acta physica slovaca vol. 49 No. 4, 579 – 583 **August 1999**

QUANTUM ELECTROMAGNETIC FIELDS IN THE NEIGHBOURHOOD OF AN ATOM*

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Received 21 April 1999, accepted 10 May 1999

Non-relativistic quantum electrodynamics is used to find the Heisenberg electric and magnetic field operators when a single atom perturbs the vacuum. The expectation values of these fields for particular quantum states are found, and the differences associated with the choice between minimal and multipolar coupling are discussed. The effect of these fields on nearby atoms is shown to give Casimir potentials. Finally an extension of the theory to allow for Roentgen currents- the source of which being moving dipoles- is made.

PACS: 42.50.Ct, 32.80.-t, 41.20.-q

Quantum Optics is mostly used with the concept of 'photon' taken as basic to the subject [1]. However this is a derived concept as the essential quantity in electrodynamics is the electromagnetic field. In fact the construct of a photon is ambiguous [2] (unlike that for the field). To show this ambiguity we consider the two alternative formalisms often used to give the dynamical equations in non-relativistic quantum electrodynamics of which quantum optics is a part. For an elementary discussion we remain within the electric dipole approximation throughout: extension to higher multipoles is not difficult but technical. Furthermore to begin we consider the interaction of the field with a single atom/molecule. As is well known [3] the generator that transforms the minimal coupling formalism to the multipolar one is $\exp(iS)$ with

$$S = \frac{1}{\hbar c}\boldsymbol{\mu}\cdot\mathbf{a}\left(\mathbf{R}\right), \tag{1}$$

where $\boldsymbol{\mu}$ is the electric dipole operator for the atom and $\mathbf{a}\left(\mathbf{R}\right)$ is the vector potential (Coulomb gauge used and thus $\mathbf{a}\left(\mathbf{R}\right)$ is transverse) at the atomic position $\mathbf{R}$. The photon is introduced into the theory through the expansion of the field operators such as

$$\mathbf{a}\left(\mathbf{r}\right) = \sum_{\boldsymbol{k},\lambda}\sqrt{\frac{2\pi\hbar c}{kV}}\left(\mathbf{e}(\lambda)\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}a_{\boldsymbol{k},\lambda} + \bar{\mathbf{e}}(\lambda)\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\dagger}_{\boldsymbol{k},\lambda}\right), \tag{2}$$

*Presented at the 6th Central-European Workshop on Quantum Optics, Château Chudobín, Czech Republic, April 30 - May 3, 1999.

with $a_{\boldsymbol{k},\lambda}$ and $a^{\dagger}_{\boldsymbol{k},\lambda}$ being annihilation and creation operators obeying

$$\left[a_{\boldsymbol{k},\lambda}, a^{\dagger}_{\boldsymbol{k}',\lambda'}\right] = \delta_{\boldsymbol{k},\boldsymbol{k}'}\ \delta_{\lambda\lambda'}\ .$$

It is straightforward to calculate the new a under the transformation (1)

$$a^{\mathrm{NEW}} = \mathrm{e}^{iS} a\, \mathrm{e}^{-iS} = a + i\,[S,a] = a - i\left(\frac{2\pi}{\hbar c k V}\right)^{1/2} \boldsymbol{\mu}\cdot\bar{\mathbf{e}}\ \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\,. \tag{3}$$

To keep track in the context of our present paper we will give labels to the two a 's, the a on the RHS of (3) to be a^{MIN} and $a^{\mathrm{NEW}} = a^{\mathrm{MULT}}$. So

$$a^{\mathrm{MULT}} = a^{\mathrm{MIN}} - i\left(\frac{2\pi}{\hbar c k V}\right)^{1/2} \boldsymbol{\mu}\cdot\bar{\mathbf{e}}\ \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\,,$$

$$a^{\dagger\mathrm{MULT}} = a^{\dagger\mathrm{MIN}} + i\left(\frac{2\pi}{\hbar c k V}\right)^{1/2} \boldsymbol{\mu}\cdot\mathbf{e}\ \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}\,. \tag{4}$$

