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Vacuum Self-Dressing of an Atom and Its Physical Effects

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Abstract: We consider a multilevel atom such as an hydrogen atom, interacting with the quantum electromagnetic field, in the dressed ground state of the interacting system. We evaluate by perturbation theory the dressed ground state of the system, within dipole approximation; we investigate and review the effect of the self-dressing of the atom on several field and atomic observables. Specifically, we obtain general expressions of the renormalized electric and magnetic field fluctuations and energy densities around the atom, and analyze their scaling with the distance from the atom, obtaining approximated expressions in the so-called near and far zone. We also investigate nonlocal spatial field correlations around the atom. We stress how the quantities we evaluate can be probed through two- and three-body nonadditive Casimir-Polder dispersion interactions. We also investigate the effect of the self-dressing, i.e. of the virtual transitions occurring in the dressed ground state, on atomic observables, for example the average potential energy of the electron in the nuclear field; this also allows us to obtain a more fundamental quantum basis for the Welton interpretation of the Lamb shift of a ground-state hydrogen atom, in terms of the atomic self-dressing processes.

Keywords: vacuum fluctuations; dressed atoms; Casimir-Polder forces; virtual photons

1. Introduction

In quantum field theory, any field source, a charged particle or an atom, for example, is surrounded by a cloud of virtual quanta and particles that are continuously emitted and reabsorbed by the source, according to the time-energy uncertainty relation [1–6]. This situation is commonly described in terms of a cloud of virtual particles surrounding the field source, that thus becomes a quite complex and spatially extended object called a *dressed source*. This research field, in the framework of nonrelativistic quantum electrodynamics, has been for many years one of the main research subjects of Prof. Francesco Saverio Persico, to whose memory this article is dedicated, and whose research activity has significantly contributed to its development.

The spatial structure of the virtual quanta cloud reflects the physical properties of the source, for example its energy level structure and its size [7]. In general, the virtual particle cloud dressing the source contributes to its mass and charge, and, according to the renormalization procedure, this contribution (or part of it) is eventually absorbed in the observable mass and charge of the source. This is very clear and well defined in a stationary condition or in a scattering matrix approach, where noninteracting asymptotically states in time, that is for $t \to \pm\infty$, are considered. In such cases, fully dressed states are used in the interaction process between asymptotic times in the past and in the future, and the interaction Hamiltonian responsible for a transition acts only for a finite time interval. However, the situation in not at all sharply defined for persistent interactions, acting at all times [8–10]. This is a quite important and fundamental point, deeply related to the very definition of a particle as an elementary object, or of any other system interacting with a quantum field (in particular when a continuous spectrum is involved), as fundamental object [11]. Specifically, it is related to the difficulty in defining a dressed (unstable) excited state [10,12–16]. Furthermore, when a time-dependent approach is used, and the time evolution of the dressing particle cloud of the field

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source between finite times is considered, bare or partially dressed states are involved [17–20]. This kind of problems is also deeply related to the fundamental question of how a (closed) physical system, initially in a nonequilibrium state, settles at long times to an equilibrium condition (local or global), also in view of the unitary time evolution of a closed quantum system [7,21].

We will investigate and review some of such fundamental questions of quantum field theory in the framework of nonrelativistic quantum electrodynamics, specifically a multilevel nonrelativistic atom interacting with the quantum radiation field in the Coulomb gauge. In this case, (virtual) photons are the only particle type surrounding the field source in its ground state. We will analyze in detail how this virtual photon cloud affects field and atomic observables, specifically electric and magnetic field fluctuations (or equivalently energy densities) as well as its spatial correlations, and electron-nucleus average distance and potential energy, respectively. Specifically, we will obtain explicit expressions of the spatial dependence of electric and magnetic field fluctuations in the dressed ground state at any distance from the atom outside the atom, as well as dressed spatial field correlations. We will also evaluate the change of the average electron-nucleus distance (and of arbitrary powers of this distance) due to the virtual processes occurring in the dressed ground state, as well as the average electron-nucleus potential energy. We will also discuss in detail the relation of these effects with observable phenomena such as intermolecular Casimir-Polder forces and atomic level shifts.

This paper is organized as follows. In section 2 we introduce our Hamiltonian model, both in the minimal and in the multipolar coupling scheme in the dipole approximation, and obtain the dressed ground state of a multilevel atom interacting with the quantum radiation field by perturbation thery. In section 3 we will evaluate electric and magnetic field fluctuations, as well as spatial field correlations, around the atom; we also discuss the relation of our results with Casimir-Polder dispersion interactions. In section 4 we explicitly show that the virtual processes occurring in the dressed ground state of the atom determine an increase of the average electron-nucleus distance and a change of the average electron-nucleus potential energy, and discuss the relation of this finding with the ground-state Lamb shift of the atom and its physical origin. Finally, section 5 is devoted to our conclusive remarks.

2. Stationary Dressed States in Nonrelativistic Quantum Electrodynamics

The physical system we consider in this section is an atom or a molecule interacting with the quantized electromagnetic field, in the nonrelativistic regime; a boundary such a reflecting or dielectric plate can be eventually present and its presence is mathematically described by the appropriate mode functions of the field operators. In the Coulomb gauge, $\nabla \cdot \mathbf{A}(\mathbf{r}) = 0$, the system is described by the Hamiltonian $H = H_0 + H_I$, where the unperturbed Hamiltonian $H_0 = H_A + H_F$ is the sum of the atomic Hamiltonian, $H_A = \sum_n E_n |\phi_n\rangle|\phi_n|$ (E_n and $|\phi_n\rangle$ are respectively the energy and the state vector of a complete set of atomic energy eigenstates), and the field Hamiltonian, $H_F = \sum_{\mathbf{k}\lambda} \hbar\omega_k a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}$ ($\mathbf{k}$ and $\lambda = 1,2$ are respectively the wavevector and the polarization of the field modes), where $a_{\mathbf{k}\lambda}$ and $a^\dagger_{\mathbf{k}\lambda}$ denote respectively the annihilation and creation operators of the field modes obeying the usual bosonic commutation rules, and the dispersion relation $\omega_k = c|\mathbf{k}|$ holds. H_I is the atom-field interaction Hamiltonian, that can be expressed in the minimal coupling scheme or in the multipolar coupling scheme, as discussed below. The expressions of the electromagnetic field operators are (we use Gauss units) [3,22,23]

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k}\lambda}\Big(\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r})a_{\mathbf{k}\lambda} + \mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r})a^\dagger_{\mathbf{k}\lambda}\Big), \tag{1}$$

$$\mathbf{E}_\perp(\mathbf{r},t) = -\frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} = \sum_{\mathbf{k}\lambda}\Big(\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})a_{\mathbf{k}\lambda} + \mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r})a^\dagger_{\mathbf{k}\lambda}\Big), \tag{2}$$

$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k}\lambda}\Big(\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r})a_{\mathbf{k}\lambda} + \mathbf{g}^*_{\mathbf{k}\lambda}(\mathbf{r})a^\dagger_{\mathbf{k}\lambda}\Big), \tag{3}$$

where the time dependence is included in the annihilation and creation operators (we often omit to explicitly indicate the time dependence of the operators). $\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r})$ are the mode functions for the

 doi:10.20944/preprints202503.1700.v1

vector potential taking into account the boundary conditions present; also, $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) = i\omega_k \mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r})/c$ and $\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r}) = \nabla \times \mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r})$ are the mode functions for the electric and magnetic field, respectively, and $\omega_k = c|\mathbf{k}|$ is the dispersion relation for the photons.

The minimal and multipolar coupling schemes mentioned above are related by a unitary transformation, the so-called Power-Zienau-Wolley transformation [24–31]. The two complete Hamiltonians are unitary related and thus equivalent, while, separately, their unperturbed and interaction parts are not unitary related to each other; thus, the separation of the Hamiltonian in its noninteracting and interacting parts in the two schemes is not connected by a unitary transformation. As it is known, this creates still unsolved problems in determining the lineshape of the photon emitted by spontaneous emission, because the initial state is usually taken as an eingenstate of the unperturbed Hamiltonian: thus the initial state is a different physical state according to the coupling scheme used [10,32–37]. Gauge ambiguities can be present also when a truncated atomic basis is used in ultra-strong coupling in cavity quantum electrodynamics [38]. In our case, however, there is not any problem of this kind because we consider a dressed ground state, which is an eigenstate of the total Hamiltonian, and, thus, we can safely use the minimal or multipolar coupling Hamiltonian, according to which coupling scheme is more convenient for making simpler specific calculations (in fact, in Sec. 3 we will use the multipolar coupling Hamiltonian while in Sec. 4 we will use the minimal coupling Hamiltonian, in both cases within the dipole approximation).

