Self-consistent frequencies of the electron-photon system

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The Heisenberg equations describing the dynamics of coupled Fermion photon operators are solved self-consistently. Photon modes, for which $\omega \approx kc$, and particlelike Bohr modes with frequencies $\omega_{nI} \approx (E_n - E_I)/\hbar$ are both approximate solutions to the system of equations that results if the current density is the source in the operator Maxwell equations. Current fluctuations associated with the Bohr modes and required by a fluctuation-dissipation theorem are attributed to the point nature of the particle. The interaction energy is given by the Casimir-force-like expression $\Delta E = \frac{1}{2}\hbar\sum(\Delta\omega_{nI} + \Delta\omega_{kc})$ or by the expectation value of $\frac{1}{2}(q\varphi - q\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}/mc + q^2A^2/mc^2)$. It is verified that the equal-time momentum-density and vector-potential operators commute if the contributions of both the Bohr modes and vacuum fluctuations are included. Both electromagnetic and Bohr or radiation-reaction modes are found to contribute equally to spontaneous emission and to the Lamb shift.

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I. INTRODUCTION

The mode structure of the electromagnetic field is modified in the presence of matter. This is evident from the fact that the speed of light is different in matter than in vacuum so that the dispersion relation becomes $\omega_i = k_i c/n$. Here c is the speed of light in vacuum, $\mathbf{k}_i$ is a wave vector, n is the index of refraction, and the subscript denotes the ith mode of the field. The Casimir force results when the zero-point energy of the electromagnetic field $\frac{1}{2}\sum_i \hbar\omega_i$ is shifted. This prediction of quantum field theory was originally developed to account for the coagulation of colloids and correctly describes the attraction between bodies such as biological membranes. The Lamb shift can also be attributed to a change in the mode structure by a beautifully simple argument originated by Feynman and elucidated by Power [1]. It is just the change in field energy due to the presence of a single atom with polarizability α which results in refractive index $n = 1 + 2\pi\alpha/V$ and a consequent change in frequency relative to the vacuum.

The Casimir force [1] and the Lamb shift can also be attributed to the interaction of the electron with its self-field, an effect called the radiation reaction. Thus all explicit reference to the zero-point field energy can be avoided. However, both contributions are needed to assure the preservation of equal-time commutators [2]. If the separation into these two effects is required to be Hermitian, it is found that both vacuum fluctuations and the radiation reaction contribute equally to spontaneous emission and the Lamb shift [3]. The same conclusion is reached in a semiclassical dispersion force calculation where the fields are real [4,5].

In the dispersion force formalism a self-consistent solution to Maxwell's equations is sought where the source term comes from polarizability multiplied by electric field [6]. A matrix equation for the modes of the electromagnetic field is obtained, and the solvability condition for this system of linear equations determines the frequencies. The physical picture implied in the dispersion force framework is unusual, in that matter interacts through changes in the mode structure of the electric and magnetic fields.

It is also possible to find a self-consistent solution to Maxwell's equations and the Schrödinger equation [4,5]. Two sets of frequencies are found: one is an electromagnetic mode for which $\omega \approx kc$, and the other is approximately the Bohr frequency $(E_n - E_I)/\hbar$. Both are shifted relative to their values when the particle and field are uncoupled. The electron is assumed to be in state $|I\rangle$ to zero order, but makes virtual transitions to all other states $|n\rangle$ under the influence of the field. This semiclassical calculation was performed in the dispersion force framework. In lowest order it gives the same results for the Lamb shift and spontaneous emission as does quantum electrodynamics (QED) [7].

In this paper the self-consistency condition for the electromagnetic and Bohr frequencies will be derived using second quantized fields. Both the minimal coupling and multipolar Hamiltonians will be discussed, and expressions for these and their relationship to the Lagrangian will be considered first. The Heisenberg equations will then be invoked to obtain the self-consistency condition. This results in an expression for the frequency shifts that can be compared to the expectation value of the interaction terms in the Hamiltonian. Finally, this formulation in terms of self-consistency and frequency shifts will be compared to other analyses of particle-field interactions.

II. LAGRANGIAN AND HAMILTONIAN

In this section the minimal coupling Hamiltonian will be used but the multipolar Hamiltonian will also be discussed to allow comparison with previous work. Second quantized electromagnetic and particle wave fields,

Gaussian units, and the Coulomb gauge will be used. The calculation is nonrelativistic and spin is ignored. The approach is similar to that of Milonni [1,2] and of Power and Thirunamachandran [8,9].

For a charge q at position $\mathbf{r}_1$ interacting with electric and magnetic fields $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ the classical Lagrangian is [10]

$$L=\tfrac{1}{2}m\dot{\mathbf{r}}_1^2-V(\mathbf{r}_1)+\frac{1}{8\pi}\int d^3r(E^2-B^2)+L_I \ . \tag{1a}$$

V is the externally produced potential energy and φ and A will denote the particle's self-potentials. They are related to the electric and magnetic self-fields by $\mathbf{E}=-\nabla\varphi-(1/c)\partial\mathbf{A}/\partial t$ and $\mathbf{B}=\nabla\times\mathbf{A}$. The momenta and the Hamiltonian then depend on the Lagrangian selected. The usual choice for the interaction Lagrangian is

$$L_I=\int d^3r\left[\frac{1}{c}\mathbf{j}\cdot\mathbf{A}-\rho\varphi\right], \tag{1b}$$

where the charge and current densities for a point particle at $\mathbf{r}_1$ are $\rho=q\delta(\mathbf{r}-\mathbf{r}_1)$ and $\mathbf{j}=q\mathbf{v}\delta(\mathbf{r}-\mathbf{r}_1)$ with $\mathbf{v}\equiv\dot{\mathbf{r}}_1$. Variation of the action gives the Lorentz force equation and Maxwell's equations with point sources ρ and $\mathbf{j}$. (For a system of charges $\mathbf{r}_1$ can be replaced by a sum over $\mathbf{r}_i$, but the dynamics of one particle will be discussed here for simplicity.) The conjugate momenta are found by differentiating the above Lagrangian (or its density in $\mathbf{r}$ space) with respect to the time rate of change of the particle and field variables $\dot{\mathbf{r}}_1$ and $\dot{\mathbf{A}}$. The particle and field momenta are then found to be $\mathbf{p}=m\mathbf{v}+q\mathbf{A}/c$ and $\Pi=-\mathbf{E}^{\perp}/4\pi c$, respectively. However, addition of the time derivative of any function does not change the equations of motion derived from L. In the dipole approximation current is the derivative of polarization, that is $\mathbf{j}=\dot{\mathbf{P}}$. If $-(d/dt)\int d^3r\,\mathbf{P}\cdot\mathbf{A}/c$ is added to L_I above, then the $\mathbf{j}\cdot\mathbf{A}$ term is canceled and the momenta become $\mathbf{p}=m\mathbf{v}$ and $\Pi=-D^{\perp}/4\pi c$ where $\mathbf{D}=\mathbf{E}+4\pi\mathbf{P}$. The superscript $\perp$ denotes components associated with electromagnetic radiation that are transverse to the direction of propagation.

