Interaction of Schrödinger electrons and photons

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The effect of transformations carried out on the Hamiltonian for the Schrödinger electron-photon system is studied. These transformations include gauge transformations and certain similarity and "hybrid" transformations. The last named involve unitary transformations of either operators or states, but not both. Unitary and hybrid transformation are discussed, which affect the transverse components of the electromagnetic vector potentials and therefore are distinct from gauge transformations. A hybrid transformation is identified which leads to a form of the Hamiltonian that contains no reference to the transverse vector potential and includes electric and magnetic fields as well as nonlocal interactions of charges and currents. The behavior of the scattering matrix under the influence of these hybrid transformations is discussed. Comments are made on two-photon absorption calculations.

I. INTRODUCTION

The electron-photon interaction has long been important in the study of photon emission and absorption by atoms and molecules. This interaction can be represented in various forms. In the first place, the theory is gauge invariant and can be formulated in any of an infinite set of gauges. Moreover, there are versions of this interaction in which, to various degrees of approximation, the electromagnetic potentials are replaced by electric and magnetic fields,[1] either when they appear in matrix elements between electron states, or as operators that appear in the Hamiltonian. The literature demonstrates that there are unresolved questions about the relation among the various forms of the Hamiltonian.[2] For example: To what extent are the different forms of the Hamiltonian equivalent? To what extent can potentials be completely eliminated when electric and magnetic fields are introduced? Which forms of the Hamiltonian can be related by gauge transformations, and which cannot? What changes ensue in a theory when the operators are unitarily transformed and the states are not? Some of these questions have not been answered previously, and the answers to others are in principle known, but have never been discussed in the context of the interaction between photons and nonrelativistic Schrödinger electrons. This paper will address itself to these topics.

II. MULTIPOLE EXPANSION

In this section we will transform the Coulomb gauge Hamiltonian that describes Schrödinger electrons interacting with photons. The transformed Hamiltonian will depend on electric and magnetic fields, and charge and current densities. Except for a surface term, that can usually be ignored, it will not depend on the vector potential. However, this transformation will not involve any change of gauge. To carry out this transformation systematically it is advantageous to quantize the Schrödinger field as well as the photon field although the quantization of the Schrödinger field leads to no new physical effects.[3] It serves only to avoid the inconvenience of dealing simultaneously with quantized electromagnetic fields and unquantized electron fields. The Hamiltonian for this theory is given by

$$H_c = H_0 - \int \vec{J}(\vec{r}) \cdot \vec{A}^T(\vec{r})\, d\vec{r} + \frac{e}{2m} \int \rho(\vec{r}) \vec{A}^T(\vec{r}) \cdot \vec{A}^T(\vec{r})\, d\vec{r} + \int \frac{\rho(\vec{r})\rho(\vec{r}')}{8\pi|\vec{r}-\vec{r}'|}\, d\vec{r}\, d\vec{r}', \tag{2.1}$$

where $\vec{A}^T$ is the transverse vector potential. H_0 is the Hamiltonian for noninteracting electrons and photons. It can be represented by

$$H_0 = H_0(e) + H_0(\gamma), \tag{2.2}$$

where

$$H_0(e) = \int \psi^\dagger(\vec{r})[-(2m)^{-1}\nabla^2 + V(\vec{r})]\psi(\vec{r})\, d\vec{r}$$

with $V(\vec{r})$ representing an external short-range potential (for example, the shielded Coulomb potential of a static nucleus). $H_0(\gamma)$ is the Hamiltonian for free transverse photons and is given by

$$H_0(\gamma) = \frac{1}{2} \int [\vec{E}^T(\vec{r})^2 + \vec{B}(\vec{r})^2]\, d\vec{r},$$

where $\vec{E}^T(\vec{r})$ and $\vec{B}(\vec{r})$ represent the transverse electric and magnetic field, respectively. In Eq. (2.1) $\rho(\vec{r})$ represents the charge density $\rho(\vec{r}) = e\psi^\dagger(\vec{r})\psi(\vec{r})$ and

$\vec{J}(\vec{r})$ represents a current

$$\vec{J}(\vec{r}) = \frac{ie}{2m}[(\vec{\nabla}\psi^\dagger(\vec{r}))\psi(\vec{r}) - \psi^\dagger(\vec{r})\vec{\nabla}\psi(\vec{r})] .$$

The commutation rules of these fields are

$$\{\psi^\dagger(\vec{r}), \psi(\vec{r}')\} = \delta(\vec{r} - \vec{r}') \tag{2.3a}$$

for the electron field; for the photon field, $-\vec{A}^T(\vec{r})$ has the transverse electric field $\vec{E}^T(\vec{r})$ as its conjugate momentum, so that the nonlocal commutation rule for the transverse components is given by

$$[A_i^T(\vec{r}), E_j^T(\vec{r}')] = -i\left(\delta_{i,j}\delta(\vec{r} - \vec{r}') + \frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}\frac{1}{4\pi|\vec{r} - \vec{r}'|}\right) . \tag{2.3b}$$

The current $\vec{J}(\vec{r})$ is conserved under the time dependence provided by the free Hamiltonian so that

$$\vec{\nabla}\cdot\vec{J}(\vec{r}) = -i[H_0, \rho(\vec{r})] . \tag{2.4a}$$

The current

$$\vec{j}(\vec{r}) = \vec{J}(\vec{r}) - (e/m)\rho(\vec{r})\vec{A}^T(\vec{r})$$

is conserved under the time dependence provided by the full Hamiltonian so that

$$\vec{\nabla}\cdot\vec{j}(\vec{r}) = -i[H_c, \rho(\vec{r})] . \tag{2.4b}$$

H_c may be expressed as

$$H_c = H_0 - \frac{1}{2}\int [\vec{J}(\vec{r}) + \vec{j}(\vec{r})]\cdot\vec{A}^T(\vec{r})\, d\vec{r} + \int \frac{\rho(\vec{r})\rho(\vec{r}')}{8\pi|\vec{r} - \vec{r}'|}\, d\vec{r}\, d\vec{r} . \tag{2.5}$$

When ψ is quantized in orbitals that are solutions of

$$[-(2m)^{-1}\nabla^2 + V(\vec{r}) - \omega_i]U_i = 0$$

(where U_i includes both bound and continuum states), $H_0(e)$ is given by

$$H_0(e) = \sum_n e_n^\dagger e_n \omega_n , \tag{2.6a}$$

where $e_n^\dagger$ and e_n designate creation and annihilation operators, respectively, for electrons in the n orbitals. $H_0(\gamma)$ can be represented as

$$H_0(\gamma) = \sum_{i=1,2}\int d\vec{k}\,|\vec{k}|\, a_{\vec{\epsilon}(i)}^\dagger(\vec{k}) a_{\vec{\epsilon}(i)}(\vec{k}) , \tag{2.6b}$$

and describes free photons in the two transverse polarization modes.