The minimal coupling interaction Hamiltonian, for a single atom located at position $\mathbf{r}_A$ and in the dipole approximation, is

$$H_I^m = -\frac{e}{mc}\mathbf{p}\cdot\mathbf{A}(\mathbf{r}_A) + \frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r}_A) \tag{4}$$

(as mentioned before, we omit the explicit time dependence of the operators). As discussed above, the multipolar coupling interaction Hamiltonian is obtained from the minimal coupling one through the Power-Zienau-Wolley unitary transformation, and in the dipole approximation it takes the following form

$$H_I^M = -\boldsymbol{\mu}\cdot\mathbf{D}_\perp(\mathbf{r}_A) = -\sum_{mn}\sum_{\mathbf{k}\lambda}\boldsymbol{\mu}^{mn}\cdot\left(a_{\mathbf{k}\lambda}\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}_A) + a^\dagger_{\mathbf{k}\lambda}\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)\right)|\phi_n\rangle\langle\phi_m|, \tag{5}$$

where $\boldsymbol{\mu} = e\mathbf{r}$ is the atomic electric dipole moment operator and $\boldsymbol{\mu}^{mn} = \langle\phi_m|\boldsymbol{\mu}|\phi_n\rangle$ its matrix elements between atomic states $|\phi_m\rangle$ and $|\phi_n\rangle$ with energy E_m and E_n respectively, $\mathbf{D}_\perp(\mathbf{r}_A)$ the transverse displacement field evaluated at the atomic position $\mathbf{r}_A$, $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})$ are the appropriate field mode functions according to the boundaries present, and $a_{\mathbf{k}\lambda}$, $a^\dagger_{\mathbf{k}\lambda}$ are the annihilation and creation operators in the multipolar coupling scheme, satisfying the usual bosonic commutation relations. The multipolar coupling interaction Hamiltonian also contains a second term of the form $2\pi\int d^3r\mathbf{P}^2_\perp(\mathbf{r})$, where $\mathbf{P}_\perp(\mathbf{r})$ is the transverse polarization field of the atom, that however is not relevant for the quantities we are going to evaluate and therefore we will neglect it. Outside the atoms, it is possible to show that $\mathbf{D}_\perp(\mathbf{r}) = \mathbf{E}(\mathbf{r}) = \mathbf{E}_\perp(\mathbf{r}) + \mathbf{E}_\parallel(\mathbf{r})$, and its mode expansion is in the same form of (2) [3,39]. This is the reason why in many cases when local field quantities are being considered, as in the next section, the multipolar coupling scheme is more convenient than the minimal coupling scheme, since the observable total electric field (longitudinal plus transverse) is directly involved.

Let us now consider the ground state of the full system. The bare state $|\phi_g, \{0_{\mathbf{k}\lambda}\}\rangle$, with the atom in its ground state $|\phi_g\rangle$ and the field in its vacuum state $|\{0_{\mathbf{k}\lambda}\}\rangle$, is an eigenstate of the free Hamiltonian H_0 but not of the total Hamiltonian H, because of the counter-rotating terms in the

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interaction Hamiltonian H_I. The true ground state can be obtained by stationary perturbation theory; up to the second order in the atom-radiation interaction we obtain

$$
\begin{aligned}
|\psi_g\rangle = &\left(1-\frac{1}{2}\sum_m\sum_{\mathbf{k}\lambda}\frac{|\boldsymbol{\mu}^{gm}\cdot\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}_A)|^2}{(E_{mg}+\hbar\omega_k)^2}\right)|\phi_g,\{0_{\mathbf{k}\lambda}\}\rangle - \sum_m\sum_{\mathbf{k}\lambda}\frac{\boldsymbol{\mu}^{mg}\cdot\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)}{E_{mg}+\hbar\omega_k}|\phi_m,1_{\mathbf{k}\lambda}\rangle \\
&+\sum_{\ell m}\sum_{\mathbf{k}\lambda\mathbf{k}'\lambda}\frac{(\boldsymbol{\mu}^{m\ell}\cdot\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A))(\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A))}{(E_{\ell g}+\hbar\omega_{k'})(E_{mg}+\hbar\omega_k+\hbar\omega_{k'})}|\phi_m,1_{\mathbf{k}\lambda}1_{\mathbf{k}'\lambda'}\rangle \\
&+\sum_{\ell m(m\neq g)}\sum_{\mathbf{k}\lambda}\frac{(\boldsymbol{\mu}^{m\ell}\cdot\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}_A))(\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A))}{E_{mg}(E_{\ell g}+\hbar\omega_k)}|\phi_m,\{0_{\mathbf{k}\lambda}\}\rangle\,,
\end{aligned}
\tag{6}
$$

where the multipolar coupling Hamiltonian (5) has been used. Here, we have defined $E_{mn}=E_m-E_n$ and $\boldsymbol{\mu}^{mn}=\langle\phi_m|\boldsymbol{\mu}|\phi_n\rangle$. In Sec. 3 we will use the state (6) for calculating relevant field quantities, specifically electric and magnetic field fluctuations and spatial correlations of the electric field. In such cases, as already mentioned, the multipolar coupling scheme is more advantageous than the minimal coupling scheme, since outside the atom the transverse displacement field coincides with the complete (transverse plus longitudinal) electric field (on the contrary, the use of the minimal coupling interaction Hamiltonian (4) would require to add the longitudinal electrostatic term to the quantum transverse electric field [40], making the calculation more complicated).

We also give here the expression of the second-order dressed ground state obtained from the minimal coupling Hamiltonian (4) in the dipole approximation, that we will use in Sec. 4 to calculate atomic quantities in the dresses ground state,

$$
\begin{aligned}
|\tilde{\psi}_g\rangle = &\left(1-\frac{1}{2}\Big(\frac{e}{mc}\Big)^2\sum_m\sum_{\mathbf{k}\lambda}\frac{|\mathbf{p}^{gm}\cdot\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r}_A)|^2}{(E_{mg}+\hbar\omega_k)^2}\right)|\phi_g,\{0_{\mathbf{k}\lambda}\}\rangle \\
&+\frac{e}{mc}\sum_m\sum_{\mathbf{k}\lambda}\frac{\mathbf{p}^{mg}\cdot\mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)}{E_{mg}+\hbar\omega_k}|\phi_m,1_{\mathbf{k}\lambda}\rangle \\
&+\Big(\frac{e}{mc}\Big)^2\sum_{\ell m}\sum_{\mathbf{k}\lambda\mathbf{k}'\lambda}\frac{(\mathbf{p}^{m\ell}\cdot\mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r}_A))(\mathbf{p}^{\ell g}\cdot\mathbf{A}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A))}{(E_{\ell g}+\hbar\omega_{k'})(E_{mg}+\hbar\omega_k+\hbar\omega_{k'})}|\phi_m,1_{\mathbf{k}\lambda}1_{\mathbf{k}'\lambda'}\rangle \\
&+\Big(\frac{e}{mc}\Big)^2\sum_{\ell m(m\neq g)}\sum_{\mathbf{k}\lambda}\frac{(\mathbf{p}^{m\ell}\cdot\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r}_A))(\mathbf{p}^{\ell g}\cdot\mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r}_A))}{E_{mg}(E_{\ell g}+\hbar\omega_k)}|\phi_m,\{0_{\mathbf{k}\lambda}\}\rangle \\
&-\frac{e^2}{2mc^2}\sum_{\mathbf{k}\lambda\mathbf{k}'\lambda}\frac{\mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)\cdot\mathbf{A}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A)}{\hbar\omega_k+\hbar\omega_{k'}}|\phi_g,1_{\mathbf{k}\lambda}1_{\mathbf{k}'\lambda'}\rangle\,,
\end{aligned}
\tag{7}
$$

where the last term comes from the $\mathbf{A}^2(\mathbf{r}_A)$ term of the interaction Hamiltonian (4), treated at first order in perturbation theory being it already a second-order quantity.