The particle's dynamical variables can be quantized by introducing the commutation relations $[r_{1i},\hat{p}_j]=i\hbar\delta_{ij}$ with $\hat{\mathbf{p}}=-i\hbar\nabla$ with $m\hat{\mathbf{v}}=\hat{\mathbf{p}}-q\mathbf{A}/c$. The Hamiltonian of the coupled system is [11]

$$\hat{H}=\tfrac{1}{2}m\hat{v}^2+V+\frac{1}{8\pi}\int d^3r(E^2+B^2)+\frac{1}{4\pi}\int d^3r\,\nabla\cdot(\varphi\mathbf{E}) \ , \tag{2}$$

where the last term reduces to a vanishing surface integral and includes $\rho\varphi$ and $\nabla\varphi\cdot\mathbf{E}/4\pi$. Equation (2) is just the kinetic plus potential energy of the particle and its field. When expressed in terms of conjugate momenta, the form of $\hat{H}$ is not unique. It is called the minimal coupling Hamiltonian for the first selection of L_I discussed above, and the multipolar Hamiltonian in the second case.

The Lagrangian becomes

$$L=\int d^3r_1\left\{\frac{i\hbar}{2}(\psi^*\dot{\psi}-\dot{\psi}^*\psi)-\psi^*(\tfrac{1}{2}m\hat{v}^2+V+q\varphi)\psi\right\}+\frac{1}{8\pi}\int d^3r_1(E^2-B^2) \ . \tag{3}$$

Here $\psi(\mathbf{r}_1,t)$ is the probability amplitude and the potentials $\varphi(\mathbf{r}_1,t)$ and $\mathbf{A}(\mathbf{r}_1,t)$ are evaluated at the position of the particle. ψ^* is the complex conjugate of ψ and $i\hbar\psi^*/2$ is canonically conjugate to it. The equations of motion required to minimize $\int L\,dt$ are the Schrödinger equation and Maxwell's equations, but with source charge density $\psi^*(\mathbf{r}_1)q\psi(\mathbf{r}_1)$ and current density $\psi^*(\mathbf{r}_1)q\hat{\mathbf{v}}\psi(\mathbf{r}_1)$. Thus $q\psi^*\psi$ looks like a real charge density with velocity $\hat{\mathbf{v}}$.

The equations will be second quantized using the boson destruction and creation operators a_i and $a_i^{\dagger}$ and the corresponding Fermion operators b_n and $b_n^{\dagger}$. The canonically conjugate pairs obey the equal-time commutation relations $[\hat{A}_i(\mathbf{r}),\hat{\Pi}_j(\mathbf{r}')]=i\hbar\delta_{ij}^{\perp}(\mathbf{r}-\mathbf{r}')$ and $[\hat{\psi}(\mathbf{r}_1),\hat{\psi}^{\dagger}(\mathbf{r}_1')]_+=i\hbar\delta(\mathbf{r}_1-\mathbf{r}_1')$ where $\hat{\psi}=\sum_n b_n|n\rangle$ and $\hat{\psi}^{\dagger}$ is its adjoint. The destruction and creation operators satisfy the commutation and anticommutation relations $[a_i,a_j^{\dagger}]=a_ia_j^{\dagger}-a_j^{\dagger}a_i=\delta_{ij}$ and $[b_n,b_m^{\dagger}]_+=b_nb_m^{\dagger}+b_m^{\dagger}b_n=\delta_{nm}$. The particle and photon operators commute with each other to any given order, as they do in the absence of particle-field coupling.

The vector potential can be expanded in plane waves as

$$\hat{\mathbf{A}}(\mathbf{r},t)=\sum_{\mathbf{k}\lambda}(\hat{\mathbf{A}}_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}}+\hat{\mathbf{A}}_{\mathbf{k}\lambda}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{r}}) \ . \tag{4a}$$

The operator

$$\hat{\mathbf{A}}_{\mathbf{k}\lambda}(t)\equiv A_{\mathbf{k}}\mathbf{e}_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}(t) \tag{4b}$$

describes the mode with wave vector $\mathbf{k}$ and polarization λ where $\mathbf{e}_{\mathbf{k}\lambda}$ is a unit vector in one of two orthogonal directions transverse to $\mathbf{k}$.

Any single-particle operator $\hat{O}$ can be expanded in Fermion operators as

$$\hat{O}=\sum_{n,m}O^{nm}b_n^{\dagger}b_m \ , \tag{5}$$

where $O^{nm}=\langle n|\hat{O}|m\rangle$. It will be convenient for writing the Heisenberg equations if δ-function charge and current density operators are defined that include the factor $\delta(\mathbf{r}-\mathbf{r}_1)=V^{-1}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_1)}$. Thus the particle density operators $\hat{O}'\equiv\delta(\mathbf{r}-\mathbf{r}_1)\hat{O}$ can be expanded in Fermion operators and in $\mathbf{k}$ space as

$$\hat{O}'=\sum_{\mathbf{k}}\sum_{n,m}O_{\mathbf{k}}^{nm}e^{i\mathbf{k}\cdot\mathbf{r}}b_n^{\dagger}b_m \ . \tag{6a}$$

The Fourier coefficients describing fluctuations between states $|n\rangle$ and $|m\rangle$ will be defined as

$$O_{\mathbf{k}}^{nm}=V^{-1}\langle n|\tfrac{1}{2}(e^{-i\mathbf{k}\cdot\mathbf{r}_1}\hat{O}+\hat{O}e^{-i\mathbf{k}\cdot\mathbf{r}_1})|m\rangle \ . \tag{6b}$$

In the Coulomb gauge the two terms in (6b) are equal for the operators needed here and can be combined. If $\hat{O}=q\hat{\mathbf{v}}$ then (6) is the expansion of the current density

operator $\hat{\mathbf{j}}$. The prime will denote multiplication by the δ function and $\hat{O}'$ contains all wave vectors and all of the Bohr frequencies ω_{nm}.

Equation (6) can be used to find the field a distance $\mathbf{r}-\mathbf{r}_1$ from a charge at $\mathbf{r}_1$ as in a recent calculation of the electromagnetic field around a free electron [12]. This procedure is mathematically equivalent to the use of a correlation function as in Ref. [1]. The operators defined in (6) can be used to evaluate

$$\int d^3r\ A'(\mathbf{r},t)B'(\mathbf{r},t)=V\sum_{\mathbf{k}}\sum_{n,m,l}A_{\mathbf{k}}^{nl}B_{-\mathbf{k}}^{lm}b_n^\dagger b_m\ . \tag{6c}$$

As an example of the relationship to the correlation function consider $B'=\rho(\mathbf{r})$ and $A'=\varphi(\mathbf{r})$. The electric potential φ can be found from $\nabla^2\varphi=-4\pi\rho$ to equal $4\pi\int d^3r_1 G(\mathbf{r}-\mathbf{r}_1)\rho(\mathbf{r}_1)$ where the Green function $G(\mathbf{r})$ satisfies $\nabla^2 G=-\delta(\mathbf{r})$. If expressed in terms of G, the Coulomb energy $\int d^3r\,\varphi(\mathbf{r})\rho(\mathbf{r})/2$ becomes $2\pi\int d^3r\int d^3r_1 G(\mathbf{r}-\mathbf{r}_1)\rho(\mathbf{r}_1)\rho(\mathbf{r})$ and the correlation function $\rho(\mathbf{r}_1)\rho(\mathbf{r})$ is required. Either expression gives (6c) above if (6a) is substituted with $\rho_{\mathbf{k}}=q/V$, $\varphi_{\mathbf{k}}=4\pi q/Vk^2$, and $G_{\mathbf{k}}=1/k^2$. The result is $E_C=\sum_{q=0}^{mc/\hbar}2\pi q^2/Vk^2$, which is the charge's Coulomb self-energy. However, if the charge density is $\rho=q\psi^*\psi$, say, for a free electron or an electron in a hydrogen atom, then the large-k modes are missing.

