proportional to the δ function, i.e., the T matrix elements, is the same in both gauges. We have thus established that the transition-matrix elements calculated in both gauges are the same. In Appendix A we shall give a more rigorous and more lengthy proof of invariance of the transition-matrix elements under gauge transformations.

In general, the scattering potential is expressed in terms of a dimensionless coupling constant λ. Let us say that V is linear in λ. However, the interaction V' need not be linear in λ. A well-known example is found in the electromagnetic interaction, when $V = \lambda\vec{E}\cdot\vec{x}$ and $V' = \lambda\vec{p}\cdot\vec{A} + \lambda^2 A^2/2m$, where $\vec{E}, \vec{x}, \vec{p}, \vec{A}$, and m have their usual meanings. Nevertheless, both T-matrix elements, whether in the interaction V or V', can be expressed as a power series in λ. Thus, our conclusion is that, to each order in λ, the transition-matrix element is the same when calculated in both gauges. This is the meaning of gauge invariance in the context of scattering theories.

V. SYSTEMS IN EXTERNAL ELECTROMAGNETIC FIELDS

In this brief section we consider a system in an external electromagnetic field. The Hamiltonian, including that of the clock, is

$$H = (\vec{p} - e\vec{A}_{\text{ext}})^2/2m + e\Phi_{\text{ext}} + \pi \, . \tag{5.1}$$

Then, under a unitary transformation $U \equiv \exp(ie\chi(x,q))$, where $\chi(x,q)$ is nonsingular, the Hamiltonian transforms to

$$H' = UHU^\dagger = [\vec{p} - e(\vec{A}_{\text{ext}} + \vec{\nabla}\chi)]^2 + e\left(\Phi_{\text{ext}} - \frac{\partial}{\partial q}\chi\right) + \pi \, . \tag{5.2}$$

This becomes the quantum analog of the classical gauge transformation on identifying the isomorphism between q and the time t. We emphasize here that no dipole approximation needs to be taken. This, together with the results in the Sec. IV, establishes quantum mechanical gauge invariance in electromagnetic interaction. In particular, if the system is in a pure external electric field, $\vec{A}_{\text{ext}} = 0$, and we can choose a regular gauge function χ[5] such that $\partial\chi/\partial q = \Phi_{\text{ext}}$, and $\vec{\nabla}\chi$ can be identified as the vector components of the quantum-mechanical electromagnetic field. More discussion follows in the Sec. VI.

VI. ELECTROMAGNETIC GAUGE INVARIANCE WITH SECOND QUANTIZATION

In Sec. III we mentioned that the clock Hamiltonian π is equivalent to the Hamiltonian of the free field that couples to the system. As an illustration we consider here a system interacting with the electromagnetic field. For simplicity we assume the dipole approximation. The Hamiltonian, including that of the photon field, is, in the "$\vec{E}\cdot\vec{x}$" gauge,

$$H = \frac{p^2}{2m} + V(\vec{x}) + \sum \omega_k a^\dagger_{k,\lambda} a_{k,\lambda} - e\vec{E}\cdot\vec{x} \, , \tag{6.1}$$

where E, the electric field, in the second-quantized form and in the dipole approximation, is

$$\vec{E} = i \sum_{k,\lambda} \left(\frac{2\pi\omega_k}{\mathcal{V}}\right)^{1/2} [a_{k,\lambda} - a^\dagger_{k,\lambda}] \vec{e}_{\vec{k},\vec{\lambda}} \, , \tag{6.2}$$

where λ is the polarization mode and $\mathcal{V}$ is the quantization volume. We now introduce a gauge function $\Phi(\vec{x}) = \vec{A}(\vec{x})\cdot\vec{x}$, where $\vec{A}(\vec{x})$ is the quantized photon field in the dipole approximation:

$$\Phi(\vec{x}) = \sum_{k,\lambda}\left(\frac{2\pi}{\omega_k \mathcal{V}}\right)^{1/2}[a_{k,\lambda}+a^\dagger_{k,\lambda}] \times \vec{E}_{k,\lambda}\cdot\vec{x} = \vec{A}(x)\cdot\vec{x}\,. \tag{6.3}$$