Straightaway we see that creating a minimal photon is different from creating a multipolar photon. The state $a^{\dagger\mathrm{MULT}}\,|\mathrm{atom};\mathrm{vac}\rangle$ is not the same as $a^{\dagger\mathrm{MIN}}\,|\mathrm{atom};\mathrm{vac}\rangle$. Also the time developments of these operators within the Heisenberg picture are different. The Hamiltonians for the two formalisms are

$$H^{\mathrm{MULT}} = H^{\mathrm{ATOM}} + H^{\mathrm{RAD}} - \boldsymbol{\mu}\cdot\mathbf{d}\,(\mathbf{R}) \tag{5}$$

and

$$H^{\mathrm{MIN}} = H^{\mathrm{ATOM}} + H^{\mathrm{RAD}} + \frac{e}{mc}\mathbf{p}\cdot\mathbf{a}\,(\mathbf{R}) + \frac{e^2}{2mc^2}\mathbf{a}^{\mathbf{2}}(\mathbf{R})\,, \tag{6}$$

so that

$$\dot{a}^{\mathrm{MULT}}(t) = -i\omega\, a^{MULT}(t) + \sqrt{\frac{2\pi c k}{\hbar V}}\boldsymbol{\mu}(t)\cdot\bar{\mathbf{e}} \tag{7}$$

and

$$\dot{a}^{\mathrm{MIN}}(t) = -i\omega\, a^{\mathrm{MIN}}(t) - i\sqrt{\frac{2\pi c}{\hbar\, k V}}\frac{e}{mc}(\mathbf{p}(t) + e\mathbf{a}(t)/c)\cdot\bar{\mathbf{e}}\,. \tag{8}$$

Thus

$$a^{\mathrm{MULT}}(t) = a^{\mathrm{MULT}}(0)\mathrm{e}^{-i\omega t} + \sqrt{\frac{2\pi c k}{\hbar V}}\mathrm{e}^{-i\omega t}\int_0^t \mathrm{d}t'\ \boldsymbol{\mu}(t')\cdot\bar{\mathbf{e}}\ \mathrm{e}^{i\omega t'} \tag{9}$$

and

$$a^{\mathrm{MIN}}(t) = a^{\mathrm{MIN}}(0)\mathrm{e}^{-i\omega t} - i\sqrt{\frac{2\pi c}{\hbar\, k V}}\mathrm{e}^{-i\omega t}\int_0^t \mathrm{d}t'\ \frac{e}{mc}(\mathbf{p}(t') + e\mathbf{a}(t')/c)\cdot\bar{\mathbf{e}}\ \mathrm{e}^{i\omega t'}\,. \tag{10}$$

It is now obvious that asking a question such as the time development of the number of photons is ambiguous, since $a^{\dagger\mathrm{MULT}}(t)a^{\mathrm{MULT}}(t)$ and $a^{\dagger\mathrm{MIN}}(t)a^{\mathrm{MIN}}(t)$ are not equal. This leads to different predictions for such properties as the line shape in the emission of radiation from an excited atom.

In contrast to the photon operators the electromagnetic field operators have less ambiguity. Since the vector potential commutes with the generator $\exp(iS)$ it is unchanged by the transformation and so is the magnetic field. On the other hand the transverse electric field operator does change. We have

$$\begin{aligned}\mathbf{e}^{\perp}(\mathbf{r}) &= \sum i\sqrt{\frac{2\pi\hbar ck}{V}}(\mathbf{e}\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\mathrm{MIN}} - \bar{\mathbf{e}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\dagger\mathrm{MIN}}) \\ &= \sum i\sqrt{\frac{2\pi\hbar ck}{V}}(\mathbf{e}\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\mathrm{MULT}} - \bar{\mathbf{e}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\dagger\mathrm{MULT}}) \\ &\quad - \left(\sum_{\boldsymbol{k},\lambda}\frac{2\pi}{V}\mathbf{e}\bar{\mathbf{e}}_j\mu_j\mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R})} + h.c.\right) \end{aligned} \tag{11}$$

and, recognising the second term on the RHS of (11) to be 4π times the transverse polarization $\mathbf{p}^{\perp}(\mathbf{r})$ for a point dipole at $\mathbf{R}$, the multipolar sum on the RHS of (11) is

$$\sum i\sqrt{\frac{2\pi\hbar ck}{V}}(\mathbf{e}\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\mathrm{MULT}} - \bar{\mathbf{e}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\dagger\mathrm{MULT}}) = \mathbf{e}^{\perp}(\mathbf{r}) + 4\pi\mathbf{p}^{\perp}(\mathbf{r}) = \mathbf{d}(\mathbf{r})\,. \tag{12}$$

We can, unambiguously, ask and answer questions as to the time dependence of the fields in the neighbourhood of an atom as long as we distinguish the electric field from Maxwell's displacement field.