The second quantized Hamiltonian of the particle plus the field is

$$\hat{H}=\sum_n E_n b_n^\dagger b_n+\sum_{\mathbf{k},\lambda}\hbar ck a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda}+\sum_{n,m}\langle n|\hat{H}_I|m\rangle b_n^\dagger b_m\ . \tag{7}$$

It has been assumed that the basis functions for the particle are eigenfunctions of its zero-order Hamiltonian, that is, $(\hat{p}^2/2m+V)|n\rangle=E_n|n\rangle$. The second term in the Hamiltonian represents the zero-order electromagnetic field and is normally ordered so that its expectation value is zero for the vacuum. The perturbation $\hat{H}_I(\mathbf{r}_1,t)$ will be taken to be that part of the Hamiltonian that is due to the electron's self-field, and is split into

$$\hat{H}_I=\hat{H}_1+\hat{H}_2+H_3\ . \tag{8}$$

If the interaction Lagrangian density is $L_I=(1/c)\mathbf{j}\cdot\mathbf{A}-\rho\varphi$ then the minimal coupling Hamiltonian is obtained. From (2), before second quantization of the particle wave field,

$$\hat{H}_1=-\frac{q}{2mc}(\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}+\hat{\mathbf{A}}\cdot\hat{\mathbf{p}})+q\varphi\ , \tag{9a}$$

$$\hat{H}_2=\frac{q^2}{2mc^2}\hat{\mathbf{A}}\cdot\hat{\mathbf{A}}\ , \tag{9b}$$

and

$$H_3=\int d^3r(E^{\parallel 2}+2\mathbf{E}\cdot\nabla\varphi)/8\pi\ . \tag{9c}$$

The longitudinal part has been included as (9c). In the Coulomb gauge $\nabla\cdot\mathbf{A}=0$, and the two momentum terms in (9a) are the same and can be combined.

If the multipolar Hamiltonian is used in the dipole approximation then, again from (2),

$$\hat{H}_1=-\int d^3r\,\mathbf{P}^\perp\cdot\hat{\mathbf{D}}\ , \tag{10a}$$

$$\hat{H}_2=2\pi\int d^3r\,\mathbf{P}^\perp\cdot\mathbf{P}^\perp\ . \tag{10b}$$

The polarization due to a point dipole atom is

$$\mathbf{P}=q\mathbf{r}_1\delta(\mathbf{r}-\mathbf{r}_1)\ . \tag{11}$$

The multipolar expansion is discussed in Ref. [9]. Here $\hat{\mathbf{p}}=m\hat{\mathbf{v}}$, that is, the particle's momentum operator is just its mass times its velocity operator. However, for the minimal coupling Hamiltonian, this is not the case.

It is straightforward to fully second quantize $\hat{H}_I$. Using (4) and (5) and the definition (6b) in the Coulomb gauge, Eq. (9a) becomes

$$\hat{H}_1=V\sum_{n,m}\left[-\sum_{\mathbf{k},\lambda}\frac{q}{mc}\left\{\mathbf{p}_{-\mathbf{k}}^{nm}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}+\mathbf{p}_{\mathbf{k}}^{nm}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}^\dagger\right\}+q\sum_{\mathbf{k}}1_{-\mathbf{k}}^{nm}\varphi_{\mathbf{k}}\right]b_n^\dagger b_m\ , \tag{12a}$$

where $\varphi=\sum_{\mathbf{k}}\varphi_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$. Also

$$\hat{H}_2=\frac{Vq^2}{2mc^2}\sum_{n,m}\sum_{\mathbf{k},\lambda}(\hat{\mathbf{A}}_{-\mathbf{k}}^{nm}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}+\hat{\mathbf{A}}_{\mathbf{k}}^{nm}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}^\dagger)b_n^\dagger b_m\ , \tag{12b}$$

where $\hat{\mathbf{A}}_{\mathbf{k}}^{nm}=V^{-1}\langle n|e^{-i\mathbf{k}\cdot\mathbf{r}_1}\hat{\mathbf{A}}(\mathbf{r}_1,t)|m\rangle$. The expressions for the multipolar $\hat{H}_I$ are analogous, with $\mathbf{p}/m$ replaced by $\mathbf{r}_1$ and $\hat{\mathbf{A}}/c$ replaced by $\hat{\mathbf{D}}$ in (12a), $q\hat{\mathbf{A}}/\sqrt{mc}$ replaced by $\sqrt{4\pi}\hat{\mathbf{P}}$ in (12b) and $q\mathbf{r}_1'=\mathbf{P}$.

III. HEISENBERG EQUATIONS AND SELF-CONSISTENCY

In the Heisenberg picture the equation for the time development of any operator is

$$i\hbar\frac{d\hat{O}}{dt}=[\hat{O},\hat{H}]+i\hbar\frac{\partial\hat{O}}{\partial t}\ . \tag{13}$$

Using the minimal coupling Hamiltonian, Eqs. (7), (8), (12), and (4), and the commutation relations, the $\mathbf{k}\lambda$th photon operators are found to satisfy the differential equations

$$i\hbar\dot{a}_{\mathbf{k}\lambda}=\hbar kca_{\mathbf{k}\lambda}-\frac{V}{c}A_{\mathbf{k}}^*\mathbf{e}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{j}}_{\mathbf{k}} \tag{14a}$$

and

$$-i\hbar\dot{a}_{\mathbf{k}\lambda}^\dagger=\hbar kca_{\mathbf{k}\lambda}^\dagger-\frac{V}{c}A_{\mathbf{k}}\mathbf{e}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{j}}_{-\mathbf{k}}\ , \tag{14b}$$

where $\hat{O}_{\mathbf{k}}\equiv\sum_{n,m}O_{\mathbf{k}}^{nm}b_n^\dagger b_m$. These equations are the minimal coupling version of those obtained by Power and Thirunamachandran [9] using the multipolar Hamiltonian. From (6a) the source can be seen to be proportional to the $\mathbf{k}$th term in the expansion of $\hat{\mathbf{j}}=\delta(\mathbf{r}-\mathbf{r}_1)q\hat{\mathbf{v}}$ where $\hat{\mathbf{p}}/m$ due to $\hat{H}_1$ and $-q\hat{\mathbf{A}}/mc$ from $\hat{H}_2$ have been added to give $\hat{\mathbf{v}}$. A factor 2 comes from $[a,\hat{\mathbf{A}}\cdot\hat{\mathbf{A}}]=[a,\hat{\mathbf{A}}]\cdot\hat{\mathbf{A}}+\hat{\mathbf{A}}\cdot[a,\hat{\mathbf{A}}]$. The source in the $a_{\mathbf{k}\lambda}^\dagger$ and $a_{\mathbf{k}\lambda}$ equations is the same except that $\mathbf{k}$ and $-\mathbf{k}$ are ex-

changed. For a solution of the form $e^{\pm i\omega t}$, the creation and destruction operators are thus related by $a^{\dagger}_{\mathbf{k}\lambda}=a_{-\mathbf{k}\lambda}(kc\pm\omega)/(kc\mp\omega)$. Both contain positive and negative frequencies, since all $b_n^{\dagger}b_m$ terms occur as coefficients of the photon destruction and creation operators in (12). However, $a^{\dagger}_{\mathbf{k}\lambda}$ is larger for positive frequencies while $a_{\mathbf{k}\lambda}$ is larger for negative frequency terms and one of these operators will dominate if $\omega\approx kc$. If the multipolar Hamiltonian is used then the last term is $VD^{*}_{\mathbf{k}}\,\mathbf{e}_{\mathbf{k}\lambda}\cdot q\mathbf{r}'_{1\mathbf{k}}$ with $D_{\mathbf{k}}=-i\omega A_{\mathbf{k}}$.