We will carry out a two-step transformation of the Hamiltonian H_c. In the first step we will use operator identities to rewrite H_c. The rewritten H_c will then be unitarily transformed to a new Hamiltonian $\bar{H}_c$ which is a nonlocal integral over charges, currents, electric and magnetic fields (modulo surface terms). The first step of the transformation begins with the identity

$$\int \partial_i [r_j J_i(\vec{r}) A_j^T(\vec{r})]\, d\vec{r} = \int \{J_j(\vec{r}) A_j^T(\vec{r}) + r_j[\partial_i J_i(\vec{r})]A_j^T(\vec{r}) + r_j J_i(\vec{r})\partial_i A_j^T(\vec{r})\}\, d\vec{r} . \tag{2.7}$$

The left-hand side is a surface integral which includes the local current $\vec{J}(\vec{r})$ and therefore vanishes when its matrix element is evaluated between two electron states, either of which is in a bound orbital. Otherwise its disappearance should not be assumed. We will suppress the possible presence of such surface terms and write all equations assuming that they vanish. The divergence $\partial_i J_i$ may be expressed as $\partial_i J_i = -i[H_0, \rho]$ (we will designate the commutator $i[H_0, \xi]$ as $\dot{\xi}$ for any operator ξ) so that

$$-\int J_j(\vec{r}) A_j^T(\vec{r})\, d\vec{r} = -\int r_j \dot{\rho}(\vec{r}) A_j^T(\vec{r})\, d\vec{r} + \int r_j J_i(\vec{r})\partial_i A_j^T(\vec{r})\, d\vec{r} . \tag{2.8}$$

We now express $\dot{\rho}A_j^T$ as

$$\dot{\rho}A_j^T = i[H_0, \rho A_j^T] - i\rho[H_0, A_j^T] , \tag{2.9}$$

and since

$$i[H_0, A_j^T] = i[H_c, A_j^T] = -E_j^T ,$$

Eq. (2.8) can be written

$$-\int J_j(\vec{r}) A_j^T(\vec{r})\, d\vec{r} = -\int r_j \rho(\vec{r}) E_j^T(\vec{r})\, d\vec{r} + i[H_0, \alpha^{(1)}] + \int r_j J_i(\vec{r})\partial_i A_j^T(\vec{r})\, d\vec{r} , \tag{2.10}$$

where

$$\alpha^{(1)} = -\int r_j \rho(\vec{r}) A_j^T(\vec{r})\, d\vec{r} .$$

The expression

$$\int r_j J_i(\vec{r})\partial_i A_j^T(\vec{r})\, d\vec{r}$$

in Eq. (2.10) can also be expressed partially in terms of electric and magnetic fields following the pattern established in Eq. (2.10). We note the identity

$$\int \partial_n [r_i r_j J_n(\vec{r})\, \partial_i A_j^T(\vec{r})]\, d\vec{r}$$

$$= \int [r_j J_i(\vec{r})\, \partial_i A_j^T(\vec{r}) + r_i J_j(\vec{r})\, \partial_i A_j^T(\vec{r}) + r_i r_j \partial_n J_n(\vec{r})\, \partial_i A_j^T(\vec{r}) + r_i r_j J_n(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})]\, d\vec{r}\,, \tag{2.11}$$

in which, as previously in Eq. (2.7), the left-hand side vanishes, leaving at most a surface term. We use Eq. (2.11) to replace one half of

$$\int r_j J_i(\vec{r})\, \partial_i A_j^T(\vec{r})\, d\vec{r}$$

and leave the other half in its original form. This procedure leads to

$$\int r_j J_i(\vec{r})\, \partial_i A_j^T(\vec{r})\, d\vec{r}$$

$$= \frac{1}{2} \int r_i r_j \dot{\rho}(\vec{r})\, \partial_i A_j^T(\vec{r})\, d\vec{r} + \frac{1}{2} \int [r_j J_i(\vec{r}) - r_i J_j(\vec{r})] \partial_i A_j^T(\vec{r})\, d\vec{r} - \frac{1}{2} \int r_i r_j J_n(\vec{r})\, \partial_i \partial_n A_j^T(\vec{r})\, d\vec{r}\,. \tag{2.12}$$

By using Eq. (2.9), we rewrite this as

$$\int r_j J_i(\vec{r})\, \partial_i A_j^T(\vec{r})\, d\vec{r}$$

$$= \frac{1}{2} \int r_i r_j \rho(\vec{r})\, \partial_i E_j^T(\vec{r})\, d\vec{r} - \frac{1}{2} \int [\vec{r} \times \vec{J}(\vec{r})] \cdot \vec{B}(\vec{r})\, d\vec{r} + i [H_0, \alpha^{(2)}] - \frac{1}{2} \int r_i r_j J_n(\vec{r})\, \partial_i \partial_n A_j^T(\vec{r})\, d\vec{r}\,, \tag{2.13}$$

where

$$\alpha^{(2)} = \frac{1}{2} \int r_i r_j \rho(\vec{r})\, \partial_i A_j^T(\vec{r})\, d\vec{r}\,.$$

Equation (2.8) and (2.13) can be combined to replace the $-\int \vec{J}(\vec{r}) \cdot \vec{A}^T(\vec{r})\, d\vec{r}$ interaction by electric dipole, electric quadropole, and magnetic dipole interaction, by $[H_0, \alpha^{(n)}]$ commutators, possible surface terms, and the remaining $\frac{1}{2} \int r_i r_j J_n(\vec{r})\, \partial_i \partial_n A_j^T(\vec{r})\, d\vec{r}$. This remainder can again be reexpressed by using the identity

$$\int \partial_k [r_n r_i r_j J_k(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})]\, d\vec{r}$$

$$= 2 \int r_i r_j J_n(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})\, d\vec{r} + \int [r_n r_i J_j(\vec{r})\, \partial_n \partial_i A_j(\vec{r}) + r_n r_i r_j \partial_k J_k(\vec{r})\, \partial_i \partial_n A_j^T(\vec{r})$$

$$+ r_i r_j r_n J_k(\vec{r})\, \partial_k \partial_i \partial_n A_j^T(\vec{r})]\, d\vec{r}\,. \tag{2.14}$$

We represent

$$\frac{1}{3} \int r_i r_j J_n(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})\, d\vec{r}$$

by using Eq. (2.14) and leave the remaining

$$\frac{2}{3} \int r_i r_j J_n(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})\, d\vec{r}$$

untransformed. With the use of Eq. (2.9) we then find that

$$-\frac{1}{2} \int r_i r_j J_n(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})\, d\vec{r}$$

$$= -(3!)^{-1} \int r_i r_j r_n \rho(\vec{r})\, \partial_n \partial_i E_j^T(\vec{r})\, d\vec{r} + (3!)^{-1} \int [\vec{r} \times \vec{J}(\vec{r})]_i r_j \partial_j \vec{B}_i(\vec{r})\, d\vec{r} + i [H_0, \alpha^{(3)}]$$

$$+ (3!)^{-1} \int r_i r_j r_n J_k(\vec{r})\, \partial_n \partial_i \partial_k A_j^T(\vec{r})\, d\vec{r}\,, \tag{2.15}$$

where

$$\alpha^{(3)} = -(3!)^{-1} \int r_i r_j r_n \rho(\vec{r})\, \partial_n \partial_i A_j^T(\vec{r})\, d\vec{r}\,.$$