The multipolar formalism is the easier to work with to find the time dependence of the fields in the Heisenberg picture and thence to calculate the probabilities for specific processes. If (9) is inserted into

$$\mathbf{d}(\mathbf{r},t) = \sum i\sqrt{\frac{2\pi\hbar ck}{V}}(\mathbf{e}\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\mathrm{MULT}}(t) - \bar{\mathbf{e}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}a^{\dagger\mathrm{MULT}}(t)) \tag{13}$$

we find

$$\mathbf{d}(\mathbf{r},t) = \mathbf{d}^{(0)}(\mathbf{r},t) + \mathbf{d}^{(s)}(\mathbf{r},t)\,, \tag{14}$$

with $\mathbf{d}^{(0)}(\mathbf{r},t)$ the free-field and the source field $\mathbf{d}^{(s)}(\mathbf{r},t)$ given by

$$d_i^{(s)}(\mathbf{r},t) = \begin{cases} (-\nabla^2\delta_{ij} + \nabla_i\nabla_j)\dfrac{\mu_j(t-r/c)}{r} & \text{for } t > r/c \\ 0 & \text{for } t < r/c \end{cases}, \tag{15}$$

where we have, for simplicity, assumed the source dipole is at the origin. An analogous calculation within the minimal coupling formalism gives

$$e_i^{\perp}(\mathbf{r},t) = e_i^{\perp(0)}(\mathbf{r},t) + \begin{cases} (-\nabla^2\delta_{ij} + \nabla_i\nabla_j)\dfrac{\mu_j(t-r/c)-\mu_j(t)}{r} & \text{for } t > r/c \\ (-\nabla^2\delta_{ij} + \nabla_i\nabla_j)\dfrac{\mu_j(0)-\mu_j(t)}{r} & \text{for } t < r/c \end{cases} \quad (16)$$

Note the clear causal behaviour within the multipolar formalism compared with the minimal case. Staying within the multipolar description we examine the electric energy density at field point $\mathbf{r}$ at time t, it is

$$\mathbf{d}^2(\mathbf{r},t)/8\pi = ((\mathbf{d}^{(0)}(\mathbf{r},t) + \mathbf{d}^{(s)}(\mathbf{r},t))^2/8\pi. \quad (17)$$

We now ask what is the expectation value of this energy density for an atom in state $|p\rangle$, and the radiation in its vacuum state. Except for the zero-point energy density $\langle \mathbf{d}^{(0)2}(\mathbf{r},t)/8\pi\rangle$ it is [4] for $t > r/c$, and to the order of the squares of the transition matrix elements,

$$\begin{aligned} &\frac{1}{4\pi}\sum_{n,E_n<E_p} \mu_i^{pn}\mu_j^{np}k_{pn}^6 f_{ik}(k_{pn}r)\,\bar{f}_{jk}(k_{pn}r) \\ &+\frac{1}{4\pi^2}\sum_{all\ n} \mu_i^{pn}\mu_j^{np}k_{pn}\int_0^\infty \mathrm{d}u\, f_{ik}(iur)\,\bar{f}_{jk}(iur)\,\frac{u^6}{u^2+k_{pn}^2}\mathrm{e}^{-2\mu r}\,, \end{aligned} \quad (18)$$

with

$$f_{ik}(kr) = -(\delta_{ik} - \hat{\mathbf{r}}_i\hat{\mathbf{r}}_k)\frac{1}{kr} + (\delta_{ik} - 3\hat{\mathbf{r}}_i\hat{\mathbf{r}}_k)\left(\frac{-i}{k^2r^2} + \frac{1}{k^3r^3}\right). \quad (19)$$

If $|p\rangle$ is the ground state the second term in (18) is the only contribution and, when evaluated, gives the electrical energy density

$$\begin{aligned} \frac{\mathbf{d}^2(\mathbf{r},t>r/c)}{8\pi} &= H^{\mathrm{elec}}(r) \\ &= \frac{\hbar c}{4\pi^2}\int_0^\infty \mathrm{d}u\,\sum_n \frac{2k_{no}\mu_{no}^2}{3\hbar c(u^2+k_{no}^2)}\left(\frac{1}{u^2r^2}+\frac{2}{u^3r^3}+\frac{5}{u^4r^4}\right. \\ &\qquad \left. +\frac{6}{u^5r^5}+\frac{3}{u^6r^6}\right)u^6\mathrm{e}^{-2\mathrm{u}r} \end{aligned} \quad (20)$$

which in terms of the polarizability of the source dipole $\alpha^{(s)}$ is

$$= \frac{\hbar c}{4\pi^2}\int_0^\infty \mathrm{d}u\,\alpha^{\mathrm{source}}(iu)\left(\frac{1}{u^2r^2}+\frac{2}{u^3r^3}+\frac{5}{u^4r^4}+\frac{6}{u^5r^5}+\frac{3}{u^6r^6}\right)u^6\mathrm{e}^{-2ur}\,. \quad (21)$$