Both expressions (6) and (7) clearly show that the interacting, i.e. dressed, ground state contains, at the second order in the atom-field coupling, admixtures of the bare ground state with states containing one or two (virtual) photons and atomic excitations. The virtual photons present are responsible of many observable effects, for example the Lamb shift [41] and the van der Waals and Casimir-Polder intermolecular interactions [5,42]. The sums over m and ℓ in Eqs. (6) and (7) are on a complete set of atomic states; due to the dipole approximation, however, only states for which $\boldsymbol{\mu}^{gm(\ell)}\neq 0$ and $\mathbf{p}^{gm(\ell)}\neq 0$ contribute.

The considerations above make very reasonable that the ground-state field fluctuations are modified by the presence of the atom with respect to those present in the bare ground state of the field, as well as relevant atomic quantities are modified by the interaction of the atom with the quantum electromagnetic field in the vacuum state.

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3. Electric and Magnetic Field Fluctuations Around a Ground-State Multilevel Atom

In this section we evaluate the average electric and magnetic field fluctuations around the atom using the multipolar coupling Hamiltonian. Apart a $1/(8\pi)$ factor they respectively coincide with the average electric and magnetic energy densities in the vacuum space around the atom in its dressed ground state (6). It is immediate to see that $\langle\psi_g|\mathbf{E}(\mathbf{r})|\psi_g\rangle = \langle\psi_g|\mathbf{B}(\mathbf{r})|\psi_g\rangle = 0$, so that the field fluctuations coincide with the corresponding averaged squared field operators. At the second order, using Eqs. (2,3,6) we find

$$\begin{aligned}\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle = &\sum_{\mathbf{k}\lambda}|\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})|^2 + 2\sum_{\ell}\sum_{\mathbf{k}\lambda\mathbf{k}'\lambda'}\left\{\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r})\cdot\mathbf{f}_{\mathbf{k}'\lambda'}(\mathbf{r})\frac{\left[\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A)\right]\left[\boldsymbol{\mu}^{g\ell}\cdot\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}_A)\right]}{(E_{\ell g}+\hbar\omega_{k'})(E_{\ell g}+\hbar\omega_k)}\right.\\ &\left.+\Re\left(2\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})\cdot\mathbf{f}_{\mathbf{k}'\lambda'}(\mathbf{r})\frac{\left[\boldsymbol{\mu}^{g\ell}\cdot\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)\right]\left[\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A)\right]}{(E_{\ell g}+\hbar\omega_{k'})(\hbar\omega_k+\hbar\omega_{k'})}\right)\right\},\end{aligned} \tag{8}$$

$$\begin{aligned}\langle\psi_g|B^2(\mathbf{r})|\psi_g\rangle = &\sum_{\mathbf{k}\lambda}|\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r})|^2 + 2\sum_{\ell}\sum_{\mathbf{k}\lambda\mathbf{k}'\lambda'}\left\{\mathbf{g}^*_{\mathbf{k}\lambda}(\mathbf{r})\cdot\mathbf{g}_{\mathbf{k}'\lambda'}(\mathbf{r})\frac{\left[\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A)\right]\left[\boldsymbol{\mu}^{g\ell}\cdot\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}_A)\right]}{(E_{\ell g}+\hbar\omega_{k'})(E_{\ell g}+\hbar\omega_k)}\right.\\ &\left.+\Re\left(2\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r})\cdot\mathbf{g}_{\mathbf{k}'\lambda'}(\mathbf{r})\frac{\left[\boldsymbol{\mu}^{g\ell}\cdot\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}_A)\right]\left[\boldsymbol{\mu}^{\ell g}\cdot\mathbf{f}^*_{\mathbf{k}'\lambda'}(\mathbf{r}_A)\right]}{(E_{\ell g}+\hbar\omega_{k'})(\hbar\omega_k+\hbar\omega_{k'})}\right)\right\},\end{aligned} \tag{9}$$

where $\Re$ stands for the real part.

The expressions above are general, valid for any multilevel atomic system within dipole approximation and in the presence of generic perfectly conducting boundaries, provided the appropriate mode functions $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})$ and $\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r})$ are used.

We now specialize to the unbounded vacuum space. In this case, the mode functions are

$$\begin{aligned}\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r}) &= \left(\frac{2\pi\hbar c^2}{\omega_k V}\right)^{1/2}\hat{\mathbf{e}}_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}},\\ \mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) &= i\left(\frac{2\pi\hbar\omega_k}{V}\right)^{1/2}\hat{\mathbf{e}}_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}},\\ \mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r}) &= i\left(\frac{2\pi\hbar\omega_k}{V}\right)^{1/2}\hat{\mathbf{b}}_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}},\end{aligned} \tag{10}$$

where V is the quantization volume, $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$ are polarization unit vectors ($\lambda = 1,2$) with $\hat{\mathbf{k}}\cdot\hat{\mathbf{e}}_{\mathbf{k}\lambda} = 0$, here assumed real without any loss of generality, and $\hat{\mathbf{b}}_{\mathbf{k}\lambda} = \hat{\mathbf{k}}\times\hat{\mathbf{e}}_{\mathbf{k}\lambda}$.

The first terms in Eqs. (8) and (9) represent the bare zero-point position-independent term, present even in the absence of the atom; they are given by

$$\begin{aligned}\sum_{\mathbf{k}\lambda}|\mathbf{f}_{\mathbf{k}\lambda}|^2 &= \frac{2\pi\hbar}{V}\sum_{\mathbf{k}\lambda}\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{e}}_{\mathbf{k}\lambda}\omega_k = \frac{4\pi\hbar}{V}\sum_{\mathbf{k}}\omega_k = z.p.t.\ ,\\ \sum_{\mathbf{k}\lambda}|\mathbf{g}_{\mathbf{k}\lambda}|^2 &= \frac{2\pi\hbar}{V}\sum_{\mathbf{k}\lambda}\hat{\mathbf{b}}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{b}}_{\mathbf{k}\lambda}\omega_k = \frac{4\pi\hbar}{V}\sum_{\mathbf{k}}\omega_k = z.p.t.\ .\end{aligned} \tag{11}$$

Both of them, as it is well known, contain an ultraviolet divergence.

The other terms in the RHS of Eqs. (8,9) are the modification of the electric and magnetic field fluctuations, proportional to the electric and magnetic energy densities, related to the presence of the ground-state atom.

Using the mode functions (10) and the polarization sum rules (A1) of Appendix A, we obtain for the renormalized fluctuations, i.e. the fluctuations obtained after subtraction of the bare vacuum ones,

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$$\begin{aligned}\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r} &= \langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle - z.p.t.\\ &= 2\left(\frac{2\pi\hbar}{V}\right)^2\sum_\ell\sum_{\mathbf{k}\mathbf{k}'}\omega_k\omega_{k'}\left(\delta_{ps}-\hat{k}_p\hat{k}_s\right)\left(\delta_{qs}-\hat{k}'_q\hat{k}'_s\right)\mu_p^{g\ell}\mu_s^{\ell g}\\ &\times\left\{\frac{e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_A)})e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}_A)}}{(E_{\ell g}+\hbar\omega_{k'})(E_{\ell g}+\hbar\omega_k)}+\Re\left(\frac{2e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_A)})e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}_A)}}{(E_{\ell g}+\hbar\omega_{k'})(\hbar\omega_k+\hbar\omega_{k'})}\right)\right\},\end{aligned} \tag{12}$$

$$\begin{aligned}\langle\psi_g|B^2(\mathbf{r})|\psi_g\rangle_{\rm r} = \langle\psi_g|B^2(\mathbf{r})|\psi_g\rangle - z.p.t. = 2\left(\frac{2\pi\hbar}{V}\right)^2\sum_\ell\sum_{\mathbf{k}\mathbf{k}'}\omega_k\omega_{k'}\epsilon_{psu}\epsilon_{qsu}\hat{k}_u\hat{k}'_v\mu_p^{g\ell}\mu_q^{\ell g}\\ \times\left\{\frac{e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_A)})e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}_A)}}{(E_{\ell g}+\hbar\omega_{k'})(E_{\ell g}+\hbar\omega_k)}+\Re\left(\frac{2e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_A)})e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}_A)}}{(E_{\ell g}+\hbar\omega_{k'})(\hbar\omega_k+\hbar\omega_{k'})}\right)\right\},\end{aligned} \tag{13}$$

where ϵ_{mnl} is the Levi-Civita totally antisymmetric symbol and the Einstein convention of repeated symbols is used.