This process can be continued indefinitely by iterating

$$R_s=(s!)^{-1}\int r_i r_j r_{n(1)}\cdots r_{n(s-2)} \times J_k(\vec{r})\partial_k\partial_{n(1)}\cdots\partial_{n(s-2)}\partial_i A_j^T(\vec{r})\,d\vec{r}$$

to generate higher-order multipoles, and successive $[H_0, \alpha^{(n)}]$ commutators. If the procedure is continued indefinitely we can consider the R_s remainder to be exhausted, and then we will be left with a complete multipole expansion, and with $i[H_0, \alpha]$, where $\alpha=\sum_{n=1}^{\infty}\alpha^{(n)}$. In that limit, we have

$$-\int \vec{J}(\vec{r})\cdot\vec{A}^T(\vec{r})\,d\vec{r}=-\int r_i\rho(\vec{r})\mathfrak{F}_r E_i^T(\vec{r})\,d\vec{r} -\int[\vec{r}\times\vec{J}(\vec{r})]_i\mathfrak{g}_r B_i(\vec{r})\,d\vec{r} + i[H_0,\alpha], \tag{2.16}$$

where $\mathfrak{F}_r$ and $\mathfrak{g}_r$ designate the operator series

$$\mathfrak{F}_r=1-\tfrac{1}{2}r_i\frac{\partial}{\partial r_i}+\frac{1}{3!}r_i r_j\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}+\cdots +\frac{(-1)^s}{(s+1)!}r_{n(1)}\cdots r_{n(s)}\frac{\partial}{\partial r_{n(1)}}\cdots\frac{\partial}{\partial r_{n(s)}}+\cdots \tag{2.16a}$$

and

$$\mathfrak{g}_r=\frac{1}{2}-\frac{1}{3!}r_i\frac{\partial}{\partial r_i}+\frac{1}{4!}r_i r_j\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}+\cdots +\frac{(-1)^s}{(s+2)!}r_{n(1)}\cdots r_{n(s)}\frac{\partial}{\partial r_{n(1)}}\cdots\frac{\partial}{\partial r_{n(s)}}+\cdots, \tag{2.16b}$$

and where α is

$$\alpha=-\int r_i\rho(\vec{r})\mathfrak{F}_r A_i^T(\vec{r})\,d\vec{r}. \tag{2.16c}$$

The argument leading to Eq. (2.16) can be modified to include the so-called "seagull" term

$$\frac{e}{2m}\int\rho(\vec{r})\vec{A}^T(\vec{r})\cdot\vec{A}^T(\vec{r})\,d\vec{r}$$

by replacing $\int\vec{J}(\vec{r})\cdot\vec{A}^T(\vec{r})\,d\vec{r}$ with

$$\frac{1}{2}\int[\vec{j}(\vec{r})+\vec{J}(\vec{r})]\cdot\vec{A}^T(\vec{r})\,d\vec{r}.$$

The identical set of transformations that we have carried out can be repeated by substituting $\vec{\nabla}\cdot\vec{j}=-i[H_c,\rho]$ for $\vec{\nabla}\cdot\vec{J}=-i[H_0,\rho]$. Since

$$-i[H_c,\vec{A}^T]=-i[H_0,\vec{A}^T]=\vec{E}^T,$$

the only change that is produced by substituting

$$\frac{1}{2}\int[\vec{j}(\vec{r})+\vec{J}(\vec{r})]\cdot\vec{A}^T(\vec{r})\,d\vec{r}$$

for $\int\vec{J}(\vec{r})\cdot\vec{A}^T(\vec{r})\,d\vec{r}$ is to replace $[H_0,\alpha]$ by $\frac{1}{2}[(H_c+H_0),\alpha]$, and $\vec{J}$ by $\frac{1}{2}[\vec{J}+\vec{j}]$ in Eq. (2.16). Equations (2.1) and (2.16) can be used, with this replacement, to give

$$H_c-i[H_c,\alpha]=H_0-\int r_i\rho(\vec{r})\mathfrak{F}_r E_i^T(\vec{r})\,d\vec{r}-\int[\vec{r}\times\vec{J}(\vec{r})]_i\mathfrak{g}_r B_i(\vec{r})\,d\vec{r}+h_c-\frac{i}{2}[H_1,\alpha]+\frac{e}{2m}\int(\vec{r}\times\vec{A}^T(\vec{r}))_i\rho(\vec{r})\mathfrak{g}_r B_i(\vec{r})\,d\vec{r}, \tag{2.17}$$

where

$$h_c=\int\rho(\vec{r})\rho(\vec{r}')(8\pi|\vec{r}-\vec{r}'|)^{-1}\,d\vec{r}\,d\vec{r}'$$

and $H_1=H_c-H_0$.

For reasons that we will discuss later, we will find an expression for the unitarily transformed Hamiltonian $\bar{H}_c$ given by

$$\bar{H}_c=e^{i\alpha}H_c e^{-i\alpha}. \tag{2.18a}$$

$\bar{H}_c$ can be given as the series

$$\bar{H}_c=H_c+i[\alpha,H_c]-\tfrac{1}{2}[\alpha,[\alpha,H_c]]. \tag{2.18b}$$

Since $[\alpha,[\alpha,H_c]]$ commutes with α, Eq. (2.18b) is exact, and represents a polynomial expression for $\bar{H}_c$; we can represent $\bar{H}_c$ in the form

$$\bar{H}_c=H_0-\int r_i\rho(\vec{r})\mathfrak{F}_r E_i^T(\vec{r})\,d\vec{r} -\int[\vec{r}\times\vec{J}(\vec{r})]_i\mathfrak{g}_r B_i(\vec{r})\,d\vec{r}+h_c+X, \tag{2.19}$$

where X designates the combination of terms given by

$$X=\frac{e}{2m}\int[\vec{r}\times\vec{A}^T(\vec{r})]_i\rho(\vec{r})\mathfrak{g}_r B_i(\vec{r})\,d\vec{r} -\tfrac{1}{2}i[H_1,\alpha]-\tfrac{1}{2}[\alpha,[\alpha,H_c]]. \tag{2.20a}$$

The expression for X in Eq. (2.20a) can be rewritten to give

$$X=\frac{e}{2m}\int\rho(\vec{r})[\vec{r}\times\mathcal{G}_r\vec{B}(\vec{r})]\cdot[\vec{r}\times\mathcal{G}_r\vec{B}(\vec{r})]\,d\vec{r}+\int r_i\rho(\vec{r})r_j'\rho(\vec{r}')\mathcal{F}_r\mathcal{F}_{r'}\left[\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}-\delta_{i,j}\nabla_r^2\right]\frac{1}{8\pi|\vec{r}-\vec{r}'|}\,d\vec{r}\,d\vec{r}'. \tag{2.20b}$$

Details of the calculation can be found in the Appendix. With the use of Eqs. (2.19) and (2.20) the Hamiltonian $\bar{H}_c$ can be expressed entirely in terms of electric and magnetic fields, the charge density ρ, and the current density $\vec{J}$, in the form

$$\bar{H}_c=H_0+\mathcal{H}_1, \tag{2.21a}$$

with

$$\mathcal{H}_1=-\int r_i\rho(\vec{r})\mathcal{F}_r E_i^T(\vec{r})\,d\vec{r}-\int[\vec{r}\times\vec{J}(\vec{r})]_i\mathcal{G}_r B_i(\vec{r})\,d\vec{r}+h_c+\frac{e}{2m}\int\rho(\vec{r})[\vec{r}\times\mathcal{G}_r\vec{B}(\vec{r})]\cdot[\vec{r}\times\mathcal{G}_r\vec{B}(\vec{r})]\,d\vec{r}$$
$$+\int r_i\rho(\vec{r})r_j'\rho(\vec{r}')\mathcal{F}_r\mathcal{F}_{r'}\left[\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j}-\delta_{i,j}\nabla_r^2\right]\frac{1}{8\pi|\vec{r}-\vec{r}'|}\,d\vec{r}\,d\vec{r}'. \tag{2.21b}$$

If the surface terms that arose in the course of this calculation had not been suppressed, H_c would also include the surface term

$$\mathcal{H}_{\text{surf}}=-\int dS\vec{n}\cdot\left(\vec{J}(\vec{r})-\frac{e}{2m}\rho(\vec{r})\vec{A}^T(\vec{r})+\frac{e}{2m}\rho(\vec{r})[\vec{r}\times\mathcal{G}_r\vec{B}(\vec{r})]\right)(r_i\,\mathcal{F}_r A_i^T(\vec{r})), \tag{2.21c}$$

where $\vec{n}$ is the unit normal to the surface element dS. In electron-photon processes in which either the initial or final electron orbitals are bound states, this surface term will not contribute. Only in cases in which both, the initial and final electron orbitals, are in the continuum, as, for example, in bremsstrahlung events, do we even need to consider $\mathcal{H}_{\text{surf}}$. To what extent $\mathcal{H}_{\text{surf}}$ contributes in these latter cases is outside the scope of this paper. Some features of $\bar{H}_c$ are important and should be noted. Most important is the fact that we can not claim to have a eliminated potentials from the Hamiltonian. Although $\bar{H}_c$ no longer involves the potential $\vec{A}^T$, $\bar{H}_c$ is not identical to the original Hamiltonian H_c, but is only unitarily equivalent to it. The significance of this fact, and the role that $\bar{H}_c$ plays in the theory, will be discussed in Sec. IV.