Under the unitary transformation $U \equiv \exp(ie\Phi(x))$ the transformed Hamiltonian becomes

$$UHU^\dagger = \frac{(\vec{p}-e\vec{A})^2}{2m} + V(\vec{x}) + \sum \omega_k a^\dagger_{k,\lambda}a_{k,\lambda} + \frac{e^2x^2}{\mathcal{V}}\,, \tag{6.4}$$

where we have used

$$i[\Phi, p^2] = -(\vec{p}\cdot\vec{A}+\vec{A}\cdot\vec{p})\,, \tag{6.5}$$

$$\tfrac{1}{2}i^2[\Phi,[\Phi,p^2]] = \vec{A}\cdot\vec{A}\,, \tag{6.6}$$

$$[a+a^\dagger, a^\dagger a] = a - a^\dagger\,, \tag{6.7}$$

and

$$[a-a^\dagger, a+a^\dagger] = 2\,. \tag{6.8}$$

In the dipole approximation the term $e^2x^2/\mathcal{V}$ in Eq. (6.4) goes to zero.[10] The results in Sec. IV then establish the complete equivalence of the electromagnetic interaction in the "$\vec{E}\cdot\vec{x}$" gauge and the "$-e\vec{p}\cdot\vec{A}+\frac{1}{2}e^2A^2$" gauge to all orders in perturbation theory. In addition, we see that the Hamiltonian of the free radiation field can indeed replace the clock Hamiltonian we introduced in Sec. III.

VII. INTERACTION OF PHOTONS WITH ATOMS NEAR RESONANCE

In a recent letter Kobe[6] pointed out that in a nonresonant photoabsorption process the matrix elements calculated in the length gauge and the velocity gauge differ by an amount of order Δ/ω, where Δ, the detuning, is of the order of the width of the excited state and ω is the photon frequency involved. He further stated that, because of gauge invariance, the results calculated in the $\vec{x}\cdot\vec{E}$ gauge are always correct. By implication, since his results in the two gauges are different, this is equivalent to stating that results calculated in the $\vec{p}\cdot\vec{A}$ gauge are wrong. He based all his analysis on transition-matrix elements calculated in terms of the complex energy bare states of the atom. The widths of the excited states are incorporated phenomenologically in the Wigner-Weisskopf perturbation scheme by the imaginary part of the complex energies. This confusion justifies a clarification. We shall point out in this section that the whole discrepancy arises because of the incorrect description of the true states in terms of the complex energy bare states and that the discrepancy disappears if the correct states are used. When the true state is approximated by a single complex energy state, the results are inaccurate to order Δ/ω in either gauge. A simpler version of the discrepancy pointed out by Kobe exists in transitions involving one-photon absorption from state i to state f, where at least one of these states has nonzero width. If one follows Kobe's incorrect line of reasoning, then for a photon of energy $\omega = E_f - E_i + \Delta$ the absorption rate will be found equal to $|M|^2\Gamma/[\Delta^2+(\frac{1}{2}\Gamma)^2]$, where $M = \langle f|V_{\text{int}}|i\rangle$ and will be different by order Δ/ω depending on whether the gauges $\vec{x}\cdot\vec{E}$ or gauge $\vec{p}\cdot\vec{A}$ is used. Hence, Kobe's analysis also leads to a discrepancy in one-photon transitions.

The discrepancy of the second-order transition-matrix elements calculated in the two different gauges, as pointed out by Kobe,[6] is due to the approximation one normally uses to describe a state near resonance. In such an approximation, as we shall show, one neglects terms of order Γ/ω, where ω is the energy separation of the bare states. For simplicity let us consider a nonrelativistic hydrogen atom, whose bare-state energies are given as ϵ_n^0, $n = 0, 1, 2, \ldots$. Suppose now we detect a photon of energy $\omega = \epsilon_1^0 - \epsilon_0^0 + \Delta$, where Δ is about the width of the first excited state. Under the usual approximation, one says the original state is a broadened first excited state whose energy is complex, $\epsilon_1 = \epsilon_1^0 - i\Gamma_1$. However, one really does not know from which state the photon has come. So the parent state must be a superposition of the first bare excited state as well as of higher excited states. This true state can be written as

$$|\omega+\epsilon_0^0,\text{true}\rangle = a_1|1,\text{bare}\rangle + a_2|2,\text{bare}\rangle + \ldots\,, \tag{7.1}$$

where

$$\begin{aligned} &a_1 = \alpha_1/(\Delta+\tfrac{1}{2}i\Gamma_1)\,, \quad a_2 \sim [\Gamma_1/(\epsilon_2^0-\epsilon_0^0)]\alpha_2 a_1\,, \\ &a_3 \sim [\Gamma_1/(\epsilon^0-\epsilon^0)]\alpha_3 a_1\,, \end{aligned} \tag{7.2}$$

etc., where the α's are essentially of the same magnitude and contain phase factors, and where the states $|2,\text{bare}\rangle$, $|3,\text{bare}\rangle, \ldots$ have quantum numbers that are the same as in the state $|1,\text{bare}\rangle$, except for the bare energy. In the crudest form of the Wigner-Weisskopf perturbation scheme one neglects $a_2, a_3, \ldots$, compared to a_1, and is therefore already making errors of the order Γ/ω. Hence, to emphasize that the transition-matrix elements calculated in two different gauges differ by order of Δ/ω when terms of order Γ/ω have been neglected from the very beginning is totally meaningless.