The coefficients $A_{\mathbf{k}}$ in (4) is

$$A_{\mathbf{k}}=\left[\frac{2\pi\hbar c}{Vk}\right]^{1/2} \tag{15}$$

for plane waves normalized in a volume V. If Eqs. (14) are multiplied by this $A_{\mathbf{k}}$, they become

$$-i\frac{d}{dt}\hat{\mathbf{A}}_{\mathbf{k}\lambda}+kc\,\hat{\mathbf{A}}_{\mathbf{k}\lambda}=\frac{2\pi}{k}\hat{\mathbf{j}}^{\perp}_{\mathbf{k}} \tag{16a}$$

and

$$i\frac{d}{dt}\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}+kc\,\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}=\frac{2\pi}{k}\hat{\mathbf{j}}^{\perp}_{-\mathbf{k}}\ . \tag{16b}$$

A differential equation for the time development of the vector-potential operator in the Coulomb gauge can be obtained by using (13) a second time resulting in

$$\left[\frac{\partial^2}{\partial t^2}-c^2\nabla^2\right]\hat{\mathbf{A}}=4\pi c\hat{\mathbf{j}}^{\perp}\ , \tag{16c}$$

where the contributions of all modes $\mathbf{k}$ have been added. The transverse current has the Fourier coefficients $\hat{\mathbf{j}}^{\perp}_{\mathbf{k}}\equiv\mathbf{e}_{\mathbf{k}\lambda}(\mathbf{e}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{j}}_{\mathbf{k}})$ which are replaced by those of the total current $\hat{\mathbf{j}}$ in the Lorentz gauge. Equation (16c) is just an operator version of Maxwell's equations where the source is the current density operator of a point charge. Thus the form of the classical Maxwell equations obtained from (1) is regained exactly, as is usual in the Heisenberg picture. This follows directly from the conventional Hamiltonian given here by (7) and (12). This correspondence between the form of the classical Maxwell equations and the operator equations in the Heisenberg picture was also noted by Milonni [1]. For the multipolar Hamiltonian the right-hand side is the derivative of polarization and can be combined with $\partial^2\hat{\mathbf{A}}/\partial t^2$ to give $\partial\hat{\mathbf{D}}/\partial t$ so that the current does not appear explicitly. Since it describes transverse modes, (16c) is then a second quantized version of $\nabla\times\mathbf{B}=c^{-1}\partial\mathbf{D}^{\perp}/\partial t$ in a nonmagnetic material.

The time development of the particle operators required in (16) is also described by (13). Substituting (7) it follows that the component associated with transitions between states $|n\rangle$ and $|m\rangle$, $\hat{O}^{nm}=O^{nm}b_n^{\dagger}b_m$, obeys the differential equation

$$i\hbar\frac{d}{dt}\hat{O}^{nm}=-\hbar\omega_{nm}\hat{O}^{nm}+[\hat{O}^{nm},\hat{H}_I]\ . \tag{17}$$

This expresses the time development of $\hat{O}$ in terms of the Bohr frequencies $\omega_{nm}=(E_n-E_m)/\hbar$. Since $\hat{H}_I=\sum_{rs}H_I^{rs}b_r^{\dagger}b_s$ and $[b_n^{\dagger}b_m,b_r^{\dagger}b_s]=\delta_{mr}b_n^{\dagger}b_s-\delta_{ns}b_r^{\dagger}b_m$,

$$i\hbar\frac{d}{dt}\hat{O}^{nm}=-\hbar\omega_{nm}\hat{O}^{nm}+O^{nm}\sum_r(b_n^{\dagger}b_r\hat{H}_I^{mr}-\hat{H}_I^{rn}b_r^{\dagger}b_m)\ . \tag{18}$$

$\hat{H}_I^{mr}$ contains the operators $a_{\mathbf{k}\lambda}$ and $a^{\dagger}_{\mathbf{k}\lambda}$, but these photon operators commute with the Fermion b's as long as both are exact. Thus the order of these operators is not crucial before any approximations have been made or if all contributions to a given order are included.

For the terms $r=n$ and $r=m$, $\hat{O}^{nm}$ oscillates at the frequency of the field due to $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ in $\hat{H}_1$. After the expectation value is taken, for a particle in state $|I\rangle$ the only terms that survive are those of the form $b_I^{0\dagger}b_I^0$. For $r=n=I$ or $r=m=I$ only fluctuations involving the state $|I\rangle$ contribute to $\hat{O}'$. Thus $\langle I|\hat{O}|I\rangle$ oscillates at the same frequency as $\hat{H}_I$ which is the frequency of the field due to $\hat{H}_1$ and is time independent for the $\hat{H}_2$ terms if two-photon effects which go as q^4 are neglected. In general, Eq. (18) is nonlinear in that it involves the product of field and particle operators. If only the one-photon terms and those diagonal in the Fermion operators are kept then a linear approximation results.

Solutions for which $\hat{\mathbf{j}}_{\mathbf{k}}$ [and thus $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ and $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ obtained from (16)] are proportional to $e^{i\omega t}$ will be considered first. Replacement of ω by $-\omega$ will then be examined and a linear combination for which $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ is the adjoint of $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ found. Multiplication of (18) by an integrating factor and integration gives

$$\hbar\hat{O}^{nm}=-O^{nm}\sum_r\left[b_n^{\dagger}b_r\frac{\hat{H}\hbar_1^{mr}}{\omega_{mr}+\omega}-\frac{\hat{H}_1^{rn}}{\omega_{rn}+\omega}b_r^{\dagger}b_m\right]\ . \tag{19}$$

There is no homogeneous solution to (19) alone, since the current and field equations will be solved as a coupled oscillator problem. Thus the relevant homogeneous solutions are those that satisfy the higher order differential equation obtained when one of the variables $\hat{\mathbf{j}}$ or $\hat{\mathbf{A}}$ is eliminated. Equations (18) and (19) apply to both $\hat{O}^{nm}$ and the Fourier components of the corresponding density operator $\hat{O}^{nm}_{\mathbf{k}}$ defined by (6),

The current and charge densities that are sources in Maxwell's equations can be expressed in terms of their expansions in the particle operators. From (19) and (12a) applied to a density operator defined in (6).

$$\hat{O}'_{\mathbf{k}}=\frac{qV}{\hbar}\sum_{n,m,r}O^{nm}_{\mathbf{k}}\left\{\sum_{\mathbf{k}',\lambda'}\left[\frac{\mathbf{p}^{mr}_{-\mathbf{k}'}b_n^{\dagger}b_r}{\omega_{mr}+\omega}-\frac{\mathbf{p}^{rn}_{-\mathbf{k}'}b_r^{\dagger}b_m}{\omega_{rn}+\omega}\right]\cdot\frac{\hat{\mathbf{C}}_{\mathbf{k}'\lambda'}}{mc}-\sum_{\mathbf{k}'}\left[\frac{1^{mr}_{-\mathbf{k}'}b_n^{\dagger}b_r}{\omega_{mr}+\omega}-\frac{1^{rn}_{-\mathbf{k}'}b_r^{\dagger}b_m}{\omega_{rn}+\omega}\right]\varphi_{\mathbf{k}'}\right\}\ . \tag{20}$$