It should also be noted that the expressions

$$h_E=-\int\rho(\vec{r})\vec{r}\cdot\mathcal{F}_r\vec{E}(\vec{r})\,d\vec{r}$$

and

$$h_B=-\int[\vec{r}\times\vec{J}(\vec{r})]\cdot\mathcal{G}_r\vec{B}(\vec{r})\,d\vec{r}$$

are not exactly multipole expansions, because the spatial integration extends over both, the fields as well as the currents. We will show how to express h_E and h_B as multipole expansions, in the usual sense, although there is no advantage to this way of expressing h_E and h_B beyond then being able to verify agreement with the well-known multipole series for the interaction of charges and currents with electromagnetic fields.[4] The expression for $\mathcal{F}_r E_i$ can be given by means of a Taylor's series,

$$\mathcal{F}_r E_i(\vec{r})=\mathcal{F}_r[(E_i)_0+r_{n(1)}(\partial_{n(1)}E_i)_0+(1/2!)r_{n(1)}r_{n(2)}(\partial_{n(1)}\partial_{n(2)}E_i)_0$$
$$+\cdots+(1/s!)r_{n(1)}r_{n(2)}\cdots r_{n(s)}(\partial_{n(1)}\partial_{n(2)}\cdots\partial_{n(s)}E_i)_0+\cdots], \tag{2.22a}$$

where the subscript zero indicates that E_i and its derivative are to be evaluated at $\vec{r}=0$. Equation (2.22a) can be rewritten as

$$\mathcal{F}_r E_i(\vec{r})=(E_i)_0+\tfrac{1}{2}r_{n(1)}(\partial_{n(1)}E_i)_0+(1/3!)r_{n(1)}r_{n(2)}(\partial_{n(1)}\partial_{n(2)}E_i)_0$$
$$+\cdots+[1/(s+1)!]r_{n(1)}r_{n(2)}\cdots r_{n(s)}(\partial_{n(1)}\partial_{n(2)}\cdots\partial_{n(s)}E_i)_0. \tag{2.22b}$$

When used in the expression for h_E this leads to

$$h_E=\sum_{s=1}^{\infty}(M_E)_{n(1),\ldots,n(s)}\times(\partial_{n(2)}\cdots\partial_{n(s)}E_{n(1)})_0, \tag{2.23}$$

where

$$(M_E)_{n(1),\ldots,n(s)}=(s!)^{-1}\int d\vec{r}\,\rho(\vec{r})r_{n(1)}\cdots r_{n(s)}.$$

Similarly, we find that

$$h_B = \sum_{s=1}^{\infty} (M_B)_{n(1),\ldots,n(s)} \times (\partial_{n(2)} \cdots \partial_{n(s)} B_{n(1)})_0 , \tag{2.24}$$

where

$$(M_B)_{n(1),\ldots,n(s)} = [(s+1)!]^{-1} s \int d\vec{r}\, (\vec{r} \times \vec{J}(\vec{r}))_{n(1)} \times r_{n(2)} \cdots r_{n(s)} .$$

Lastly, we will make a comment about the interaction term

$$\int r_i \rho(\vec{r}) r'_j \rho(\vec{r}') \mathfrak{F}_r \mathfrak{F}_{r'} \times \left(\frac{\partial}{\partial r_i} \frac{\partial}{\partial r_j} - \delta_{i,j} \nabla_r^2 \right) \frac{d\vec{r}\, d\vec{r}'}{8\pi |\vec{r} - \vec{r}'|} .$$

Superficially this term may appear to describe a Coulomb-like interaction between electric multipoles, but that appearance is illusory. The interaction described by this term is mediated by transverse photons, as is indicated by the transverse projection operator

$$\left(\frac{\partial}{\partial r_i} \frac{\partial}{\partial r_j} - \delta_{i,j} \nabla_r^2 \right)$$

that acts on $(8\pi|\vec{r} - \vec{r}'|)^{-1}$. Dynamical effects that appear upon iteration of the Green's function, generated by $\bar{H}_c$, retard this interaction as is required for interactions transmitted by transverse photons.

III. THEORY IN DIFFERENT GAUGES

In classical electrodynamics, gauge transformations affect longitudinal and timelike components of the vector potential. Gauge transformations never change transverse components of the vector potential, and it is trivial to demonstrate that physical predictions are independent of the choice of gauge. The situation is the same in quantum electrodynamics but the gauge independence of its physical predictions is not as immediately obvious as it is in the classical case. One reason is that the time derivative that is part of a gauge transformation involves a commutator with a Hamiltonian, and the Hamiltonian itself depends on the gauge. For example, in its most common form, the Hamiltonian for the electron-photon interaction in the Lorentz gauge bears little resemblance to the Coulomb gauge form. This can be illustrated by writing the Lagrangian for the Lorentz gauge case,

$$\mathfrak{L} = -(1/2m)[\partial_j + ieA_j]\psi^\dagger [\partial_j - ieA_j]\psi + \psi^\dagger V \psi - i\psi^\dagger(\partial_0 - ieA_4)\psi - \tfrac{1}{4} F_{\mu\nu} F_{\mu\nu} - G\partial_\mu A_\mu + \tfrac{1}{2}(1-\gamma)G^2 , \tag{3.1}$$

where $F_{\mu\nu} = \partial_\nu A_\mu - \partial_\mu A_\nu$ and G is a so-called "gauge-fixing" field. Inclusion of the gauge-fixing field makes the canonical quantization procedure possible by providing A_4 with a nonvanishing conjugate momentum. The parameter γ selects one of a number of Lorentz gauges[5]; $\gamma = 0$ identifies the Feynman gauge for example, and $\gamma = 1$ the Landau gauge.[6] The commutation rules for the theory are Eq. (2.3a) for the electron field and, for the photon field, the canonical commutation relation

$$[A_\mu(\vec{r}), \Pi_\nu(\vec{r}')] = i\delta_{\mu\nu}\delta(\vec{r} - \vec{r}') , \tag{3.2}$$

where $\Pi_j = -E_j$ and $\Pi_4 = iG$. The Hamiltonian generated by the Lagrangian in Eq. (3.1) is given by

$$H_L = \int \{ \tfrac{1}{2}\Pi_\mu(\vec{r})\Pi_\mu(\vec{r}) - \tfrac{1}{2}\gamma\Pi_4(\vec{r})\Pi_4(\vec{r}) + \tfrac{1}{4}F_{ij}(\vec{r})F_{ij}(\vec{r}) + i[\Pi_j(\vec{r})\partial_j A_4(\vec{r}) - \Pi_4(\vec{r})\partial_j A_j(\vec{r})] + (1/2m)\partial_j\psi^\dagger(\vec{r})\partial_j\psi(\vec{r}) - \tfrac{1}{2}A_l(\vec{r})[J_l(\vec{r}) + j_l(\vec{r})] - i\rho(\vec{r})A_4(\vec{r})\} d\vec{r} . \tag{3.3}$$

Since the Hamiltonian has a crucial role both in defining the eigenspectrum of the theory and in determining its time evolution, the lack of identifiable correspondence between H_L in Eq. (3.3) and H_c in Eq. (2.1), needs to be discussed.