Next, we must bear in mind that any physical state must be a true eigenstate of the total Hamiltonian. In this case the atom and the radiation field responsible for the decay of the excited state constitute the total system, describable by the Hamiltonian

$$H = p^2/2m + V(X) - e\vec{x}\cdot\vec{E}_{RF} + H_{RF}, \tag{7.3}$$

where the subscript RF stands for the radiation field. The interaction $-e\vec{x}\cdot\vec{E}_{RF}$ is responsible for the widths of the bare states, and the dipole approximation is usually sufficient for this interaction if one deals with atomic systems. The true states of this Hamiltonian are not given by the bare states (eigenstates of $p^2/2m + V + H_{RF}$) multiplied by phenomenological Wigner-Weisskopf factors. For example, the true ground state is a linear superposition of the bare states:

$$|\text{ground true}\rangle = \sum_n g_n |n\text{ bare}\rangle , \tag{7.4}$$

where $|n,\text{bare}\rangle$, can be considered as product states of the isolated atom and the isolated radiation field. In the right-hand side of Eq. (7.4), $|\text{ground, isolated atom, no photon}\rangle$ is most dominant, and if the dipole approximation has been taken to first order in e in the interaction $e\vec{x}\cdot\vec{E}_{RF}$, the only other states that enter the right-hand side of Eq. (7.4) are of the form $|\text{excited isolated atom, one photon}\rangle$. The sum $\sum_n$ should, of course, include photon energies and polarizations. Above the ground-state energy level any energy would have a corresponding energy eigenstate, allowing for degeneracies among different angular momenta states as well as free photon states. In particular, because of the weakness of the EM coupling constant, for energies close to the eigenenergies of the bare atom, these eigenstates of the true Hamiltonian exhibit resonance behavior. When we describe a realistic atom in an excited state, say hydrogen for simplicity, it is insufficient to specify the principal quantum number; we must also specify the energy. The principal quantum number serves only as a reminder that the atom and radiation field exhibit a resonance structure at energies corresponding to the bare states of this principal quantum number. Hence, a true state of an excited realistic atom "in the state m" is given by

$$|\omega, m, \text{true}\rangle = \sum f_n(\omega)\,|n\text{bare}\rangle \equiv |\omega\text{ true}\rangle , \tag{7.5}$$

where $f_n(\omega)$ displays resonance structure in the neighborhood of $\omega = \alpha/2am^2$.

Next we consider the system being acted on by an external field. This can be introduced as a perturbation and the external field can be described by a c-number field, and the Hamiltonian becomes

$$H' = H - e\vec{x}\cdot\vec{E}_{\text{ext}}. \tag{7.6}$$

As is well known, Fermi's "golden rule" states that physical transitions take place only when energy is conserved. This is true to any order in perturbation theory. A nonresonant absorption by a detuning of Δ in the context used by Kobe[6] is in reality an absorption from the initial state to a final state whose energy is $\alpha/2an_f^2 - \Delta$, and it is totally incorrect to say that energy conservation need not hold in an nonresonant transition. Now the Hamiltonian in (7.6) can be transformed to the form

$$H' = H - \frac{e(\vec{p}\cdot\vec{A}_{\text{ext}} + \vec{A}_{\text{ext}}\cdot\vec{p})}{2m} + \frac{e^2 A^2{}_{\text{ext}}}{2m} \tag{7.7}$$

by a unitary transformation. Hence, according to the theorem we stated in Sec. IV, the transition-matrix elements to any order in e calculated in the two gauges must be the same when the true states are used. On applying this result to a first-order transition between two true atomic states of energy ν' and ν with emission of a photon of energy $\nu' - \nu$, we have

$$\left\langle \nu'\text{ true, atom; no photon}\left|\frac{-\vec{p}\cdot\vec{A}_{\text{ext}}}{m}\right|\nu\text{ true, atom; one photon with energy } \nu' - \nu\right\rangle$$