In the continuum limit, $\sum_{\mathbf{k}}\to V/(2\pi)^3\int_0^\infty dkk^2\int d\Omega_k$, setting $\mathbf{R}=\mathbf{r}-\mathbf{r}_A$ and performing the angular integrations exploiting the relations (A2,A3) of Appendix A, after some algebra we obtain

$$\begin{aligned}\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r} &= \frac{2}{\pi^2}\sum_\ell\mu_p^{g\ell}\mu_q^{\ell g}\left(\nabla^2\delta_{ps}-\nabla_p\nabla_s\right)^R\left(\nabla^2\delta_{sq}-\nabla_s\nabla_q\right)^{\bar{R}}\frac{1}{R\bar{R}}\\ &\times\int_0^\infty dk\int_0^\infty dk'\left[\frac{1}{(k_{\ell g}+k)(k_{\ell g}+k')}+\frac{2}{(k_{\ell g}+k')(k+k')}\right]\sin(kR)\sin(k'\bar{R})\Big|_{R=\bar{R}},\end{aligned} \tag{14}$$

$$\begin{aligned}\langle\psi_g|B^2(\mathbf{r})|\psi_g\rangle_{\rm r} &= \frac{2}{\pi^2}\epsilon_{psu}\epsilon_{qsv}\sum_\ell\mu_p^{g\ell}\mu_q^{\ell g}\nabla_u^R\nabla_v^{\bar{R}}\frac{1}{R\bar{R}}\\ &\times\int_0^\infty dk\int_0^\infty dk'kk'\left[\frac{1}{(k_{\ell g}+k)(k_{\ell g}+k')}-\frac{2}{(k_{\ell g}+k')(k+k')}\right]\sin(kR)\sin(k'\bar{R})\Big|_{R=\bar{R}},\end{aligned} \tag{15}$$

where $k_{\ell g}=E_{\ell g}/(\hbar c)$. In these expressions, two different variables R and $\bar{R}$ have been introduced and, after the derivatives have been taken, one must take $R=\bar{R}$.

Eqs. (14) and (15) are general and valid at any distance from the atom outside the atomic size, that is for distances sufficiently larger than the Bohr's radius a_0. In both equations, the contributions from the first term in the square bracket is factorized in k and k' and can be evaluated analytically, while the second term is not factorized. We give here approximated expressions valid in the so-called near- and far-zone. These two zones of space are defined with reference to the typical length scale in the problem given by $k_{\ell g}^{-1}$. In the multilevel case we are considering here, this lengthscale should be intended as an appropriate average of $k_{\ell g}^{-1}$ over all atomic states ℓ, similarly to what is done in the well known Bethe nonrelativistic calculation of the Lamb shift [22,43].

We start with the electric field fluctuations (14).

In the near zone, $R\ll k_{\ell g}^{-1}$, we can approximate $k\gg k_{\ell g}$: thus, $1/[(k_{\ell g}+k)(k_{\ell g}+k')]\simeq 1/(kk')$ and $1/[(k_{\ell g}+k')(k+k')]\simeq 1/[k'(k+k')]$. The double integral in the second term in the square brackets can be factorized by using the identity $\int_0^\infty du\exp(-u(k+k'))=(k+k')^{-1}$. After performing the integrals over k and k', we get

$$\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r} = \sum_\ell\mu_p^{g\ell}\mu_q^{\ell g}\left[\left(\nabla^2\delta_{ps}-\nabla_p\nabla_s\right)^R\frac{1}{R}\right]\left[\left(\nabla^2\delta_{sq}-\nabla_s\nabla_q\right)^{\bar{R}}\frac{1}{\bar{R}}\right]\Big|_{R=\bar{R}}. \tag{16}$$

After some algebra, using the relations given in Appendix A, we finally obtain

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$$\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r}=\sum_\ell \mu_p^{g\ell}\mu_q^{\ell g}\left(\delta_{pq}+3\hat{R}_p\hat{R}_q\right)\frac{1}{R^6}\,, \tag{17}$$

where $\hat{\mathbf{R}}=\mathbf{R}/R$ is the unit vector along the direction of $\mathbf{R}$. Our result (17) shows that in the near zone the renormalized electric field fluctuations scale as R^{-6}, and they are essentially given by the longitudinal field contribution (the transverse field contribution is negligible at short distances, as indeed expected) [40]. Both one- and two-photon components of the dressed ground state (6) contribute in this region.

In the far zone, $R\gg k_{\ell g}^{-1}$, we can approximate $k\ll k_{\ell g}$: thus, $1/[(k_{\ell g}+k)(k_{\ell g}+k')]\simeq 1/k_{\ell g}^2$ and $1/[(k_{\ell g}+k')(k+k')]\simeq 1/[k_{\ell g}(k+k')]$, and we obtain

$$\begin{aligned}\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r}=&\frac{2}{\pi^2}\sum_\ell \mu_p^{g\ell}\mu_q^{\ell g}\left(\nabla^2\delta_{ps}-\nabla_p\nabla_s\right)^R\left(\nabla^2\delta_{sq}-\nabla_s\nabla_q\right)^{\bar R}\frac{1}{R\bar R}\\&\times\int_0^\infty dk\int_0^\infty dk'\left[\frac{1}{k_{\ell g}^2}+\frac{2}{k_{\ell g}(k+k')}\right]\sin kR\sin k'\bar R\Big|_{R=\bar R}\,.\end{aligned} \tag{18}$$

The spatial dependence obtained from the two terms in the square bracket inside the k,k' integrals in the second row of (18) can be immediately obtained from a dimensional analysis, and they are as R^{-8} for the first term and as R^{-7} for the second one. In the far zone we can thus neglect the first term. After some algebra and using various relations given in Appendix A, we finally get

$$\langle\psi_g|E^2(\mathbf{r})|\psi_g\rangle_{\rm r}=\frac{1}{2\pi}\sum_\ell\frac{\mu_p^{g\ell}\mu_q^{\ell g}}{k_{\ell g}}\left(13\delta_{pq}+7\hat{R}_p\hat{R}_q\right)\frac{1}{R^7}\,, \tag{19}$$

showing a R^{-7} decay law with the distance from the atom, faster than the R^{-6} near-zone case of Eq. (17), due to retardation effects.

The expressions obtained above are valid for a generic multilevel atomic system, and they show a decay law for the renormalized electric field fluctuations as R^{-6} in the near zone and R^{-7} in the far zone. We also note that in the far zone there is a proportionality to the static polarizability of the atom $(\alpha_s)_{pq}=(2/c)\sum_\ell \mu_p^{g\ell}\mu_q^{\ell g}/k_{\ell g}$. In this region, contrarily to the near-zone region, the leading contribution comes from the two-photon component of the dressed ground state (6). Electric field fluctuations in the far zone decay with the distance faster than in the near zone, and this behavior is essentially due to retardation effects given by the transverse electric field.

We now turn to the magnetic field fluctuations, starting from Eq. (15) and approximating it in the near and far zones.