The equations of motion in the Lorentz gauge follow from the form of the Lagrangian [Eq. (3.1)] and are[7]

$$\partial_\lambda F_{\mu\nu} + \partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} = 0 , \tag{3.4a}$$

$$\partial_\nu F_{\mu\nu} - j_\mu = \partial_\mu G , \tag{3.4b}$$

and

$$\Box G = 0 . \tag{3.4c}$$

These equations are not identical to Maxwell's equations, but differ from them by the inclusion of $\partial_\mu G$ in Eq. (3.4b). Gauss's law, as well as the equation $\vec{\nabla} \times \vec{B} - \partial\vec{E}/\partial t = \vec{j}$, are not operator identities in this formulation of the theory. In Eq. (3.3) the operators for free (or "bare") electrons describe electrons detached from all electromagnetic fields, longitudinal, timelike and transverse (we are considering V to be a phenomenological potential due to an external source, and not part of the electromagnetic field of a participating particle). In the process of developing the "exact" electron wave function, superpositions of free electrons, and longitudinal, timelike, and transverse photons need to be combined to assemble the electron's Coulomb field, as well as its transverse field com-

ponent. The representation of an "exact" electron wave function is fraught with severe technical difficulties, and the finished product must have an electric field, properly flattened to include the effect of the electron's motion, as well as the magnetic field of a moving charge. But the free-electron operator has none of these effects. The one-particle state for a free electron has a vanishing expectation value of its electric field (transverse and longitudinal) as well as of its magnetic field. In the Coulomb gauge the situation is different. Gauss's law is explicitly used to eliminate the longitudinal electric field from the Coulomb gauge Hamiltonian[8] to arrive at the form given in Eq. (2.1). The free-electron states in the Coulomb gauge therefore are automatically consistent with Gauss's law, even without further photon "dressing." The expectation value of transvere electric or magnetic fields for free-electron states vanishes in the Coulomb gauge as well as in the Lorentz gauge. But the longitudinal electric field in the Coulomb gauge is not an independent variable, and is given by

$$-\nabla_r \int d\vec{r}\,' \rho(\vec{r}\,')(4\pi|\vec{r}-\vec{r}\,'|)^{-1},$$

which has a nonvanishing expectation value even for "free" electrons. The bare electron operators in the two different formulations (i.e., the Coulomb gauge and the Lorentz gauge) really refer to different particles. The so-called "bare" or free electron obeys Gauss's law in the Coulomb gauge formulation, but does not obey it in the Lorentz gauge version of the theory. It is therefore not surprising that the two Hamiltonians [H_c in Eq. (2.1) and H_L in Eq. (3.3)] differ considerably in appearance when expressed in terms of the two different electron operators, particularly since these different electron operators are generally represented by the same symbol.

We can understand this aspect of the problem better by studying how the Lagrangian in Eq. (3.1) and the Hamiltonian in Eq. (3.3) lead to electrodynamics in the Lorentz gauge, even though the equations of motion [Eqs. (3.4)] differ from Maxwell's equations. The fact that G is a free field [Eq. (3.4c)] allows us to restore the validity of Maxwell's equations by the following device. A constraint is imposed in the form of a subsidiary condition that selects a "physical" subspace of the indefinite metric space in which the Lorentz gauge theory must be embedded.[9] This subsidiary condition[10] makes use of the positive frequency part of the free field G, and is

$$G^{(+)}|\nu\rangle = 0. \tag{3.5}$$

This condition defines the states $|\nu\rangle$ that constitute the physical subspace. All of the dynamical processes of the theory are confined to the physical subspace, and, within it, Maxwell's equations are valid.

The extraction of the positive frequency part of G can be carried out in a straightforward manner.[11] It is most useful to give the results in the momentum representation. We define

$$a_Q(\vec{k}) = [a_L(\vec{k}) + i a_4(\vec{k})]/\sqrt{2}, \tag{3.6a}$$

$$a_R(\vec{k}) = [a_L(\vec{k}) - i a_4(\vec{k})]/\sqrt{2}, \tag{3.6b}$$

$$a_Q^*(\vec{k}) = [a_L^\dagger(\vec{k}) + i a_4^\dagger(\vec{k})]/\sqrt{2}, \tag{3.6c}$$

$$a_R^*(\vec{k}) = [a_L^\dagger(\vec{k}) - i a_4^\dagger(\vec{k})]/\sqrt{2}, \tag{3.6d}$$

where a_L ($a_L^\dagger$) designates annihilation (creation) operators for photons polarized in the direction of propagation, and a_4 ($a_4^\dagger$) designates the corresponding operators for timelike photons. $a_Q^*|0\rangle$ designates zero-helicity photons and $a_R^*|0\rangle$ scalar photons. Both states have zero norm and are called "ghosts." The momentum transform of Eq. (3.5) is

$$[a_Q(\vec{k}) + \rho(\vec{k})/2|\vec{k}|^{3/2}]|\nu\rangle = 0. \tag{3.7}$$

We see, for example, that a single free-electron state $e_i^\dagger|0\rangle$ fails to satisfy Eq. (3.7), because

$$\rho(\vec{k}) = \int \rho(\vec{r}) e^{-i\vec{k}\cdot\vec{r}}\, d\vec{r}$$

gives $\rho(\vec{k})e_i^\dagger|0\rangle \neq 0$. The subsidiary condition properly refuses to let us use electrons without their Coulomb field, because that would lead to a violation of Gauss's Law.

To simplify the solution of Eq. (3.7) we resort to a unitary transformation within the indefinite metric space[12] (these are often called "pseudounitary" transformations). We transform all operators O by $\hat{O} = UOU^{-1}$ and states by $|\hat{\nu}\rangle = U|\nu\rangle$. This transformation carried out simultaneously on all operators and states leaves all matrix elements unaffected, and if we choose

$$U = e^D \tag{3.8}$$

with

$$D = i \int \frac{d\vec{r}\, d\vec{r}\,'}{4\pi|\vec{r}-\vec{r}\,'|}[\partial_j A_j(\vec{r}) - \tfrac{1}{2}G(\vec{r})]\rho(\vec{r}\,'),$$

we get

$$U[a_Q(\vec{k}) + \rho(\vec{k})/2|\vec{k}|^{3/2}]U^{-1} = a_Q(\vec{k}). \tag{3.9}$$