$$= \langle \nu'\text{ true, atom; no photon}|-\vec{x}\cdot\vec{E}_{\text{ext}}|\nu\text{ true, atom; one photon with energy } \nu' - \nu\rangle , \tag{7.8}$$

where we have made use of the transversality of the photon. This gives rise to an interesting sum rule involving the functions $f_n(\nu)$ defined in Eq. (7.5):

$$\sum_{m,n} f_m^*(\nu')f_n(\nu)(E_m^0 - E_n^0)\langle m\text{bare}|x|n\text{bare}\rangle = (\nu' - \nu)\sum_{m,n} f_m^*(\nu')f_n(\nu)\langle m\text{bare}|x|n\text{bare}\rangle , \tag{7.9}$$

where the superscript 0 stands for bare energies. This equation actually places a constraint for consistency on the functions f_n. For example, in the usual approximation one takes as expressed in Eqs. (7.1) and (7.2), Eq. (7.9) places a constraint on the a's to be chosen. It is our conjecture that by using all possible gauge transformations and the fact that the transition-matrix elements are equal in both gauges, one should be able to establish a sufficient number of constraint equations to determine uniquely these a's. We intend to discuss this further in a future paper.

CONCLUSION

In this paper we have vigorously established the gauge invariance of physical transition-matrix elements. One can expect such invariance on grounds that any violation would imply that one can generate perturbations that can cause physical transitions merely by the use of gauge transformations. Hence, the difference between two Hamiltonians as a result of a gauge transformation can only be regarded as a pseudoperturbation. We have stated and proved the theorem that such pseudoperturbations cannot cause any physical transitions. In particular, we have applied our study to electromagnetic interactions and shown that the real transition-matrix elements calculated in both gauges are always the same when the true states are used. The usually accepted expression for off-resonant (with respect to bare states) transition rate in the form $|M|^2\Gamma/(\Delta^2+\frac{1}{4}\Gamma^2)$ is only an approximation in which terms of order Γ/ω have already been neglected. In such an approximation the emphasis, as stressed by Kobe,[6] on the difference between transition-matrix elements in different gauges, which turns out to be of order Δ/ω, is totally meaningless. In Appendix B we shall also show that our theorem on pseudoperturbations enables us to establish interesting sum rules and on-shell identies which may serve as useful constraints in variational calculations.

ACKNOWLEDGMENT

The authors are grateful to Professor K. Haller for pointing out some previous work[4] by Haller and Haller *et al.* that is relevant to the subject discussed in this paper.

APPENDIX A: GAUGE INVARIANCE OF TRANSITION-MATRIX ELEMENTS

In this appendix we would like to give an alternative proof of the results in Sec. IV. To make this appendix self-contained, we state the theorem once again. If a Hamiltonian $H=H_0+V$, where H_0 is the "unperturbed Hamiltonian" and V is the scattering potential, is related to another Hamiltonian $H'=H_0+V'$ via a unitary transformation $U\equiv\exp(i\Phi)$, where Φ is an acceptable gauge function, then the transition-matrix elements calculated in terms of the unperturbed states in either gauge V or V' are equal to all orders in perturbation theory on the energy shell. As in Sec. IV in the text, we denote the eigenfunctions of H_0, H, and H' by $|\phi\rangle$, $|\psi\rangle$, and $|\psi'\rangle$. Under our assumption, $UHU^\dagger=H'$, and so $|\psi'\rangle=U|\psi\rangle$ and H and H' have the same spectrum. We also denote the precollision and postcollision states by $|\psi_+\rangle$ and $|\psi_-\rangle$ for the Hamiltonian H, and by $|\psi'_+\rangle$ and $|\psi'_-\rangle$ for the Hamiltonian H'. Then, according to the Lippmann-Schwinger equation,

$$|\psi_{\alpha\pm}\rangle=|\phi_\alpha\rangle+\lim_{\eta\to0}\frac{1}{E_\alpha-H\pm i\eta}(H-E_\alpha)|\phi_\alpha\rangle \tag{A1}$$

$$=|\phi_\alpha\rangle+G_{0^\pm}(E_\alpha)V|\phi_\alpha\rangle+G_{0^\pm}(E_\alpha)VG_{0^\pm}(E_\alpha)V|\phi_\alpha\rangle+\dots, \tag{A2}$$

where

$$H_0|\phi_\alpha\rangle=E_\alpha|\phi_\alpha\rangle \tag{A3}$$

and

$$G_{0^\pm}(E_\alpha)=\lim_{\eta\to0}\frac{1}{E_\alpha-H_0\pm i\eta}. \tag{A4}$$

Hereafter we assume that the limiting process $\eta\to0$ is understood and we drop the notation $\eta\to0$. From Eq. (A1) we have

$$(E_\alpha-H)|\psi_{\alpha^\pm}\rangle=\pm i\eta(|\phi_\alpha\rangle-|\psi_{\alpha^\pm}\rangle)=0\text{ as }\eta\to0. \tag{A5}$$