In the near one, $R\ll k_{\ell g}^{-1}$, which yields $k\gg k_{\ell g}$, if we approximate the denominators in the square bracket of (15) at zeroth order in $k_{\ell g}/k$ as we did for the electric case, an explicit calculation shows that we get zero because the contributions from the two terms inside the square bracket cancel with each other. We thus need to go to the first order in $k_{\ell g}/k$. We thus use

$$\frac{1}{(k_{\ell g}+k)(k_{\ell g}+k')}\simeq\frac{1}{kk'}\left(1-\frac{k_{\ell g}}{k}-\frac{k_{\ell g}}{k'}\right),\quad \frac{1}{(k_{\ell g}+k)(k+k')}\simeq\frac{1}{k'(k+k')}\left(1-\frac{k_{\ell g}}{k'}\right). \tag{20}$$

After some algebra we obtain

$$\begin{aligned}\langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r}=&\frac{2}{\pi^2}\epsilon_{psu}\epsilon_{qsv}\sum_\ell\mu_p^{g\ell}\mu_q^{\ell g}k_{\ell g}\nabla_u^R\nabla_v^{\bar R}\frac{1}{R\bar R}\\&\times\int_0^\infty dk\int_0^\infty dk'\left[-\frac{1}{k}-\frac{1}{k'}+\frac{2k}{k'(k+k')}\right]\sin kR\sin k'\bar R|_{R=\bar R}\,.\end{aligned} \tag{21}$$

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Factorizing the integrals over k and k' using $\int_0^\infty du \exp(-u(k+k')) = (k+k')^{-1}$ as already done for the electric case, exploiting some of the relations reported in the Appendix A, we finally get

$$\langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r} = -\frac{5}{2}\epsilon_{psu}\epsilon_{qsv}\sum_\ell \mu_p^{g\ell}\mu_q^{\ell g}k_{\ell g}\hat{R}_u\hat{R}_v\frac{1}{R^5}\,. \tag{22}$$

This result shows a near-zone scaling of the renormalized magnetic field fluctuations as R^{-5}, different from the R^{-6} scaling found for the near-zone electric field fluctuations.

In the far zone, $R \gg k_{\ell g}^{-1}$, we have $k, k' \ll k_{\ell g}$, and (15) is approximated as

$$\begin{aligned}\langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r} = \frac{2}{\pi^2}\epsilon_{psu}\epsilon_{qsv}\sum_\ell \mu_p^{g\ell}\mu_q^{\ell g}k_{\ell g}\nabla_u^R\nabla_v^{\bar{R}}\frac{1}{R\bar{R}}\\ \times\int_0^\infty dk\int_0^\infty dk' kk'\left[\frac{1}{k_{\ell g}^2}-\frac{2}{k_{\ell g}(k+k')}\right]\sin kR\sin k'\bar{R}|_{R=\bar{R}}\,.\end{aligned} \tag{23}$$

Using the relations reported in Appendix A, factorizing the k, k' as in the previous cases, we finally obtain

$$\langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r} = -\frac{7}{2\pi}\epsilon_{psu}\epsilon_{qsv}\sum_\ell \frac{\mu_p^{g\ell}\mu_q^{\ell g}}{k_{\ell g}}\hat{R}_u\hat{R}_v\frac{1}{R^7}\,. \tag{24}$$

Analogously to the electric case analyzed before, the far-zone scaling is as R^{-7} and proportional to the ground-state static (electric) polarizability of the atom.

All expressions obtained up to now are valid for a generic multilevel atom when one-electron virtual transitions are considered, and contain a sum over a complete set of atomic states. If we specify them to the simpler case of a two-level system consisting of a ground state $|g\rangle$ with energy E_g and an excited state $|e\rangle$ with energy E_e, transition frequency $\omega_{eg} = (E_e - E_g)/\hbar c$ and a well-defined direction of the transition dipole moment, let say along the z axis, from the expressions (17,19,22,24) we recover previous results in the literature [3,44,45]. We also recover previous results for the energy density of the virtual photon cloud obtained in the framework of relativistic quantum field theory in the ground and in the excited state of the hydrogen atom [46], as well as results obtained with different Hamiltonian schemes [40,47]; an extension to an excited atom can be found in [48].

In the near zone, $R \ll c/\omega_{eg}$, we obtain

$$\begin{aligned}\langle\psi|E^2(\mathbf{r})|\psi\rangle_{\rm r} &= |\mu_z^{ge}|^2\left(1+3\cos^2\theta\right)\frac{1}{R^6}\,,\\ \langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r} &= -\frac{5}{2}|\mu_z^{ge}|^2 k_{eg}\sin^2\theta\frac{1}{R^5}\,,\end{aligned} \tag{25}$$

where θ is the angle between $\mathbf{R}$ and the z axis, that is with the direction of the atomic transition dipole moment.

In the far zone, $R \gg c/\omega_{eg}$, we obtain

$$\begin{aligned}\langle\psi|E^2(\mathbf{r})|\psi\rangle_{\rm r} &= \frac{1}{2\pi}\frac{|\mu_z^{ge}|^2}{k_{eg}}\left(7+13\cos^2\theta\right)\frac{1}{R^7}\,,\\ \langle\psi|B^2(\mathbf{r})|\psi\rangle_{\rm r} &= -\frac{7}{2\pi}\frac{|\mu_z^{ge}|^2}{k_{eg}}\sin^2\theta\frac{1}{R^7}\,.\end{aligned} \tag{26}$$

The near- and far-zone expressions (25) and (26) for the two-level case show also an angular dependence of the electric and magnetic field fluctuations with respect to the transition dipole moment. In the case of a ground-state hydrogen atom, however, we expect from symmetry considerations that the field fluctuations around the atom should have a spherical symmetry, provided a sum over the

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relevant intermediate atomic states (specifically, the sum over ℓ in our previous expressions) is properly done. We now discuss explicitly this point.

In Eqs. (14) and (15) the sum over the atomic intermediate states $|\phi_\ell\rangle$ involves in principle all atomic states for which the matrix elements of a cartesian component of the dipole moment operator with the ground state $|\phi_g\rangle$ is not vanishing. These states can be explicitly written in the form $|\psi_\ell\rangle = |\phi_{nlm}\rangle = |R_{nl}\rangle|Y_l^m\rangle$, where n is the quantum number determining the energy of the state (we use the same symbol for both discrete and continuum states), and l, m are the usual orbital angular momentum quantum numbers, while $R_{nl}(r)$ and $Y_n^l(\theta,\phi)$ are respectively the radial and angular (spherical harmonics) parts of the atomic wavefunction. The bare atomic ground state is $|\phi_g\rangle = |\phi_{100}\rangle = |R_{10}\rangle|Y_0^0\rangle$. Due to our dipole approximation, dipole selection rules impose that only intermediate atomic states with $l = 1$ contribute. Thus the summation over ℓ reduce to a summation over n, that includes both discrete and continuum states, and over $m = 0, \pm 1$, while l is fixed to 1. Given n, the contribution of a single state with a specific value of m, that specifies the z component of the orbital angular momentum, gives a contribution to the field fluctuations that depends also on the polar angles, as we have explicitly seen in the two-level case. However, it is easy to show that when we sum over the three allowed values of m, the result is spherically symmetric and the angular dependence disappears, also yielding a more compact expression. We first apply these considerations to our general expressions for the electric and magnetic field fluctuations, Eqs. (14) and (15), and then in more detail for their approximations in the near and far zones, Eqs. (19) and (24). The indices p and q in these expressions are cartesian components $p, q = x, y, z$; concerning the sum over the magnetic quantum number m, it is more convenient to change basis for the spherical harmonics, introducing a new orthonormal basis set in the subspace with $l = 1$: $Y_1^x = (Y_1^{-1} - Y_1^1)/\sqrt{2}$, $Y_1^y = i(Y_1^{-1} + Y_1^1)/\sqrt{2}$, $Y_1^z = Y_1^0$, so that $\mu_{x,y,z} = \mu\sqrt{4\pi/3}Y_1^{x,y,z}$. Thus, we straightforwardly obtain

$$\sum_{m=x,y,z} \langle\phi_{100}|\mu_p|\phi_{n1m}\rangle\langle\phi_{n1m}|\mu_q|\phi_{100}\rangle = \frac{1}{3}|\langle R_{10}|\mu|R_{n1}\rangle|^2\delta_{pq}. \tag{27}$$

Substituting (27) into (19) and (24) and using the relations (A7) and (A8) of Appendix A, we can show that summation over m yields, as expected, a dependence of (19) and (24) from R only and not from the spherical angles. We report here only the final results in the near and far zone limits, starting from our results (17) and (19) for the electric component and (22) and (24) for the magnetic component. After some straightforward algebra, we get

$$\begin{aligned} \langle\psi|E^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} &= 2\sum_n |\langle R_{10}|\mu|R_{n1}\rangle|^2 \frac{1}{R^6} \quad \text{(near zone)}\,, \\ \langle\psi|E^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} &= \frac{23}{3\pi}\sum_n \frac{|\langle R_{10}|\mu|R_{n1}\rangle|^2}{k_{n1}} \frac{1}{R^7} \quad \text{(far zone)} \end{aligned} \tag{28}$$

for the electric field fluctuations, and

$$\begin{aligned} \langle\psi|B^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} &= -\frac{5}{3}\sum_n |\langle R_{10}|\mu|R_{n1}\rangle|^2 k_{n1} \frac{1}{R^5} \quad \text{(near zone)}\,, \\ \langle\psi|B^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} &= -\frac{7}{3\pi}\sum_n \frac{|\langle R_{10}|\mu|R_{n1}\rangle|^2}{k_{n1}} \frac{1}{R^7} \quad \text{(far zone)} \end{aligned} \tag{29}$$

for the magnetic field fluctuations. In these expressions the sum over n, as already stated, includes both the discrete and continuous parts of the energy spectrum of the atom.