The wave vector $\mathbf{k}'$ was replaced with $-\mathbf{k}'$ in the $\hat{\mathbf{A}}^{\dagger}$ terms and $\hat{\mathbf{C}}_{\mathbf{k}\lambda}\equiv\hat{\mathbf{A}}_{\mathbf{k}\lambda}+\hat{\mathbf{A}}^{\dagger}_{-\mathbf{k}\lambda}$. The commuting particle and field operators $C_{\mathbf{k}'\lambda'}$ and $b_n^{\dagger}b_r$ have been interchanged. Equation (20) gives the current density as $\hat{\mathbf{p}}'-q\,\hat{\mathbf{A}}'/c$ for the minimal coupling Hamiltonian. If the

multipolar Hamiltonian is used in the dipole approximation then $\mathbf{p}^{mn}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}_{\mathbf{k}'\lambda'}/mc$ can be replaced by $(\mathbf{r}_1)^{mn}_{-\mathbf{k}}\cdot\mathbf{D}_{\mathbf{k}'\lambda'}$ and the $\mathbf{A}$ term can be omitted in (16) as noted previously. The second-order Hamiltonian $\hat{H}_2$ gives $-4\pi\hat{\mathbf{P}}_{\mathbf{k}}\cdot(q\mathbf{r}_1)^{mn}_{-\mathbf{k}}$ which can be added to $(q\mathbf{r}_1)^{mn}_{-\mathbf{k}}\cdot\mathbf{D}_{\mathbf{k}\lambda}$, resulting in $(q\mathbf{r}_1)^{mn}_{-\mathbf{k}}\cdot\hat{\mathbf{E}}_{\mathbf{k}\lambda}$. The physics of the particle equation, (20), and the field equations, (16), is the same for either choice of $\hat{H}$. The net field drives the particle oscillations and the particle velocity determines the current density which in turn is the source in the operator Maxwell equations.

Equations (16) and (20) each give a relationship between the vector potential and current operators. The self-consistency condition can be obtained by substituting (20) into (16a) and using $\hat{\mathbf{A}}^{\dagger}_{-\mathbf{k}\lambda}=\hat{\mathbf{A}}_{\mathbf{k}\lambda}(kc+\omega)/(kc-\omega)$. After the expectation value over particle states is taken, then for potentials of frequency ω, substitution of (20) with $\hat{O}'=\hat{\mathbf{j}}$ into (16a) gives

$$\hat{\mathbf{C}}_{\mathbf{k}\lambda}=\frac{4\pi q^2V_c}{\hbar m(k^2c^2-\omega^2)}\sum_m\left\{\sum_{\mathbf{k}',\lambda'}\left[\frac{\mathbf{p}^{\perp Im}_{\mathbf{k}}\mathbf{p}^{mI}_{-\mathbf{k}'}}{\omega_{mI}+\omega}-\frac{\mathbf{p}^{\perp mI}_{\mathbf{k}}\mathbf{p}^{Im}_{-\mathbf{k}'}}{\omega_{Im}+\omega}\right]\cdot\frac{\hat{\mathbf{C}}_{\mathbf{k}'\lambda'}}{mc}-\sum_{\mathbf{k}'}\left[\frac{\mathbf{p}^{\perp Im}_{\mathbf{k}}1^{mI}_{-\mathbf{k}'}}{\omega_{mI}+\omega}-\frac{\mathbf{p}^{\perp mI}_{\mathbf{k}}1^{Im}_{-\mathbf{k}'}}{\omega_{Im}+\omega}\right]\varphi_{\mathbf{k}'}\right\}-\frac{4\pi q^2}{Vm(k^2c^2-\omega^2)}\hat{\mathbf{C}}_{\mathbf{k}\lambda} \tag{21a}$$

neglecting dc and two-photon terms. If the expectation value is not taken, then the operator form in (20) is retained. The expectation value is over the particle state which can be taken to be the uncoupled state $|I\rangle$ when calculating the lowest order frequency shifts. The frequencies of both the Bohr and electromagnetic modes satisfy the same eigenvalue equation. Since $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ is transverse, only components of $\mathbf{p}$ parallel to $\hat{\mathbf{A}}$ and thus perpendicular to $\mathbf{k}$ contribute as indicated by the superscript $\perp$.

In the Coulomb gauge the scalar electric potential satisfies $\nabla^2\varphi=-4\pi\rho$. If $O_{\mathbf{k}}$ is taken to be $1_{\mathbf{k}}$ in (20) then, since $\rho^{nm}_{\mathbf{k}}=V^{-1}q\langle n|e^{-i\mathbf{k}\cdot\mathbf{r}}|m\rangle$,

$$\varphi_{\mathbf{k}}=\frac{4\pi q^2V}{\hbar k^2}\sum_m\left\{\sum_{\mathbf{k}',\lambda'}\left[\frac{1^{Im}_{\mathbf{k}}\mathbf{p}^{mI}_{-\mathbf{k}'}}{\omega_{mI}+\omega}-\frac{1^{mI}_{\mathbf{k}}\mathbf{p}^{Im}_{-\mathbf{k}'}}{\omega_{Im}+\omega}\right]\cdot\frac{\hat{\mathbf{C}}_{\mathbf{k}'\lambda'}}{mc}-\sum_{\mathbf{k}'}\left[\frac{1^{Im}_{\mathbf{k}}1^{mI}_{-\mathbf{k}'}}{\omega_{mI}+\omega}-\frac{1^{mI}_{\mathbf{k}}1^{Im}_{-\mathbf{k}'}}{\omega_{Im}+\omega}\right]\varphi_{\mathbf{k}'}\right\}. \tag{21b}$$

The self-consistency condition (21) is a matrix equation for the two components of $\hat{\mathbf{C}}_{\mathbf{k}\lambda}$ and a third component $\varphi_{\mathbf{k}}$ for each $\mathbf{k}$. If N wave vectors are included, there are $3N$ equations and an equal number of unknowns. The solvability condition for this linear system, that the determinant of the matrix equal zero, gives the frequencies ω that satisfy the Heisenberg equations for both $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ and $\hat{\mathbf{j}}_{\mathbf{k}}$.

The operator referred to as $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ will not be the adjoint of $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ if positive (or negative) frequencies alone are taken. However $\hat{\mathbf{j}}^{\dagger}_{\mathbf{k}}=\hat{\mathbf{j}}_{-\mathbf{k}}$ according to (6a), and comparison of the equation obtained by taking the adjoint of (16a) with (16b) implies that $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ and $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ are conjugate if both positive and negative frequencies are included. If $b^{\dagger}_nb_m\sim e^{i\omega t}$, the corresponding negative frequency term is $\mathbf{j}^{mn}_{\mathbf{k}}b^{\dagger}_mb_n=(\mathbf{j}^{nm}_{-\mathbf{k}}b^{\dagger}_nb_m)^{\dagger}$ so that the positive and negative frequency contributions are related by $\hat{\mathbf{j}}_{\mathbf{k}}(-\omega)=\hat{\mathbf{j}}^{\dagger}_{-\mathbf{k}}(\omega)$. The frequencies satisfy an equation of the form $|D_k(\omega)\delta_{\mathbf{k}\lambda,\mathbf{k}'\lambda'}-M_{\mathbf{k}\lambda,\mathbf{k}'\lambda'}(\omega)|=0$. Here M is a Hermitian matrix and the $\varphi_{\mathbf{k}}$ terms have been included as a third λ. If ω is replaced by $-\omega$, then M is merely transposed with the signs of $\mathbf{k}$ and $\mathbf{k}'$ changed. Thus if ω is an eigenvalue then so is $-\omega$ provided all wave vectors are replaced by their negatives. The vector potential due to the positive and negative frequency source terms is