Thus, $\psi_{\alpha^\pm}$ are asymptotic eigenstates of H with eigenvalue E_α. Similarly we can construct the asymptotic state of H':

$$|\psi'_{\alpha\pm}\rangle=|\phi_\alpha\rangle+\lim_{\eta\to0}\frac{1}{E_\alpha-H'\pm i\eta}(H'-E_\alpha)|\phi_\alpha\rangle \tag{A6}$$

$$=|\phi_\alpha\rangle+G_{0^\pm}(E_\alpha)V'|\phi_\alpha\rangle+G_{0^\pm}(E_\alpha)V'G_{0^\pm}(E_\alpha)V'|\phi_\alpha\rangle+\dots, \tag{A7}$$

and $|\psi'_{\alpha\pm}\rangle$ also have eigenvalues E_α. Then, for two unperturbed states $|\phi_i\rangle$ and $|\phi_f\rangle$ on the same energy shell, $E_i=E_f$, and

$$H'|\psi'_{i+}\rangle=E_i|\psi'_{i+}\rangle \tag{A8}$$

and

$$\langle\psi_{f-}|H=\langle\psi_{f-}|E_f, \tag{A9}$$

Thus,

$$\langle\psi_{f-}|H'-H|\psi'_{i+}\rangle=0, \tag{A10}$$

or

$$\langle\psi_{f-}|V'|\psi'_{i+}\rangle=\langle\psi_{f-}|V|\psi'_{i+}\rangle. \tag{A11}$$

Using Eq. (A7) we have

$$|\psi'_{i+}\rangle=|\phi_i\rangle+G_{0+}(E_i)V'|\phi_i\rangle+G_{0+}(E_i)V'G_{0+}(E_i)V'|\phi_i\rangle+\dots \tag{A12}$$

and

$$\langle\psi'_{f-}|=\langle\phi_f|+\langle\phi_f|VG^\dagger_{0-}(E_f)+\langle\phi_f|VG^\dagger_{0-}(E_f)VG^\dagger_{0-}(E_f)+\dots. \tag{A13}$$

On using the on-shell condition $E_i = E_f$, we have

$$G^{\dagger}_{0-}(E_f) = G_{0+}(E_i) \equiv G \text{ on the energy shell,} \tag{A14}$$

where we have simply denoted them by G. On substituting Eqs. (A12)–(A14) into (A11), we have

$$\begin{aligned}(\langle\phi_f| + \langle\phi_f| VG + \langle\phi_f| VGVG + \ldots)\, V'(|\phi_i\rangle + GV'|\phi_i\rangle \\ + GV'GV'|\phi_i\rangle + \ldots) \\ = (\langle\phi_f| + \langle\phi_f| VG + \langle\phi_f| VGVG + \ldots)\, V(|\phi_i\rangle + GV'|\phi_i\rangle \\ + GV'GV'|\phi_i\rangle + \ldots)\,.\end{aligned} \tag{A15}$$

This equation is of the form

$$\begin{aligned}\Big(\sum_i \langle \text{bra}, i|\Big) V' \Big(\sum_j |\text{ket}, j\rangle\Big) \\ = \Big(\sum_i \langle \text{bra}, i|\Big) V \Big(\sum_j |\text{ket}, j\rangle\Big)\end{aligned} \tag{A16}$$

or

$$\sum_{ij} L_{ij} = \sum_{ij} R_{ij}\,, \tag{A17}$$

where L and R stand for the left-hand side and right-hand side terms, respectively. For example,

$$L_{1,3} = \langle\phi_f| V'GV'GV'|\phi_i\rangle\,, \tag{A18}$$

and

$$R_{2,2} = \langle\phi_f| VGVGV'|\phi_i\rangle\,, \tag{A19}$$

and so on. From this we see that

$$L_{(i+1)j} = R_{i(j+1)}\,, \quad i,j \neq 0\,, \tag{A20}$$

and we are left with

$$\sum_j L_{1j} = \sum_i R_{i1}\,. \tag{A21}$$

Now

$$\begin{aligned}\sum_j L_{1j} &= \langle\phi_f|V'|\phi_i\rangle + \langle\phi_f|V'GV'|\phi_i\rangle \\ &\quad + \langle\phi_f|V'GV'GV'|\phi\rangle + \ldots \\ &= \langle\phi_f|\mathcal{T}'|\phi_i\rangle\end{aligned} \tag{A22}$$