These field fluctuations extend over a large distance from the atom, and they can be detected through their interaction with an electrically or magnetically polarizable body, an atom or a molecule for example, placed at some distance from the atom: this interaction energy is indeed the van der

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Waals or Casimir-Polder interaction between them [3,22]. This point gives a direct and clear physical interpretation on the origin of such quantum interactions between atoms or molecules.

Thus, electric and magnetic field fluctuations are directly observable thorough intermolecular van der Waals and Casimir-Polder interactions, that is long-range dispersion interactions between neutral atoms or molecules placed at distances larger than the typical distance of electron wavefunctions overlap, typically at a distance larger than a few nanometer. For example, if a second (test) isotropic atom is placed in the space around our (source) atom in the far zone, when their distance R is larger than $k_{\ell g}^{-1}$ and low-frequency virtual photons are involved in the renormalized field fluctuations, the test atom will respond to electric and magnetic fluctuations through its static electric and magnetic polarizability, α_T^E and α_T^M, yielding an interaction energy given by [3,5,22,40,49,50]

$$\begin{aligned} \Delta E_{CP}^{EE} &= -\frac{1}{2}\alpha_T^E \langle\psi|E^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} = -\frac{23\hbar c}{4\pi}\frac{\alpha_A^E \alpha_T^E}{R^7}, \\ \Delta E_{CP}^{EM} &= -\frac{1}{2}\alpha_T^M \langle\psi|B^2(\mathbf{r})|\psi\rangle_{\mathrm{r}} = \frac{7\hbar c}{4\pi}\frac{\alpha_A^E \alpha_T^M}{R^7}, \end{aligned} \tag{30}$$

where we have used the far-zone expressions of (28) and (29) and introduced the static ground-state electric polarizability of atom A, $\alpha_A^E = 2/(3\hbar c)\sum_n \frac{|\langle R_{10}|\mu|R_{n1}\rangle|^2}{k_{n1}}$. The expressions so obtained exactly concide with the Casimir-Polder interaction between the two atoms as obtained from fourth-order perturbation theory [39,51]. An analogous relationship exists in the near zone too, even if it is more complicated because the dynamical polarizability of the test atom, $\alpha_T(\omega)$, is involved since in this case high-frequency virtual photons play a main role [52,53].

Another important consequence of the self-dressing of an atom is the change of the vacuum field correlations. In the bare vacuum state, i.e. in the absence of any field source, equal-time vacuum field correlations are spatially correlated. For example, in the unbounded space, for the equal-time spatial correlation of the electric field, using (2) and (A2) we have [54,55]

$$\langle\{0_{\mathbf{k}\lambda}\}|E_i(\mathbf{r},t)E_j(\mathbf{r}',t)|\{0_{\mathbf{k}\lambda}\}\rangle = \frac{2\pi\hbar}{V}\sum_{\mathbf{k}}\omega_k\left(\delta_{ij}-\hat{k}_i\hat{k}_j\right)e^{i\mathbf{k}\cdot\mathbf{R}} = -\frac{4\hbar c}{\pi}\left(\delta_{ij}-2\hat{R}_i\hat{R}_j\right)\frac{1}{R^4}, \tag{31}$$

where $\mathbf{R} = \mathbf{r}-\mathbf{r}'$. Eq. (31) shows that quantum vacuum fluctuations have relevant nonlocal features and scale as R^{-4} with the distance. This is a quite important point with a fundamental interest, also in view of recent experimental measurements of vacuum fluctuations, their correlations including their nonlocality, exploiting electro-optic sampling techniques [56–59]. The presence of such vacuum field correlations is directly related to two-body dispersion interactions between atoms or molecules, because they induce and correlate dipole moments in them [60–63].

In the presence of the atom, also vacuum field correlations are modified. A direct calculation shows that, in the unbounded space [55],

$$\begin{aligned} &\langle\psi_g|E_i(\mathbf{r})E_j(\mathbf{r}')|\psi_g\rangle_r = \langle\psi_g|E_i(\mathbf{r})E_j(\mathbf{r}')|\psi_g\rangle - \langle\{0_{\mathbf{k}\lambda}\}|E_i(\mathbf{r},t)E_j(\mathbf{r}',t)|\{0_{\mathbf{k}\lambda}\}\rangle \\ &= \frac{2}{\pi}\sum_{\ell}\mu_p^{g\ell}\mu_q^{\ell g}\left(-\nabla^2\delta_{qi}+\nabla_q\nabla_i\right)^R\left(-\nabla^2\delta_{pj}+\nabla_p\nabla_j\right)^{R'}\frac{1}{RR'}f[k_{\ell g}(R+R')], \end{aligned} \tag{32}$$

where $\mathbf{R} = \mathbf{r}-\mathbf{r}_A$, $\mathbf{R}' = \mathbf{r}'-\mathbf{r}_A$, and $f(z) = \mathrm{ci}(z)\sin(z) - \mathrm{si}(z)\cos(z)$ is the auxiliary function of the sine and cosine integral functions, $\mathrm{si}(z)$ and $\mathrm{ci}(z)$ respectively [64]. In the far zone, that is $R, R' \gg c/\omega_{\ell g}$, we have $f(\omega_{\ell g}(R+R')/c) \simeq (\omega_{\ell g}(R+R')/c)^{-1}$ [64]; thus, the renormalized field correlation (32) asymptotically scales with the inverse seventh power of the distance from the atom A. Such R^{-7} distance scaling should be compared with the R^{-4} scaling of the bare vacuum field correlation given by (31). This scaling can be related to the distance dependence in the far zone of the three-body component of dispersion Casimir-Polder interaction energy between three-atoms [55,65,66];

 doi:10.20944/preprints202503.1700.v1

in other words, three-body Casimir-Polder interactions allow to probe the change of spatial vacuum field correlations due to the presence of a polarizable body such as an atom or a molecule or, in general, a polarizable body.

It is worthwhile to notice from the equations above, specifically from Eqs. (28) and (29), that, both in the near and in the far zone, the renormalized field fluctuations (or, equivalently, the related field energy densities) obtained in this section are positive for the electric part and negative for the magnetic part. This means that the presence of the atom increases the electric field fluctuations and decreases the magnetic field fluctuations, with respect to those present even in the absence of any field source and given by (11). This fact, in our opinion, is an important point to stress, since it shows that neglecting the (spatially uniform) zero-point terms would yield a negative value of $\langle \psi_g | B^2(\mathbf{r}) | \psi_g \rangle$. In other words, if the bare vacuum fluctuations were eliminated, for example using a normal ordering of the field operators [67,68], a negative energy density of the magnetic field would be obtained. This fact would be quite unsatisfactory from a physical point of view, supporting the importance and reality of quantum zero-point field fluctuations in the vacuum space, even if it has been shown that the Casimir effect and Casimir-Polder interactions, usually considered as a proof of the existence of vacuum fluctuations, can be indeed obtained also without mention the vacuum energy [69].

4. Effect of the Self-Dressing on Atomic Observables

In the previous section we have analyzed in detail the effects of the ground-state self-dressing of the atom, that is the fact that it continuously emits and reabsorbs virtual photons, on field quantities, namely electric and magnetic field fluctuations and energy densities in the space around the atom, and on equal-time spatial correlations of the electric field.