$$\hat{\mathbf{A}}_{\mathbf{k}\lambda}=\frac{\pi}{k}\left[\frac{\hat{\mathbf{j}}_{\mathbf{k}}(0)e^{i\omega_{\mathbf{k}}t}}{kc+\omega_{\mathbf{k}}}+\frac{\hat{\mathbf{j}}^{\dagger}_{-\mathbf{k}}(0)e^{-i\omega_{-\mathbf{k}}t}}{kc-\omega_{-\mathbf{k}}}\right], \tag{21c}$$

and $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ calculated using (16b) is the adjoint of this $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ as required. Then, in the limit as $\omega\to kc$, $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ includes only negative frequencies while $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ has only positive frequency terms as expected for photon annihilation and creation operators.

IV. FREQUENCY SHIFTS AND INTERACTION ENERGY

In dispersion force calculations, the interaction energy is written as

$$\Delta E=\tfrac{1}{2}\hbar\sum_i\Delta\omega_i\ , \tag{22}$$

where $\Delta\omega_i$ is the shift in the angular frequency of the ith mode that results from interactions. For the frequencies ω_{kc} this is just the change in zero-point energy of the field. Its application to the Bohr modes for which $\omega\approx\omega_{mI}$ can be justified if an oscillator model of the atom is used. More generally, this expression for the sum of the frequency shifts can be based on the fluctuation-dissipation theorem [13,5]. It is conventional to write this interaction energy as the contour integral [6]

$$\Delta E=\frac{\hbar}{4\pi i}\sum_i\oint d\omega\,\omega\frac{d}{d\omega}\ln\left[\frac{\omega-(\omega_i+\Delta\omega_i)}{\omega-\omega_i}\right]$$
$$=-\frac{\hbar}{4\pi i}\sum_i\oint d\omega\ln\left[\frac{\omega-(\omega_i+\Delta\omega_i)}{\omega-\omega_i}\right] \tag{23}$$

after integrating by parts. The solvability condition for Eqs. (21) is of the form $|\delta_{ij}-\chi_{ij}|=0$. The matrix $\delta_{ij}-\chi_{ij}$ can be diagonalized without changing its trace to give $|\delta_{ij}(\omega-\omega_i-\Delta\omega_i)/(\omega-\omega_i)|=0$. After expanding the logarithm, the interaction energy may be written as a sum over the trace of powers of the matrix χ as

$$\Delta E=\frac{\hbar}{4\pi i}\oint d\omega\sum_{r=1}^{\infty}\mathrm{Tr}(\chi)^r/r\ . \tag{24}$$

The contour should include the positive ω axis and there should be no poles or branch points other than those at ω_i. Since χ is proportional to q^2, each successive term in the expansion (24) is of higher order in the coupling constant $\alpha=q^2/\hbar c$.

The lowest order contributions to ΔE come from the contour integral of the first or $r=1$ term. This is the sum over the diagonal terms, $\mathbf{k}=\mathbf{k}'$ and $\lambda=\lambda'$ with the same components of $(1,\mathbf{p}/mc)$. Equivalently, the lowest order contribution to the frequency shift can be found by solving (21) directly, taking the diagonal terms to give a first approximation. For a particle in state $|I\rangle$ the transverse modes are frequency shifted by

$$\Delta\omega_{kc}\approx\frac{2\pi q^2V}{\hbar m^2}\sum_m\frac{1}{kc}\left[-\frac{\mathbf{p}_{\mathbf{k}}^{\perp Im}\cdot\mathbf{p}_{-\mathbf{k}}^{\perp mI}}{kc+\omega_{mI}}+\frac{\mathbf{p}_{\mathbf{k}}^{\perp mI}\cdot\mathbf{p}_{-\mathbf{k}}^{\perp Im}}{kc-\omega_{mI}}\right]+\frac{2\pi q^2}{Vmkc} \tag{25a}$$

and

$$\Delta\omega_{mI}^t\approx\frac{2\pi q^2V}{\hbar m^2}\sum_{\mathbf{k},\lambda}\frac{1}{kc}\left[-\frac{\mathbf{p}_{\mathbf{k}}^{\perp mI}\cdot\mathbf{p}_{-\mathbf{k}}^{\perp Im}}{kc+\omega_{mI}}-\frac{\mathbf{p}_{\mathbf{k}}^{\perp mI}\cdot\mathbf{p}_{-\mathbf{k}}^{\perp Im}}{kc-\omega_{mI}}\right], \tag{25b}$$

as discussed in Refs. [4] and [5]. The last contribution in (25a) gives the A^2 term (9b). It can be obtained more directly when $\mathbf{p}_{\mathbf{k}}^{nI}=0$ by substituting $\mathbf{j}=-q^2\mathbf{A}/Vmc$ in (16b) to give $\omega-kc=2\pi q^2/Vmck$. For the longitudinal modes, from (21b),

$$\tfrac{1}{2}\hbar\sum_m\Delta\omega_{mI}^1\approx\frac{2\pi q^2}{V}\sum_{\mathbf{k},m}\frac{\langle m|e^{i\mathbf{k}\cdot\mathbf{r}}|I\rangle\langle I|e^{-i\mathbf{k}\cdot\mathbf{r}}|m\rangle}{k^2}=\frac{2\pi q^2}{V}\sum_{\mathbf{k}}\frac{1}{k^2}, \tag{25c}$$

which is just the energy in the Coulomb field of a point charge [4]. Equation (22) then becomes

$$\Delta E_I=\tfrac{1}{2}\hbar\left[\sum_{\mathbf{k}}\Delta\omega_{\mathbf{k}c}+\sum_m(\Delta\omega_{mI}^t+\Delta\omega_{mI}^1)\right]. \tag{25d}$$

Equations (21) fix the frequencies while (20) and (16) give current in terms of the field and vice versa. As coupling goes to zero, the momentum density operator components must be $\hat{\mathbf{p}}'^{nm}$ from (6) while the field modes have the amplitude $A_{\mathbf{k}}$ given by (15). When coupling is turned on, Eqs. (16) and (20), respectively, then give the field at the Bohr frequency ω_{nm} and the momentum operator at $\omega_{\mathbf{k}c}$. It is the sum of these zero- and first-order contributions that results in particle and field operators $\mathbf{p}_{\mathbf{k}}^{nm}b_n^\dagger b_m$ and $\hat{\mathbf{A}}_{\mathbf{k}\lambda}$ that commute. The transverse particle and field operators are, to first order,

$$\hat{\mathbf{A}}_{\mathbf{k}\lambda}=\hat{\mathbf{A}}_{\mathbf{k}\lambda}^0+\frac{2\pi q}{mk}\sum_{r,s}\mathbf{p}_{\mathbf{k}}^{\perp rs}b_r^{0+}b_s^0\frac{1}{kc+\omega_{rs}} \tag{26a}$$