In the transformed representation (in which operators and states are "hatted"), the subsidiary condition has the simple form

$$a_Q(\vec{k})|n\rangle = 0, \tag{3.10}$$

and ordinary "free"-electron states satisfy it. These "free"-electron states incorporate the effect of the unitary transformation of Eq. (3.8) and refer

to electrons that have their Coulomb field, even without any further "photon dressing." They are therefore the same electron states as are used in the Coulomb gauge theory. The Hamiltonian $\hat{H}_L$ is the Hamiltonian for the Lorentz gauge theory in terms of these transformed operators. It is given by

$$\hat{H}_L = H_0 + h_c + H_T + H'_Q \,, \tag{3.11}$$

where h_c and H_T are given by

$$h_c = \int \frac{d\vec{k}}{2|\vec{k}|^2}\,\rho(\vec{k})\rho(-\vec{k})\,, \tag{3.11a}$$

$$H_T = -\int d\vec{k} \sum_{\lambda=1}^{2}\sum_{l=1}^{3} \hat{\epsilon}_l^{\lambda}(\vec{k})[\,a_\lambda(\vec{k})J_l(-\vec{k}) + a_\lambda^\dagger(\vec{k})J_l(\vec{k})\,]$$
$$+ \frac{e}{2m(2\pi)^{3/2}} \int d\vec{k}\,d\vec{k}' \sum_{\lambda,\lambda'}^{2} \hat{\epsilon}^{\lambda}(\vec{k})\cdot\hat{\epsilon}^{\lambda'}(\vec{k}')\ [\,a_\lambda(\vec{k})a_{\lambda'}(\vec{k}')\rho(-\vec{k}-\vec{k}') + a_\lambda^\dagger(\vec{k})\,a_{\lambda'}^\dagger(\vec{k}')\rho(\vec{k}'+\vec{k})$$
$$+ a_\lambda^\dagger(\vec{k})a_{\lambda'}(\vec{k}')\rho(\vec{k}-\vec{k}') + a_{\lambda'}^\dagger(\vec{k}')a_\lambda(\vec{k})\rho(\vec{k}'-\vec{k})\,]\,. \tag{3.11b}$$

H'_Q is given by

$$H'_Q = H_Q + \gamma \int d\vec{k}\,|\vec{k}|\,a_Q^*(k)a_Q(k)$$

and H_Q by

$$H_Q = -\int \frac{d\vec{k}}{2|\vec{k}|^{3/2}}\left(1-\frac{\gamma}{2}\right)[\vec{k}\cdot\vec{J}(-\vec{k})a_Q(\vec{k}) + \vec{k}\cdot\vec{J}(\vec{k})a_Q^*(\vec{k})] - \int \frac{d\vec{k}}{2(|\vec{k}|)^{1/2}}\left(1+\frac{\gamma}{2}\right)[\,\rho(-\vec{k})a_Q(\vec{k}) + \rho(\vec{k})a_Q^*(\vec{k})\,]$$
$$+ \frac{e}{m(2\pi)^{3/2}} \int \frac{d\vec{k}\,d\vec{k}'(1-\gamma/2)}{(2|\vec{k}|)^{1/2}2|\vec{k}'|^{1/2}} \sum_{\lambda=1}^{2} \hat{\epsilon}^{\lambda}(\vec{k})\cdot\hat{k}'\{\,a_\lambda(\vec{k})[\,\rho(-\vec{k}-\vec{k}')a_Q(\vec{k}') + \rho(\vec{k}'-\vec{k})a_Q^*(\vec{k}')\,]$$
$$+ a_\lambda^\dagger(\vec{k}')[\,\rho(\vec{k}+\vec{k}')a_Q^*(\vec{k}') + \rho(\vec{k}-\vec{k}')a_Q(\vec{k}')\,]\}$$
$$+ \frac{e}{2m(2\pi)^{3/2}} \int \frac{d\vec{k}\,d\vec{k}'\,\hat{k}\cdot\hat{k}'}{4|\vec{k}|^{1/2}|\vec{k}'|^{1/2}}\{\,\rho(-\vec{k}-\vec{k}')a_Q(\vec{k})a_Q(\vec{k}') + \rho(\vec{k}+\vec{k}')a_Q^*(\vec{k})a_Q^*(\vec{k}') + 2\rho(\vec{k}-\vec{k}')a_Q^*(\vec{k})a_Q(\vec{k}')\}\,. \tag{3.11c}$$

Inspection of Eq. (3.11) demonstrates that $\hat{H}_L$ consists of two parts. One part, $H_0 + h_c + H_T$, is independent of γ and is identical to the Coulomb gauge Hamiltonian except for the trivial difference that H_0 in the Lorentz gauge also counts noninteracting zero-norm scalar and zero-helicity photons. The other part, H'_Q, depends on γ but each term in it incorporates either a_Q or a_Q^* operators (or both) but never a_R or a_R^* operators. Since

$$[\,a_R(\vec{k}), a_Q^*(\vec{k}')] = [\,a_Q(\vec{k}), a_R^*(\vec{k}')] = \delta(\vec{k}-\vec{k}')$$

but

$$[\,a_Q(\vec{k}), a_Q^*(\vec{k}')] = [\,a_R(\vec{k}), a_R^*(\vec{k}')] = 0\,,$$

H'_Q can never have any observable effect on state vectors. It can never destroy any $a_R^*(k)$ photon states because none may appear in the initial wave function; none can ever appear at a subsequent time, because the time evolution operator $\exp - i\hat{H}_L t$ never generates them. H'_Q therefore can cannot generate internal photon loops. It can only generate $a_Q^*(\vec{k})$ zero-helicity photon states, which have no norm and no energy, and can never be annihilated by $\hat{H}_L$. The time evolution operator $\exp - i\hat{H}_L t$ can never shift any state vector from the physical subspace to the unphysical. The dynamical predictions made by the Coulomb gauge Hamiltonian and by $\hat{H}_L$ are trivially identical. We can therefore conclude that when the same operators correspond to equivalent particles the Coulomb gauge and the Lorentz gauge versions of the theory are just as closely related in quantum electrodynamics as in classical electrodynamics.

Once we have expressed the Coulomb and Lorentz gauge formulations in forms that use identical operators, i.e., H_c [Eq. (2.1)] and $\hat{H}_L$ [Eq. (3.11)], respectively, we can carry out gauge transformations in the quantized theory.[13] For example, we can gauge transform from the Lorentz to the Coulomb gauge by using $\vec{A}_c = \vec{A}_L + \nabla\chi$ and $\phi_c = \phi_L - i[\hat{H}, \chi]$, with $\nabla^2\chi = -\nabla\cdot\vec{A}_L$, so that $\nabla\cdot\vec{A}_c = 0$. Since $\hat{H}_L$ and H_c differ only by the inclusion of H'_Q in the former, the time derivative operator $i[\hat{H}_L, \ ]$ is appropriate for this transformation. We find that the gauge-transformed theory has the appropriate commutation rules and equations of motion for the Coulomb gauge. Similar transformations can be made to other gauges, and, in fact, the method works for all gauges.

It is worth noting that the kind of transformation that we have carried out in Sec. II can never be the

result of a gauge transformation. Gauge transformations never affect transverse field components, while the transformation that leads to $\overline{H}_c$ only affects the transverse components.

IV. GAUGE, UNITARY, AND HYBRID TRANSFORMATIONS

In Sec. III of this paper we have shown that, although the Hamiltonian for the electron-photon system is gauge dependent, physical predictions can never depend on the choice of gauge. In Sec. II we have discussed a transformation that replaces the Hamiltonian H_c by another, $\overline{H}_c$, in which the electromagnetic potentials have been eliminated everywhere except in a surface term. We have also pointed out that the gauge transformation, and the transformation that replaces H_c by $\overline{H}_c$, are basically different and apply to disparate components of the vector potential. One important question, however, applies to both of these transformations and we would like to raise and answer this question in this section. In the case of gauge transformations the question takes the following form: We have related the Coulomb gauge version of the theory with the Lorentz gauge version. The latter is characterized by the Hamiltonian H_L [Eq. (3.3)] and a constraint equation in the form of the subsidiary condition [Eq. (3.7)]. But there is a very common form of the theory that we have not yet discussed. This form consists of the Hamiltonian H_L [Eq. (3.3)] but fails to take account of the subsidiary condition [Eq. (3.7)]. This is the form that is used when the Lorentz gauge theory is applied computationally. The only concession that is made to the subsidiary condition in actual calculations is that, when incident states are chosen, free electrons and photons are selected and nontransverse incident photons are rejected as unphysical. But the incident free electrons lack a Coulomb field and violate Eqs. (3.5) and (3.7). This form of the theory is not appropriate for *any* gauge. Nevertheless it is simple to use and always gives right answers. The question is: Why does it work?