and

$$\begin{aligned}\sum_i R_{i1} &= \langle\phi_f|V|\phi_i\rangle + \langle\phi_f|VGV|\phi_i\rangle \\ &\quad + \langle\phi_f|VGVGV|\phi_i\rangle + \ldots \\ &= \langle\phi_f|\mathcal{T}|\phi_i\rangle\,,\end{aligned} \tag{A23}$$

which give the transition-matrix elements calculated, respectively, in the gauges V' and V in terms of the unperturbed eigenstates of H_0. This proves our theorem in Sec. IV in a more vigorous way. Thus, as explained in the text in Sec. IV, if the scattering potential is expressible in terms of a coupling constant λ, the transition-matrix elements, calculated in either gauge to a given order in λ, are equal on the energy shell.

APPENDIX B: SUM RULES AND ON-SHELL IDENTITIES

In this appendix we wish to show that the theorem we proved in Sec. I and further extended in Sec. III leads to some interesting sum rules and operator identifies valid only on the energy shell. We consider a Hamiltonian of the following form:

$$H = H_0 + \pi\,, \tag{B1}$$

where π is the clock Hamiltonian we introduced in Sec. III and H_0 is the Hamiltonian of the system. We now switch on a pseudoperturbation by a unitary transformation $U \equiv \exp(i\lambda\Phi(x,q))$, where $\Phi(x,q)$ is a regular function of the system and clock coordinates alone. Under this unitary transformation we generate the following pseudoperturbation:

$$V = \sum \lambda^n V_n\,, \tag{B2}$$

where the V_n's are given in Eqs. (1.3) and (1.4). In fact, Φ can be either a quantized field or classical field. We now consider all possible transition-matrix elements to a given order in λ, between two states $|i\rangle$ and $|f\rangle$ that are on the same energy shell, i.e., degenerate states of the Hamiltonian H. According to the theorem we proved in Secs. I and III, the sum of all matrix elements to the same order in λ must vanish. We shall denote these matrix elements by M^N_α, where N is the order of λ under consideration and $\alpha \in \mathfrak{C}(N)$, where $\mathfrak{C}(N)$ is the class of all Feyman diagrams generated by the pseudoperturbation V to order N in λ, and $M^N = \sum_{\alpha\in\mathfrak{C}(N)} M^N$. The cases $N=1$ and 2 are trivial and we shall not consider them. In addition, if the system under consideration is a nonrelativistic atom, we denote it by

$$H_0 = p^2/2m + V(x) \tag{B3}$$

and in this case $V_n = 0$ for $n \geq 3$. Henceforth, we shall denote the Green's operator by G,

$$G = (E_i - H)^{-1} = (E_f - H)^{-1}\,, \tag{B4}$$

and shall drop factors of $i\eta$ when no ambiguity arises. We first consider $N=3$. Now

$$M^{\text{III}}_{(1,1,1)} \equiv \langle f| V_1 G V_1 G V_1 |i\rangle = -\langle f|\Phi[\Phi, H]\Phi|i\rangle\,, \tag{B5}$$

$$\begin{aligned}M^{\text{III}}_{(2,1)} &\equiv \langle f| V_2 G V_1 |i\rangle \\ &= (1/2!)\langle f|[\Phi, [\Phi, H]]\Phi|i\rangle\,,\end{aligned} \tag{B6}$$

$$\begin{aligned}M^{\text{III}}_{(1,2)} &= \langle f| V_1 G V_2 |i\rangle \\ &= -(1/2!)\langle f|\Phi[\Phi, [\Phi, H]]|i\rangle\,,\end{aligned} \tag{B7}$$

and

$$M^{\mathrm{III}}_{(3)} = \langle f|\, V_3 |i\rangle$$

$$= (1/3!)\langle f|[\Phi, [\Phi, [\Phi, H]]]|i\rangle \,. \tag{B8}$$

Thus,

$$M^{\mathrm{III}} = -\langle f|\Phi[\Phi, H]\Phi + \tfrac{1}{3}[\Phi, [\Phi, [\Phi, H]]]|i\rangle = 0 \,. \tag{B9}$$

As an application of this identity we consider a nonrelativistic atom H_0, as given by Eq. (B3). Then we see that

$$\langle f|\Phi(\vec{x})[\Phi(\vec{x}), p^2]\Phi(\vec{x})|i\rangle = 0 \tag{B10}$$

between two degenerate states for any regular function of x. A word of caution is in order here. Gauge functions of the form $\Phi(x) = 1/x$ are classified as singular, and cannot be used here, if the states involved are S states.