Furthermore if a second *test* atom with polarizability α^{test} is placed at $\mathbf{r}$ the energy shift is $-\frac{1}{2}\alpha^{\mathrm{test}}\mathbf{d}^2(\mathbf{r})$ which, with equation (21) for the energy density, leads to exactly the Casimir-Polder potential [5].

If on the other hand $|p\rangle$ is an excited state the dominant term in (18) for large r is the first and is

$$\frac{2}{3}\sum_{\substack{\text{states n}\\ \text{below p}}}\mu_{pn}^2 k_{pn}^4 \frac{1}{4\pi r^2} \tag{22}$$

which corresponds to real energy emission. The rate of total energy flow, out of a sphere with radius r, is $\sum_{\substack{\text{states n}\\ \text{below p}}} A_{pn}(\hbar c k_{pn})$, with A_{pn} the Einstein A-coefficients.

In the above theory the atom was considered fixed. Recent studies of translational effects make it important to extend the theory to include the motion of the atom. This introduces the Roentgen current as an additional source for the electromagnetic field. We illustrate the consequence of this by showing how the familiar field of a fixed point dipole is generalized when the motion of the atomic centre is taken into account. If we express the field (15) to the first power of the transition moments we find, with $\boldsymbol{\rho} = \mathbf{r} - \mathbf{R}$ and $\rho > r/c$, that the i-th component of the field of a fixed ($\dot{\boldsymbol{\rho}} = 0$) dipole is the familiar

$$\mu_j \frac{\delta_{ij} - 3\hat{\boldsymbol{\rho}}_i\hat{\boldsymbol{\rho}}_j}{\rho^3} + \frac{\mathrm{d}}{c\mathrm{d}t}\mu_j \frac{\delta_{ij} - 3\hat{\boldsymbol{\rho}}_i\hat{\boldsymbol{\rho}}_j}{\rho^2} + \frac{\mathrm{d}^2}{c^2\mathrm{d}t^2}\mu_j \frac{\delta_{ij} - \hat{\boldsymbol{\rho}}_i\hat{\rho}_j}{\rho}\,. \tag{23}$$

On the other hand if the atom moves, so that $\dot{\boldsymbol{\rho}} = -\dot{\mathbf{R}}$, we find, a new result, that the i-th component of the field is

$$\begin{aligned}&\mu_j \frac{\delta_{ij} - 3\hat{\boldsymbol{\rho}}_i\hat{\boldsymbol{\rho}}_j}{\rho^3}\frac{1}{1+\dot{\rho}/c} + \frac{\mathrm{d}}{c\mathrm{d}t}\mu_j \frac{\delta_{ij} - 3\hat{\boldsymbol{\rho}}_i\hat{\boldsymbol{\rho}}_j}{\rho^2}\frac{1}{1+\dot{\rho}/c} + \frac{\mathrm{d}^2}{c^2\mathrm{d}t^2}\mu_j \frac{\delta_{ij} - \hat{\boldsymbol{\rho}}_i\hat{\rho}_j}{\rho}\frac{1}{1+\dot{\rho}/c}\\ &+\frac{\mathrm{d}}{c^2\mathrm{d}t}(\mu_j\dot{R}_i - \mu_i\dot{R}_j)\frac{\hat{\boldsymbol{\rho}}_j}{\rho^2}\frac{1}{1+\dot{\rho}/c} + \frac{\mathrm{d}^2}{c^3\mathrm{d}t^2}(\mu_j\dot{R}_i - \mu_i\dot{R}_j)\frac{\hat{\boldsymbol{\rho}}_j}{\rho}\frac{1}{1+\dot{\rho}/c}\,,\end{aligned} \tag{24}$$

where the time derivatives act on all the variables $\boldsymbol{\mu}$, $\boldsymbol{\rho}$ and $\mathbf{R}$.

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