We can also represent this common form of the theory in its unitarily transformed version, in which the Hamiltonian is $\hat{H}_L$ [Eq. (3.11)] and the subsidiary condition is given by Eq. (3.10). The "common" form of the theory can then also be understood as using the correct states (i.e., "bare" electrons and transverse photons), but an inappropriate Hamiltonian (i.e., H_L instead of $\hat{H}_L$). It appears, in substance, that the "common" form of the Lorentz gauge theory is related to the correct form by a transformation in which the Hamiltonian is unitarily transformed, but the states are not (or, alternatively the states are unitarily transformed and the Hamiltonian is not). We will refer to this as a "hybrid transformation."

It becomes clear that the change from H_c to $\overline{H}_c$ in Sec. II also is a hybrid transformation. In this case, too, we have unitarily transformed H_c to $\overline{H}_c$. However, we do not also want to unitarily transform the states since we want to be able to apply $\overline{H}_c$ to the same electron and photon states to which we originally applied the Hamiltonian H_c.

In general, quantum theory does not support the use of hybrid transformations. It is easy to show that when both, the states as well as the operators, are unitarily transformed all matrix elements remain unchanged and the physical content of the theory is unaffected. But no such general result applies when the states, or the operators alone, are unitarily transformed. It is therefore necessary to study hybrid transformations to determine what kind of equivalence can be demonstrated for them.

We will prove an identity for the hybrid transformations we have made that relates the scattering transition amplitudes of the untransformed and transformed theories. The identity was originally developed in connection with the gauge problem,[14] but we will first give the proof as it applies to the $H_c \to \overline{H}_c$ transformation. The two cases are very similar, although in the $H_c \to \overline{H}_c$ case the underlying space is a Hilbert space, and in the $H_L \to \hat{H}_L$ case it has an indefinite metric.

We begin with

$$\mathcal{K}_1 = H_1 e^{-i\alpha} + (1 - e^{-i\alpha})\overline{H}_c - H_0(1 - e^{-i\alpha}) \qquad (4.1a)$$

and

$$H_1 = e^{-i\alpha}\mathcal{K}_1 + H_c(1 - e^{-i\alpha}) - (1 - e^{-i\alpha})H_0 , \qquad (4.1b)$$

where $\mathcal{K}_1$ is given in Eq. (2.21), α in Eq. (2.16c), and $H_1 = H_c - H_0$. The "outgoing" scattering wave function for an incident state in the "hybrid" version of the theory (designated by $|\overline{\psi}_i\rangle$) is

$$|\overline{\psi}_i\rangle = |i\rangle + (E_i - \overline{H}_c + i\epsilon)^{-1}\mathcal{K}_1|i\rangle , \qquad (4.2)$$

where $(H_0 - E_i)|i\rangle = 0$. This wave function reflects the fact that the untransformed eigenspectrum of H_0 still describes the noninteracting incident and final states before the onset and after the termination of the collision process. However, the Hamiltonian that is used is $\overline{H}_c$ instead of H_c. We rewrite Eq. (4.2) as

$$|\overline{\psi}_i\rangle = |i\rangle + e^{i\alpha}(E_i - H_c + i\epsilon)^{-1}e^{-i\alpha}\mathcal{K}_1|i\rangle \qquad (4.2b)$$

and, with Eq. (4.1b),

$$|\overline{\psi}_i\rangle = e^{i\alpha}|\psi_i\rangle - i\epsilon(E_i - \overline{H}_c + i\epsilon)^{-1}(e^{i\alpha} - 1)|i\rangle , \qquad (4.3)$$

where $|\psi_i\rangle$ is the scattering wave function for the untransformed theory and is given by

$$|\psi_i\rangle = |i\rangle + (E_i - H_c + i\epsilon)^{-1}H_1|i\rangle . \qquad (4.4)$$

The transition amplitude for the hybrid formulation

is given by

$$\overline{T}_{f,i} = \langle f | \mathcal{H}_1 | \overline{\psi}_i \rangle , \tag{4.5a}$$

where $|f\rangle$ is the final state, for which $(H_0 - E_f)|f\rangle = 0$. Use of Eq. (4.3) leads to

$$\overline{T}_{f,i} = \langle f | \mathcal{H}_1 e^{i\alpha} | \psi_i \rangle - i\epsilon \langle f | \mathcal{H}_1 (E_i - \overline{H}_c + i\epsilon)^{-1} (e^{i\alpha} - 1) | i \rangle , \tag{4.5b}$$

and Eq. (4.5b) can be rewritten by using Eqs. (4.1) and the relation

$$(H_c - E_i)|\psi_i\rangle = i\epsilon (E_i - H_c + i\epsilon)^{-1} H_1 |i\rangle , \tag{4.6}$$

leading to

$$\overline{T}_{f,i} = T_{f,i} + (E_f - E_i)\langle f | (1 - e^{i\alpha}) | \psi_i \rangle + i\epsilon \langle f | (e^{i\alpha} - 1)(E_i - H_c + i\epsilon)^{-1} H_1 - \mathcal{H}_1 (E_i - \overline{H}_c + i\epsilon)^{-1} (e^{i\alpha} - 1) | i \rangle , \tag{4.7}$$

with $T_{f,i} = \langle f | H_1 | \psi_i \rangle$.

A similar derivation can be given for the relation between the two forms of the Lorentz gauge theory that are governed by the Hamiltonians H_L and $\hat{H}_L$, respectively, both operating on states $|n\rangle$ that obey $(H_0 - E_n)|n\rangle = 0$ and both constrained by the subsidiary condition as given in Eq. (3.10). In that case we have

$$\hat{T}_{f,i} = \langle n_f | {}^* \hat{H}_1 | \hat{\psi}_i \rangle , \quad T_{f,i} = \langle n_f | {}^* H_1 | \psi_i \rangle ,$$

and

$$T_{f,i} = \hat{T}_{f,i} + (E_f - E_i)\langle n_f | {}^* (1 - e^{-D}) | \hat{\psi}_i \rangle - i\epsilon \langle n_f | {}^* (1 - e^{-D})(E_i - \hat{H}_L + i\epsilon)^{-1} \hat{H}_1 - H_1 (E_i - H_L + i\epsilon)^{-1} (1 - e^{-D}) | n_i \rangle . \tag{4.8}$$

Equations (4.7) and (4.8) notify us that the transition amplitudes are not invariant to hybrid transformations. However, the changes in the transition amplitudes are so benign that the hybrid-transformed version of the theory may safely be used. The discrepancy between $T_{f,i}$ and $\overline{T}_{f,i}$ (and between $T_{f,i}$ and $\hat{T}_{f,i}$) has one part that vanishes on the energy shell (when $E_f = E_i$). Since overall energy conservation in scattering processes is guaranteed, scattering cross sections involve only transition amplitudes with $E_f = E_i$. That part of the discrepancy therefore has no physical consequences. The other part of the discrepancy is proportional to $i\epsilon$, the displacement of the Green's-function pole from the real axis. That discrepancy vanishes as $i\epsilon \to 0$, unless there are $(i\epsilon)^{-1}$ singularities in

$$\langle f | (e^{i\alpha} - 1)(E_i - H_c + i\epsilon)^{-1} H_1 - \mathcal{H}_1 (E_i - \overline{H}_c + i\epsilon)^{-1} (e^{i\alpha} - 1) | i \rangle$$