and

$$\hat{\mathbf{p}}_{\mathbf{k}}'^{\perp nm}=\mathbf{p}_{\mathbf{k}}^{\perp nm}b_n^{0\dagger}b_m^0+\frac{qV}{mc\hbar}\mathbf{p}_{\mathbf{k}}^{\perp nm}\sum_r\left\{\left[-\frac{\mathbf{p}_{-\mathbf{k}}^{mr}b_n^{0\dagger}b_r^0}{kc-\omega_{mr}}+\frac{\mathbf{p}_{-\mathbf{k}}^{rn}b_r^{0\dagger}b_m^0}{kc-\omega_{rn}}\right]\cdot\frac{\hat{\mathbf{A}}_{\mathbf{k}\lambda}^0}{mc}+\left[\frac{\mathbf{p}_{-\mathbf{k}}^{mr}b_n^{0\dagger}b_r^0}{kc+\omega_{mr}}-\frac{\mathbf{p}_{-\mathbf{k}}^{rn}b_r^{0\dagger}b_m^0}{kc+\omega_{rn}}\right]\cdot\frac{\hat{\mathbf{A}}_{-\mathbf{k}\lambda}^{0\dagger}}{mc}\right\}, \tag{26b}$$

where $\hat{\mathbf{p}}_{\mathbf{k}}'^{nm}\equiv\mathbf{p}_{\mathbf{k}}^{nm}b_n^\dagger b_m$. It can be verified by substitution that $[\hat{\mathbf{p}}_{\mathbf{k}}'^{nm},\hat{\mathbf{A}}_{\mathbf{k}\lambda}]=0$ and $[\hat{\mathbf{p}}_{\mathbf{k}}'^{nm},\hat{\mathbf{A}}_{\mathbf{k}\lambda}^\dagger]=0$, that is, the particle and field operators commute to first order in the coupling constant. The equations are also valid if $\mathbf{p}^{nm}$ is replaced by O^{nm} for an arbitrary particle operator.

The relevant energy here is that of the particle plus the field. The momentum $q\mathbf{A}/c$ equals [14] $\mathbf{E}^\parallel\times\mathbf{B}/4\pi c$ since the Coulomb field is $\mathbf{E}^\parallel=-i\mathbf{k}4\pi q/Vk^2$ and $\mathbf{B}=i\mathbf{k}\times\mathbf{A}$. Thus $\mathbf{p}_I=m\mathbf{v}+q\mathbf{A}/c$ is the momentum of the particle plus the additional field momentum that it produces. In the "rest" frame K' where $\mathbf{p}_I=0$, the total momentum is zero and the field's energy is $cP_e'^0\equiv\int d^3r(E'^2+B'^2)/8\pi$. In K' the combined particle and field energy is $cP'^0=mc^2+cP_e'^0$ where $m_ec^2\equiv\int d^3r\,E^{\parallel2}/8\pi$ is the longitudinal part of the field energy. At the frequency $kc+\Delta\omega_{kc}$ of the $q^2A'^2/2mc^2$ term, $\Delta(E'^2+B'^2)V/8\pi=kc\Delta\omega_{kc}A'^2/4\pi$ reduces to $\frac{1}{2}\hbar\Delta\omega_{kc}$ with the aid of (15). This photonlike term will be absorbed in the transverse part of $cP_e'^0$ as a frequency shift. In the laboratory frame K the covariant electromagnetic energy [15] is the zeroth component of the second rank stress tensor contracted with the four-volume's normal $(\gamma,\gamma\beta)$. This gives $\gamma^2\int d^3r(E^2+B^2-2\beta\cdot\mathbf{E}\times\mathbf{B})/8\pi$ where $\beta=\mathbf{p}_I/mc$. Since the magnetic field due to a moving charge is $\mathbf{B}=c\beta\times\mathbf{E}^\parallel$, the last term in brackets $-2B^2$ and the Coulomb energy γm_ec^2 becomes the ω_{nI} contribution to $\gamma^2\int d^3r(E^2-B^2)/8\pi$. The electromagnetic field energy density at ω_{kc} can be written as $(E'^2-B'^2+2B'^2)/8\pi$ where the $2B'^2$ term equals the energy density of the pure vacuum field since $E^2=B^2$ for $\omega=kc$. The terms $E'^2-B'^2$ form an invariant and again give $\gamma^2\int d^3r(E^2-B^2)/8\pi$ in K. But, for self-fields, time averaging results in $\int dt\int d^3r(E^2-B^2)/8\pi=\int dt\int d^3r(\rho\varphi-\mathbf{j}\cdot\mathbf{A}/c)/2$ after integration by parts [18]. Using $\mathbf{j}=q(\mathbf{p}_I-q\mathbf{A}/c)/m$ this energy can be seen to be $\langle\hat{H}_I\rangle$ except that the $\hat{H}_1$ contribution has acquired a factor $\frac{1}{2}$. In terms of the fields in the laboratory frame K both the Bohr and electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$ have transverse components.

The contributions to the interaction energy $\frac{1}{2}\hbar\Delta\omega_i$ will now be compared with $\langle\frac{1}{2}\hat{H}_1+\hat{H}_2+H_3\rangle$. For the Bohr modes the zero-order current fluctuations from (26b) combine with the first-order vector potential, the second term of (26a), to give the interaction energy. Taking the expectation value

$$\langle I,\text{vac}|-\frac{1}{2}\frac{Vq}{mc}(\hat{\mathbf{p}}'^{0nm}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}+\hat{\mathbf{p}}'^{0nm}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}^{\dagger}_{-\mathbf{k}\lambda})|I,\text{vac}\rangle$$
$$=\frac{\pi q^2 V}{m^2 kc}\left[-\frac{\mathbf{p}^{\perp Im}_{-\mathbf{k}}\cdot\mathbf{p}^{\perp mI}_{\mathbf{k}}}{kc+\omega_{mI}}-\frac{\mathbf{p}^{\perp Im}_{-\mathbf{k}}\cdot\mathbf{p}^{\perp mI}_{\mathbf{k}}}{kc-\omega_{mI}}\right]. \quad (27a)$$

For $\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}$ the order of the Fermion operators is reversed, and thus $\omega_{Im}=-\omega_{mI}$ is obtained. This is the $\mathbf{k}\lambda$ contribution to $\frac{1}{2}\hbar\Delta\omega_{mI}$, in agreement with (25b). For vacuum fluctuations the first term of (26a) and the last term of (26b) give for the energy in the $\omega_{\mathbf{k}c}$ mode

$$\langle I,\text{vac}|-\frac{1}{2}\frac{qV}{mc}\hat{\mathbf{p}}'^{nm}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}^{0\dagger}_{-\mathbf{k}\lambda}|I,\text{vac}\rangle$$
$$=\frac{1}{2\hbar}\left[\frac{qV}{mc}\right]^2 A^2_{\mathbf{k}}\sum_m\left[-\frac{\mathbf{p}^{\perp Im}_{\mathbf{k}}\cdot\mathbf{p}^{\perp mI}_{-\mathbf{k}}}{kc+\omega_{mI}}+\frac{\mathbf{p}^{\perp mI}_{\mathbf{k}}\cdot\mathbf{p}^{\perp Im}_{-\mathbf{k}}}{kc-\omega_{mI}}\right] \quad (27b)$$

consistent with (25a). The coefficient of the factor in brackets is the same in (27a) and (27b) after substitution of (15). The last term in (25a) multiplied by $\frac{1}{2}\hbar$ is $\langle\hat{H}_2\rangle$. The longitudinal part (25c) is the expectation value of $\frac{1}{2}\rho\varphi$.