In this section we discuss some aspects of how the virtual processes leading to the ground-state dressing photon cloud affect atomic observables. One of them is, of course, an energy shift leading, after renormalization, to the well-known Lamb shift [3,41,43]. A new aspect that we want to investigate is the change of the average atomic radius due to the virtual processes when the virtual photon is emitted, and the consequent change of the average value of the electron-nucleus potential energy. In fact, during such virtual processes, the atom goes to an excited state that has an average radius larger than that in the ground state. Even if this virtual excited state lives for a short time according to the time-energy uncertainty relation, we expect that the average dimension of the electronic structure of the dressed atom should be larger than that of the bare atom. This is also truly consistent with the well-known Welton interpretation of the Lamb shift, ascribed to a change of the average electron-nucleus electrostatic energy due to the fluctuating motion of the electron caused by its interaction with the electric vacuum fluctuations [70–72].

In the present calculation it is more convenient to work in the minimal coupling scheme and we will use the dressed ground state (7) in the dipole approximation.

We now evaluate the average value of the operator r^n, where r is the distance of the electron from the atomic nucleus, on the dressed ground state (7). We expect it should be different than that on the bare ground state, due to the possibility of virtual transitions of the atom to an excited state. We obtain

$$\begin{aligned} \langle \tilde{\psi}_g | r^q | \tilde{\psi}_g \rangle = & \left[1 - \left(\frac{e}{mc} \right)^2 \frac{1}{(\hbar c)^2} \sum_{\ell} \sum_{\mathbf{k}\lambda} \frac{|\mathbf{p}^{g\ell} \cdot \mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r}_A)|^2}{(k_{\ell g} + k)^2} \right] \langle \phi_g | r^q | \phi_g \rangle \\ & + \left(\frac{e}{mc} \right)^2 \frac{1}{(\hbar c)^2} \sum_{\ell\ell'} \sum_{\mathbf{k}\lambda} \frac{\left(\mathbf{p}^{g\ell'} \cdot \mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r}_A) \right) \left(\mathbf{p}^{\ell g} \cdot \mathbf{A}^*_{\mathbf{k}\lambda}(\mathbf{r}_A) \right)}{(k_{\ell' g} + k)(k_{\ell g} + k)} \langle \phi_{\ell'} | r^q | \phi_{\ell} \rangle \, . \end{aligned} \tag{33}$$

Using the well-known relation between atomic matrix elements of the position $\mathbf{r}$ and of the momentum $\mathbf{p}$, $p_j^{\ell n} = imck_{\ell n} r_j^{\ell n}$ (the subscript j indicates the cartesian component), in the unbounded space where the mode functions $\mathbf{A}_{\mathbf{k}\lambda}$ are given by (10), we find

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$$\langle\tilde{\psi}_g|r^q|\tilde{\psi}_g\rangle = \left[1 - \frac{2\pi e^2}{\hbar c V}\sum_{\ell}\sum_{\mathbf{k}\lambda}\frac{|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{g\ell}|^2 k_{\ell g}^2}{k(k_{\ell g}+k)^2}\right]\langle\phi_g|r^q|\phi_g\rangle + \frac{2\pi e^2}{\hbar c V}\sum_{\ell\ell'}\sum_{\mathbf{k}\lambda}\frac{\left(\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{g\ell'}\right)\left(\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{\ell g}\right)k_{\ell g}k_{\ell' g}}{k(k_{\ell' g}+k)(k_{\ell g}+k)}\langle\phi_{\ell'}|r^q|\phi_\ell\rangle\,. \tag{34}$$

Eq. (34) clearly shows that the virtual processes of emission/absorption of photons occurring in the dressed ground state of the interacting system also yields a change in the average value of r^n, compared to that in the bare ground state $|\phi_g\rangle$. A thorough evaluation of this change, that involves the summation over all intermediate atomic states, and its precise relation with the previously mentioned Welton model for the ground-state Lamb shift of the hydrogen atom will be the subject of a future work. Here we only wish to stress some relevant conceptual aspects obtained exploiting some reasonable approximations. In particular, including only the contribution of intermediate atomic levels with principal quantum number $n = 2$, we obtain

$$\langle\tilde{\psi}_g|r^q|\tilde{\psi}_g\rangle \simeq \left[1 - \frac{2\pi e^2}{\hbar c V}\sum_{m=0,\pm1}\sum_{\mathbf{k}\lambda}\frac{|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{gm}|^2 k_{21}^2}{k(k_{21}+k)^2}\right]\langle R_{10}|r^q|R_{10}\rangle + \frac{2\pi e^2}{\hbar c V}\sum_{m=0,\pm1}\sum_{\mathbf{k}\lambda}\frac{|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{gm}|^2 k_{21}^2}{k(k_{21}+k)^2}\langle R_{21}|r^q|R_{21}\rangle\,, \tag{35}$$

where $\mathbf{r}^{gm} = \langle\phi_{100}|\mathbf{r}|\phi_{21m}\rangle$. From (35) we obtain that the expectation value of r^q in the dressed ground state is larger than in the bare ground state. For example, for the significant cases $q = 1$ and $q = 2$ of a hydrogen atom, we have: $\langle R_{10}|r|R_{10}\rangle = 3a_0/2$, $\langle R_{21}|r|R_{21}\rangle = 5a_0$, $\langle R_{10}|r^2|R_{10}\rangle = 3a_0^2$, $\langle R_{21}|r^2|R_{21}\rangle = 30a_0^2$, where a_0 is the Bohr's radius [73]. Substitution into (35) immediately yields

$$\langle\tilde{\psi}_g|r|\tilde{\psi}_g\rangle > \langle\phi_{100}|r|\phi_{100}\rangle\,,\quad \langle\tilde{\psi}_g|r^2|\tilde{\psi}_g\rangle > \langle\phi_{100}|r^2|\phi_{100}\rangle\,, \tag{36}$$

showing an increase of the average atomic size due to the virtual excitation processes resulting from its ground-state self-dressing.

Moreover, $\langle R_{10}|r^{-1}|R_{10}\rangle = a_0^{-1}$ and $\langle R_{21}|r^{-1}|R_{21}\rangle = (4a_0)^{-1}$ [73]: thus, our result (35) immediately yields that the (negative) average value of the electron-nucleus potential energy $V(r) = -e^2/r$ in the dressed ground state is larger than in the bare ground state, yielding a positive contribution to the ground-state energy shift, fully consistent with the Welton model and interpretation for the ground-state Lamb shift [11,70],

$$\langle\tilde{\psi}_g|V(r)|\tilde{\psi}_g\rangle = -e^2\langle\tilde{\psi}_g|\frac{1}{r}|\tilde{\psi}_g\rangle > \langle\phi_{100}|V(r)|\phi_{100}\rangle\,. \tag{37}$$

The summation over $\mathbf{k}$ in (35), and present in the potential energy shift (37), can be easily evaluated in the continuum limit, $V \to \infty$. After polarization sum evaluated using (A1) and angular integration, the integrand over k scales at high frequencies as k^{-1}, yielding a logarithmic ultraviolet divergence in the integration upper limit, that can be cured with a nonrelativistic ultraviolet wavenumber cutoff at $k_M \sim mc^2/(\hbar c)$. Taking into account $k_M \gg k_{21}$, we obtain

$$\frac{1}{V}\sum_{\mathbf{k}\lambda}\frac{|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{gm}|^2 k_{21}^2}{k(k_{21}+k)^2} \simeq \frac{|\mathbf{r}^{gm}|^2 k_{21}^2}{6\pi^2}\log\left(\frac{k_M}{k_{21}}\right)\,. \tag{38}$$

Therefore the shift of the average value of $V(r)$ in the dressed ground state has only a logarithmic ultraviolet divergence, without need of renormalization (in fact, there is not any linearly divergent term in $\langle V(r)\rangle$, as found in the Welton model too [70]). This seems related to the fact that nonrelativistic linearly diverging terms appear in the electron's kinetic energy only [22,43].

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The new results obtained in this section quantitatively show, as expected from physical basis, that the virtual processes due to the counterrotating terms in the Hamiltonian change atomic quantities such as for example the electron-nucleus average distance and the average squared distance, as well as the average potential energy of the electron in the nuclear electric field. This gives a quantitative and fundamental quantum basis to the Welton interpretation of the Lamb shift of an hydrogen atom [22,70,74]. The original Welton interpretation of the Lamb shift is based on (bare) vacuum fluctuation of the quantum electromagnetic field, that yields a fluctuating motion of the atomic electron, evaluated classically, which adds to its orbital motion. The Lamb shift is then obtained from the consequent change of the average electron's potential energy in the nucleus Coulomb field. In our case the fluctuating motion of the electron is related to quantum processes due to its interaction with the transverse radiation field (specifically virtual transitions from ground to excited states), and thus it is entirely obtained from quantum mechanical considerations. We will address in more detail this point, including the summation over all intermediate atomic states, in a future publication.