Next we turn to fourth-order diagrams and use them to illustrate a sum rule.

$$M^{\mathrm{IV}}_{(1,1,1,1)} = \langle f|\, V_1 G V_1 G V_1 G V_1 |i\rangle = -\sum_m \langle f|\Phi[\Phi, H]|m\rangle \frac{1}{E_i - E_m} \langle m|[\Phi, H]\Phi|i\rangle \,, \tag{B11}$$

$$M^{\mathrm{IV}}_{(1,2,1)} = \langle f|\, V_1 G V_2 G V_1 |i\rangle = -\tfrac{1}{2}\langle f|\Phi[\Phi, [\Phi, H]]\Phi|i\rangle \,, \tag{B12}$$

$$M^{\mathrm{IV}}_{(1,1,2)} = \langle f|\, V_1 G V_1 G V_2 \,|i\rangle = \sum_m -\tfrac{1}{2}\langle f|\Phi[\Phi, H]|m\rangle \frac{1}{E_i - E_m} \langle m|[\Phi, [\Phi, H]]|i\rangle \,, \tag{B13}$$

$$M^{\mathrm{IV}}_{(2,1,1)} = \langle f|\, V_2 G V_1 G V_1 |i\rangle = \sum_m \tfrac{1}{2}\langle f|[\Phi, [\Phi, H]]|m\rangle \frac{1}{E_i - E_m} \langle m|[\Phi, H]\Phi|i\rangle \,, \tag{B14}$$

$$M^{\mathrm{IV}}_{(2,2)} = \langle f|\, V_2 G V_2 |i\rangle = \tfrac{1}{4}\sum_m \langle f|[\Phi, [\Phi, H]]|m\rangle \frac{1}{E_i - E_m} \langle m|[\Phi[\Phi, H]]|i\rangle \,, \tag{B15}$$

$$M^{\mathrm{IV}}_{(3,1)} = \langle f|\, V_3 G V_1 |i\rangle = (1/3!)\langle f|[\Phi, [\Phi, [\Phi, H]]]\Phi|i\rangle \,, \tag{B16}$$

$$M^{\mathrm{IV}}_{(1,3)} = \langle f|\, V_1 G V_3 |i\rangle = -(1/3!)\langle f|\Phi[\Phi, [\Phi, [\Phi, H]]]|i\rangle \,, \tag{B17}$$

$$M^{\mathrm{IV}}_{(4)} = \langle f|\, V_4 |i\rangle = (1/4!)\langle f|\, [\Phi, [\Phi, [\Phi, [\Phi, H]]]]|i\rangle \,. \tag{B18}$$

Now

$$M^{\mathrm{IV}}_{(3,1)} + M^{\mathrm{IV}}_{(1,3)} + M^{\mathrm{IV}}_{(4)}$$

$$= -\tfrac{1}{8}\langle f|[\Phi, [\Phi, [\Phi, [\Phi, H]]]|]|i\rangle \tag{B19}$$

and we have the sum rule

$$M^{\mathrm{IV}}_{(1,1,1,1)} + M^{\mathrm{IV}}_{(1,1,2)} + M^{\mathrm{IV}}_{(2,1,1)} + M^{\mathrm{IV}}_{(2,2)} = \tfrac{1}{8}\langle f|[\Phi, [\Phi, [\Phi, [\Phi, H]]]] + 4\Phi[\Phi, [\Phi, H]]\Phi|i\rangle \,, \tag{B20}$$

where the left-hand side involves summing over intermediate states. The left-hand side of Eq. (B20) can actually be summed to give

$$M^{\mathrm{IV}}_{(1,1,1,1)} + M^{\mathrm{IV}}_{(1,1,2)} + M^{\mathrm{IV}}_{(2,1,1)} + M^{\mathrm{IV}}_{(2,2)} = -\tfrac{1}{4}\langle f|[\Phi^2, H]\Phi^2|i\rangle = -\tfrac{1}{8}\langle f|[[\Phi^2, H], \Phi^2]|i\rangle \,, \tag{B21}$$

where we have used $\langle f|[H, \Phi^4]|i\rangle = 0$ in the last step. Combining equations (B20) and (B21), we have the on-shell identity

$$\langle f|[\Phi, [\Phi, [\Phi, [\Phi, H]]]] + [[\Phi^2, H], \Phi^2] + 4\Phi[\Phi, [\Phi, H]]\Phi|i\rangle = 0 \,. \tag{B22}$$