(or its counterpart in the $H_L \to \hat{H}_L$ case). Such singularities only arise in expressions for wave function renormalization constants and never any where else, so this discrepancy too cannot affect physical quantities.[14] The overall effect is that, when scattering cross sections are evaluated, the use of $\overline{H}_c$ in place of H_c (or H_L instead of $\hat{H}_L$) is permissible. A similar argument holds for bound state energy levels and the appropriateness of the substitution of $\overline{H}_c$ for H_c (or H_L for $\hat{H}_L$) is thereby extended to all scattering processes and to calculations of energy levels.[14]

V. ENERGY CONSERVATION IN SCATTERING EVENTS

The proof that we gave, that scattering cross sections are unaffected by the hybrid transformations that transform H_c into $\overline{H}_c$ and $\hat{H}_L$ into H_L, is crucially dependent on the well-known result that the scattering matrix vanishes unless the total energy of the incident and final states agree identically. We emphasize this point because some authors, in discussing the various forms of the electron-photon interaction, treat the nonresonant two photon absorption by hydrogen as though it had observable off-energy-shell scattering matrix elements.[15] For the process in which hydrogen in its $1s$ state absorbs photons γ_1 and γ_2, and is excited to its $2s$ state, these authors define

$$\Delta = E_{2s} - E_{1s} - \omega_{\gamma(1)} - \omega_{\gamma(2)}$$

and consider the nonresonant transitions to be those for which $\Delta \neq 0$. In this work, the transition amplitude for the process $H(1s) + \gamma(1) + \gamma(2) \to H(2s)$ is evaluated off its energy shell, and the off-energy-shell amplitude (with $\Delta \neq 0$) is used to simulate the fact that the $2s$ state has a finite lifetime, and therefore a finite width. We believe that this description of the process is not consistent with the formalism of scattering theory.[16] Our view is that two-photon (nonresonant) absorption is an energy conserving collision, in which the virtual transition through the $H(2s)$ resonance makes an important contribution, although the transition proceeds near, rather than directly at, the resonance maximum. It has been asserted[17] that in such calculations one should use the $\vec{r} \cdot \vec{E}(0)$ operator [leading term in our $\mathcal{H}_1$, given in Eq. (2.21b)], rather than the $\vec{p} \cdot \vec{A}(0)$ operator [leading term in H_1 given in Eq. (2.1)]. For on-shell transition amplitudes (which, in our opinion, includes the case of nonresonant two-photon absorption) $\mathcal{H}_1$ and H_1 must give identical results, except insofar as they are approximated in different ways. In view of the fact that $\overline{H}_c = H_0 + \mathcal{H}_1$ and $H_c = H_0 + H_1$ are only connected by a hybrid transformation, they are bound to give different results for off-shell amplitudes. We can find no general theoretical basis for preferring $\mathcal{H}_1$ to H_1 in the calculation of off-shell amplitudes, be they approximate or exact.

APPENDIX

In this appendix we will show how Eq. (2.20b) can be derived from Eq. (2.20a). The expression $i[H_c, \alpha]$ is the operator time derivative of α and is given by

$$i[H_c, \alpha] = \int r_i \rho(\vec{r}) \mathfrak{F}_r E_i^T(\vec{r})\, d\vec{r} + \int r_j \partial_i j_i(\vec{r}) \mathfrak{F}_r A_j^T(\vec{r})\, d\vec{r}\,. \tag{A1}$$

The commutator $\frac{1}{2}[\alpha, [H_c, \alpha]]$ is given by

$$\tfrac{1}{2}[\alpha, [H_c, \alpha]] = Y_1 + Y_2\,, \tag{A2}$$

where

$$Y_1 = \frac{i}{2} \int r_i r_j' [\mathfrak{F}_r A_i^T(\vec{r})][\mathfrak{F}_{r'} A_j^T(\vec{r}')] \times \frac{\partial}{\partial r_n'} [\rho(\vec{r}), J_n(\vec{r}')]\, d\vec{r}\, d\vec{r}' \tag{A3}$$

and

$$Y_2 = \frac{i}{2} \int r_i r_j' \rho(\vec{r}) \rho(\vec{r}') \mathfrak{F}_r \mathfrak{F}_{r'} \times [A_j^T(\vec{r}'), E_i^T(\vec{r})]\, d\vec{r}\, d\vec{r}'\,. \tag{A4}$$

Equations (A3) and (A4) can be evaluated by using the commutator

$$[\rho(\vec{r}), J_i(\vec{r}')] = -\frac{ie}{2m}\left[\left(\frac{\partial}{\partial r_i}\rho(\vec{r})\right)\delta(\vec{r}-\vec{r}') + e[\psi^\dagger(\vec{r}')\psi(\vec{r}) + \psi^\dagger(\vec{r})\psi(\vec{r}')]\frac{\partial}{\partial r_i}\delta(\vec{r}-\vec{r}')\right], \tag{A5}$$

which leads to

$$Y_1 = \frac{e}{2m} \int W_i(\vec{r}) W_i(\vec{r}) \rho(\vec{r})\, d\vec{r}\,, \tag{A6}$$

where

$$W_i(\vec{r}) = \frac{\partial}{\partial r_i}[r_j \mathfrak{F}_r A_j^T(\vec{r})]\,.$$

Equation (2.16a) and (2.16b) can be used to show that

$$W_i(\vec{r}) = A_i^T(\vec{r}) + [\vec{r} \times \mathfrak{g}\vec{B}(\vec{r})]_i\,. \tag{A7}$$

The commutator $-\frac{1}{2}i[H_1, \alpha]$ is evaluated using Eqs. (A5) and (A7), and is given by

$$-\tfrac{1}{2}i[H_1, \alpha] = -\frac{e}{2m} \int \rho(\vec{r}) A_i^T(\vec{r})[\mathfrak{F}_r A_i^T(\vec{r}) + r_j \mathfrak{g}_r \partial_i A_j^T(\vec{r})]\, d\vec{r}\,. \tag{A8}$$

We use the identity

$$\mathfrak{F}_r A_i^T(\vec{r}) = A_i^T(\vec{r}) - r_j \mathfrak{g}_r \partial_j A_i^T(\vec{r}) \tag{A9}$$

and find that the sum $Z_1 = Y_1 - \frac{1}{2}i[H_1, \alpha]$ is given by

$$Z_1 = \frac{e}{2m} \int \rho(\vec{r})[\vec{r} \times \mathfrak{g}_r \mathrm{B}(\vec{r})] \cdot [\vec{A}^T(\vec{r}) + \vec{r} \times \mathfrak{g}_r \vec{B}(\vec{r})]\, d\vec{r}\,. \tag{A10}$$

X therefore can be written in the form

$$X = \frac{e}{2m} \int [\vec{r} \times \vec{A}^T(\vec{r})]_i \rho(\vec{r}) \mathfrak{g}_r B_i(\vec{r})\, d\vec{r} + Z_1 + Y_2\,. \tag{A11}$$

Use of the commutator given in Eqs. (2.3b) and (A4) combined with Eq. (A11) leads to Eq. (2.20b).

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