The contributions of the vacuum fluctuations and the Bohr or radiation reaction modes to the expectation value of the interaction energy can be modified by the choice of ordering. If either $\langle\hat{\mathbf{p}}'^{nm}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}+\hat{\mathbf{p}}'^{mn}_{\mathbf{k}}\cdot\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}\rangle$ or $\langle\hat{\mathbf{A}}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{p}}'^{nm}_{-\mathbf{k}}+\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{p}}'^{mn}_{\mathbf{k}}\rangle$ is evaluated, then the result is the sum of (27a) and (27b). The vacuum fluctuation and radiation reaction contributions to the photon absorption or $(kc-\omega_{mI})^{-1}$ terms cancel, leaving equal photon emission or $(kc+\omega_{mI})^{-1}$ terms which add. For normal ordering $\langle\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{p}}'^{mn}_{\mathbf{k}}+\hat{\mathbf{p}}'^{nm}_{-\mathbf{k}}\cdot\hat{\mathbf{A}}_{\mathbf{k}\lambda}\rangle$ gives the same final result, but only the Bohr modes contribute with each giving $-(kc+\omega_{mI})^{-1}$ and there are no photon absorption terms. In the case of antinormal ordering, $\langle\hat{\mathbf{A}}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{p}}'^{mn}_{-\mathbf{k}}+\hat{\mathbf{p}}'^{nm}_{\mathbf{k}}\cdot\hat{\mathbf{A}}^{\dagger}_{\mathbf{k}\lambda}\rangle$ gives $2(kc-\omega_{mI})^{-1}$ and $-2(kc+\omega_{mI})^{-1}$ due to vacuum fluctuations, with an additional $-2(kc-\omega_{mI})^{-1}$ from the Bohr modes. Thus the net result is again the sum of (27a) and (27b) and it is due entirely to vacuum fluctuations. However, the radiation reaction modes were necessary to cancel the photon absorption terms. This is consistent with conclusions reached previously [2,3,16,17].

V. DISCUSSION

The generality of the Casimir force expression $\Delta E=\frac{1}{2}\hbar\sum_i\Delta\omega_i$ is perhaps surprising and the physics underlying it will now be examined. For an electromagnetic mode, $\frac{1}{2}\hbar\Delta\omega_{kc}$ is just the change in its zero-point energy that results from the presence of the particle. In the case of the Bohr modes there is no zero-point energy $\frac{1}{2}\hbar\omega_{nI}$ and a less direct explanation must be sought. Charge-density fluctuations with wave vector $\mathbf{k}$ can be attributed to a charge making virtual transitions between states $|I\rangle$ and $|n\rangle$. It has an associated energy $2E_C=\int d^3r\,\rho\varphi$ giving it an excess energy of $E_n-E_I+2E_C$. Thus the Bohr frequency ω_{nI} is shifted upward by $2E_C/\hbar$. The Coulomb self-energy can thus be attributed to this frequency shift and equals $\frac{1}{2}\hbar\Delta\omega_{nI}$. It leads to the radiation reaction when moving particles are viewed from the laboratory frame where the fields acquire transverse components.

There is a close mathematical connection between frequency shifts and the fluctuation-dissipation relation as discussed in Ref. [5]. There the potential in the presence of matter due to an external potential $\mathbf{A}^a$ was written as $\mathbf{A}=\chi(\omega)\mathbf{A}^a$ where $\chi=C(\omega-\omega_i)^{-1}=C[P(\omega-\omega_i)^{-1}+i\pi\delta(\omega-\omega_i)]$. The susceptibility χ is inversely proportional to the complex dielectric constant or conductivity. The self-consistency condition is $\chi=1$, since this means that the applied field and the field in the presence of the particle are the same. The frequency shift is then $\Delta\omega_i=C$ while the fluctuation-dissipation relation requires that $\hbar\int d\omega\,\text{Im}\chi(\omega)/2\pi=\frac{1}{2}\hbar C$ equal the field energy. The calculation of frequency shifts and the use of $\Delta E=\frac{1}{2}\hbar\Delta\omega$ is thus equivalent to the fluctuation-dissipation theorem.

In the present derivation, $\hat{\mathbf{j}}=\psi^*(q\hat{\mathbf{v}})\psi$ is not the primary current source for the Bohr modes that give the radiation reaction. It would require that $\psi^*\psi=\delta(\mathbf{r}-\mathbf{r}_1)$ and this is not the probability density for a free charge or an electron bound to a nucleus. As a consequence of working in the Heisenberg picture, the operator equations have exactly the form of the classical equations and the source is a point charge as it is classically. Equations (25b) and (25c) come from the field of a point charge as they must in the semiclassical version of the present theory [4]. Most semiclassical calculations have been based on the original Schrödinger interpretation of the wave function [19], but this does not give agreement with experiment. The point charge interpretation might help to explain the controversial [20] $\psi=\sum_n|n\rangle e^{-iE_nt/\hbar}$ expansion used in the self-field formulation of Barut and co-workers. Their expression for the Lamb shift is the relativistic extension of (27a) and can be interpreted as the energy in the field of a point charge expressed in terms of the current correlation function.

As a result of fluctuations at the Bohr frequencies the particle radiates electromagnetic energy as it must classically. This is balanced, say for a system in its ground state, by absorption from the field. The rate of energy emission will equal the rate of absorption only if the fields have the amplitudes that are deduced from QED. There is a balance between self-reaction and vacuum fluctuations implied by the dispersion force formalism. As discussed in Ref. [5], it is the interplay of these two sets of modes that gives an imaginary component to the frequency shifts in the case of a particle that is not in its ground state. The same conclusion is reached here based on a second quantized formalism, since the equation for the frequencies is essentially the same. It is not necessary to invoke the $i\varepsilon$ prescription to describe emission by a system in an excited state, since imaginary frequency shifts arise naturally in the dispersion force formalism. Emission of electromagnetic radiation by a particle in its ground state is exactly canceled by absorption due to the electromagnetic modes. For a particle that can make a transition to a lower-energy state, these terms add and a photon can be emitted.

Equal contributions from the electromagnetic and Bohr modes to emission are also a feature of the master-equation approach of Cohen-Tannoudji and co-workers [3,7]. They obtain this result by requiring that the separation into electromagnetic and Bohr modes be Hermitian so that they are observables. Fain also came to the conclusion that the vacuum fluctuation and radiation-reaction modes contribute equally [15]. The order of operators can modify the role of the electromagnetic and Bohr modes if the source terms are normally or antinormally ordered by separation of the electric field into its positive and negative frequency parts [2]. However, if the particle and field operators are to commute to a given order, then both these terms must be present in the field and current density operators and in the field modes themselves [8,9]. The electromagnetic and Bohr modes are found to make equal contributions in the present calculation, but by a different argument. In the dispersion force formalism, the frequencies of both modes are shifted as would be the case for classical oscillators and thus both contribute to the interaction energy or to emission.

In summary, I have demonstrated that it is possible to find an approximate self-consistent solution of the second quantized particle and field Heisenberg equations. The equation for the allowed frequencies is the same as that previously derived semiclassically [4]. The solutions are the electromagnetic and Bohr frequencies, but both are shifted in relation to their values in the absence of particle-field coupling. The Bohr or radiation-reaction modes are a consequence of the point nature of the particle. The present derivation based on self-consistency uses a formalism developed for Casimir-force calculations. Within this framework it is independently concluded that electromagnetic and Bohr modes make equally significant contributions to spontaneous emission and to the Lamb shift energy.

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