For the fifth-order diagrams, we simply state the result of the sum of 16 diagrams:

$$\begin{aligned} M^{V} = \langle f|\, & V_1 G V_1 G V_1 G V_1 G V_1 + V_2 G V_1 G V_1 G V_1 + V_1 G V_2 G V_1 G V_1 + V_1 G V_1 G V_2 G V_1 + V_1 G V_1 G V_1 G V_2 + V_2 G V_2 G V_1 \\ & + V_2 G V_1 G V_2 \\ & + V_1 G V_2 G V_2 + V_3 G V_1 G V_1 + V_1 G V_3 G V_1 + V_1 G V_1 G V_3 + V_3 G V_2 + V_2 G V_3 + V_4 G V_1 + V_1 G V_4 + V_5 |i\rangle \end{aligned} \tag{B23}$$

$$= \tfrac{1}{20}\langle f|[\Phi, [\Phi, [\Phi, [\Phi, [\Phi, H]]]]] + 5\Phi[\Phi, [\Phi, [\Phi, H]]]\Phi + 5\Phi^2[\Phi, H]\Phi^2|i\rangle \,. \tag{B24}$$

For the benefit of some readers who wish to check our result, we point out that the first term in the right-hand side of (B24) comes from the sum of the ninth through sixteenth terms on the right-hand side of (B23); the second term on the right-hand side of (B24) comes from the sum of the third, fourth, sixth, and eighth terms of (B23); and the last term of (B24) comes from the sum of the first, second, fifth, and seventh terms of (B23). As an application of this identity, we see that

$$\langle f|\Phi^2[\Phi,p^2]\Phi^2|i\rangle = 0 \tag{B25}$$

between any two degenerate atomic states for any regular gauge function Φ.

As we go to higher orders in λ, more complex sum rules and on-shell identities can be generated. In addition, we can vary Φ as long as we keep it regular. We must also state that the on-shell identities can be generated by starting out with the relation

$$\langle f|[H,\Phi^n]|i\rangle = 0\,. \tag{B26}$$

However, in such a process the sum rules are not manifested.

These on-shell identities can serve as useful constraints in the variational calculation of wave functions. In addition, if we include the clock Hamiltonian or the Hamiltonian corresponding to the free field in Eq. (B3), these on-shell identities enable us to put constraints on wave functions of other states that can be connected by the emission or absorption of a finite number of photons to a state whose wave function is known accurately.

---

*On leave from the University of Tel Aviv, Israel.

[1] See, for example, G. Baym, *Lectures on Quantum Mechanics* (Benjamin, New York, 1969).

[2] F. Bassani, J. J. Forney, and A. Quattropani, Phys. Rev. Lett. 39, 1070 (1977).

[3] J. J. Forney, A. Quattropani, and F. Bassani, Nuovo Cimento B 37, 78 (1977); E. A. Power and T. Thirunamachandran, Am. J. Phys. 46, 370 (1978).

[4] After this wrok was completed, we were informed by Professor K. Haller that the same results were obtained by K. Haller and L. F. Landovitz [Phys. Rev. D 2, 1498 (1970)] and by K. Haller [Acta Phys. Austriaca 42, 163 (1975)]. Except for wave-function renormalization terms, which we do not consider here, our results are in agreement with those of Haller. See also K. Haller and R. B. Sohn, Phys. Rev. A 20, 1541 (1979).

[5] The condition that the gauge function vanishes at infinity is required if we discuss perturbations acting on scattering states. However, this condition can be relaxed if only bound states are involved. In the case where one is concerned with photon-atom interactions, the constraints on gauge functions to vanish at infinity implies that the line integral of the field vanishes. This is of no consequence as far as the external field in the vicinity of the atom is concerned.

[6] D. H. Kobe, Phys. Rev. Lett. 40, 538 (1978).

[7] B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950).

[8] See, for example, M. Born, ***Problems of Atomic Dynamics*** (MIT, Cambridge, Mass., 1926).

[9] M. Goldberger and K. Watson, ***Collision Theory*** (Wiley, New York, 1968).

[10] The factor $1/\mathcal{V}$ can be looked upon as the photon-phase space which is of order ω^3. Hence, the term $e^2x^2/\mathcal{V}$ is negligible in the dipole approximation.