5. Conclusion

In this paper we have considered the self-dressing of a multilevel atom, such as an hydrogen atom, interacting with the quantum electromagnetic field within dipole approximation, in its interacting ground state. We have evaluated the dressed ground state of the atom at the second order in perturbation theory both in the minimal and in the multipolar coupling scheme, and evaluated on this state relevant field and atomic quantities. We have first investigated the change of the quantum fluctuations of the electric and magnetic field around the atom with respect to the bare ones, obtaining general expressions valid at any distance from the atom; then, we approximated them in the so-called near (nonretarded) and far (retarded) zone. We have discussed their distance scaling, stressing that the presence of the atom enhances electric field fluctuations and reduces magnetic field fluctuations, with respect to those present in the bare field vacuum state. We have also discussed the observability of such renormalized field fluctuations through dispersion (van der Waals and Casimir-Polder) interactions. We have also investigated the structure of the equal-time spatial correlations of the electric field in the dressed ground state and discussed their nonlocal features and the strict relation with non-additive three-body Casimir-Polder interactions.

We have finally investigated the effect of the self-dressing of the atom on atomic observables, such as the average electron-nucleus distance and the average squared distance, as well the change of the average potential energy of the atomic electron in the nuclear electric field, due to the virtual processes related to the self-dressing. This has allowed us to give a fundamental quantum basis of the Welton interpretation of the ground-state Lamb shift of the hydrogen atom, in terms of atomic self-dressing processes.

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Appendix A

We list here some useful formula for handling polarization sums and angular integrations, frequently used in this article [3,23,39].

Polarization sums:

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$$\begin{aligned}\sum_\lambda (\hat{\mathbf{e}}_{\mathbf{k}\lambda})_m (\hat{\mathbf{e}}^*_{\mathbf{k}\lambda})_n &= \sum_\lambda \left(\hat{\mathbf{b}}_{\mathbf{k}\lambda}\right)_m \left(\hat{\mathbf{b}}^*_{\mathbf{k}\lambda}\right)_n = \delta_{mn} - \hat{k}_m \hat{k}_n, \\ \sum_\lambda (\hat{\mathbf{e}}_{\mathbf{k}\lambda})_m \left(\hat{\mathbf{b}}^*_{\mathbf{k}\lambda}\right)_n &= \epsilon_{mnl} \hat{k}_l, \end{aligned} \tag{A1}$$

where $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$ are polarization unit vectors ($\lambda = 1, 2$), orthogonal to each other and to the wavevector $\mathbf{k}$, $\hat{\mathbf{b}}_{\mathbf{k}\lambda} = \mathbf{k} \times \hat{\mathbf{e}}_{\mathbf{k}\lambda}$, ϵ_{mnl} is the Levi-Civita totally antisymmetric symbol, and the Einstein convention of repeated symbols has been used.

Angular integrations:

$$\int d\Omega_{\mathbf{k}} \hat{k}_m e^{\pm i\mathbf{k}\cdot\mathbf{R}} = \mp \frac{i}{k} \nabla^R_m \int d\Omega_{\mathbf{k}} e^{\pm i\mathbf{k}\cdot\mathbf{R}} = \mp \frac{4\pi i}{k^2} \nabla^R_m \frac{\sin(kR)}{R}, \tag{A2}$$

$$\begin{aligned}\int d\Omega_{\mathbf{k}} \left(\delta_{\ell m} - \hat{k}_\ell \hat{k}_m\right) e^{\pm i\mathbf{k}\cdot\mathbf{R}} &= -\frac{1}{k^2} \left(\delta_{\ell m} \nabla^2 - \nabla_\ell \nabla_m\right)^R \int d\Omega_{\mathbf{k}} e^{\pm i\mathbf{k}\cdot\mathbf{R}} \\ &= -\frac{4\pi}{k^3} \left(\delta_{\ell m} \nabla^2 - \nabla_\ell \nabla_m\right)^R \frac{\sin(kR)}{R}, \end{aligned} \tag{A3}$$

where the superscript R indicates the variable with respect to which the derivatives are taken.

We report here other useful formulas, frequently used in the main text of this paper, are

$$\begin{aligned}\nabla_i f(R) &= \hat{R}_i \frac{df(R)}{dR}, \quad \nabla^2 f(R) = \frac{2}{R}\frac{df(R)}{dR} + \frac{d^2 f(R)}{dR^2}, \\ \nabla_i \nabla_j f(R) &= \delta_{ij} \frac{1}{R}\frac{df(R)}{dR} + \hat{R}_i \hat{R}_j \left(-\frac{1}{R}\frac{df(R)}{dR} + \frac{d^2 f(R)}{dR^2}\right), \\ \left(-\nabla^2 \delta_{ij} + \nabla_i \nabla_j\right) f(R) &= \left(-\delta_{ij} - \hat{R}_i \hat{R}_j\right) \frac{1}{R}\frac{df(R)}{dR} + \left(-\delta_{ij} + \hat{R}_i \hat{R}_j\right) \frac{d^2 f(R)}{dR^2}. \end{aligned} \tag{A4}$$

where i, j indicate cartesian components and we have introduced the unit vector $\hat{\mathbf{R}} = \mathbf{R}/R$. Speficic cases are

$$\begin{aligned}\nabla^2 \left(\frac{\sin kR}{kR}\right) &= -\frac{k}{R} \sin kR, \\ \nabla_j \left(\frac{\sin kR}{kR}\right) &= \hat{R}_j \left(\frac{\cos kR}{R} - \frac{\sin kR}{kR^2}\right), \\ \nabla_i \nabla_j \left(\frac{\sin kR}{kR}\right) &= \delta_{ij} \left(\frac{\cos kR}{R^2} - \frac{\sin kR}{kR^3}\right) + \hat{R}_i \hat{R}_j \left(-\frac{k \sin kR}{R} - 3\frac{\cos kR}{R^2} + 3\frac{\sin kR}{kR^3}\right), \end{aligned} \tag{A5}$$

From (A5), we then obtain

$$\begin{aligned}\left(\nabla^2 \delta_{ij} - \nabla_i \nabla_j\right)^R \frac{\sin kR}{kR} &= -\frac{k^2}{4\pi} \int d\Omega \left(\delta_{ij} - \hat{k}_i \hat{k}_j\right) e^{\pm i\mathbf{k}\cdot\mathbf{R}} \\ &= -k^2 \left[\left(\delta_{ij} - \hat{R}_i \hat{R}_j\right) \frac{\sin kR}{kR} + \left(\delta_{ij} - 3\hat{R}_i \hat{R}_j\right) \left(\frac{\cos kR}{k^2 R^2} - \frac{\sin kR}{k^3 R^3}\right)\right]. \end{aligned} \tag{A6}$$

Finally, for a generic regular function $f(k)$ of $k = |\mathbf{k}|$, we have the following relations

$$\begin{aligned}\sum_{\mathbf{k}} f(k) \left(\delta_{ij} - \hat{k}_i \hat{k}_j\right) e^{\pm i\mathbf{k}\cdot\mathbf{R}} &= -\frac{1}{2\pi^2} D^R_{ij} \int_0^\infty dk \frac{1}{k} f(k) \sin kR \\ \left(\nabla^2 \delta_{ij} - \nabla_i \nabla_j\right)^R \left[\frac{1}{R} \int_0^\infty \frac{1}{k} f(k) \sin kR\right] &= D^R_{ij} \int_0^\infty dk \frac{1}{k} f(k) \sin kR, \end{aligned} \tag{A7}$$

 doi:10.20944/preprints202503.1700.v1

where we have defined the following differential operator acting on the coordinate R

$$D_{ij}^{R} = \frac{1}{R}\left[(\delta_{ij} - \hat{R}_i\hat{R}_j)\frac{\partial^2}{\partial R^2} + (\delta_{ij} - 3\hat{R}_i\hat{R}_j)\left(\frac{1}{R^2} - \frac{1}{R}\frac{\partial}{\partial R}\right)\right]. \tag{A8}$$

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