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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 a hydrogen atom, interacting with the quantum electromagnetic field in the dressed ground state of the interacting system. Using perturbation theory within the dipole approximation, we evaluate the dressed ground state and investigate the effect of atomic self-dressing 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 zones. 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 self-dressing—namely, the virtual transitions occurring in the dressed ground state—on atomic observables, such as 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—such as a charged particle or an atom—is surrounded by a cloud of virtual quanta and particles that are continuously emitted and reabsorbed by the source, in accordance with the time–energy uncertainty relation [1–6]. This is commonly described in terms of a cloud of virtual particles surrounding the field source, which thus becomes a complex and spatially extended object called a dressed source.

The spatial structure of the virtual quanta cloud reflects the physical properties of the source, including its energy level structure and spatial extent [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 well defined in stationary conditions or in a scattering matrix approach, where noninteracting asymptotically states in time, that is for time $t \to \pm\infty$, 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, this is clearly defined for persistent interactions, acting at all times [8–10]. This point is essential and fundamental being deeply related to the very definition of a particle, or of any other system interacting with a quantum field (in particular when a continuous spectrum is involved),

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as a fundamental object [11]. Specifically, it is related to the difficulty of 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 source between finite times is considered, bare or partially dressed states are involved [17–20]. This kind of problem 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].

In this paper, we investigate and review some of the above-described fundamental questions of quantum field theory using nonrelativistic quantum electrodynamics (QED). Specifically, we consider a multilevel nonrelativistic atom interacting with the quantum radiation field in the Coulomb gauge. In this scenario, (virtual) photons are the only quanta or particles surrounding the field source in its ground state. We examine how this virtual photon cloud affects field and atomic observables, in particular electric and magnetic field fluctuations (or equivalently energy densities) as well as spatial field correlations, and electron–nucleus average distance and potential energy, respectively. Specifically, we 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 also evaluate the change in the average electron–nucleus distance (and of arbitrary powers of this distance) due to virtual processes occurring in the dressed ground state, along with the average electron–nucleus potential energy. We also explore 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 in both the minimal and multipolar coupling schemes under the dipole approximation, and obtain the dressed ground state of a multilevel atom interacting with the quantum radiation field using perturbation theory. In Section 3, we evaluate the electric and magnetic field fluctuations and spatial field correlations around the atom, and we discuss their connection 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 in the average electron–nucleus distance and a change in 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 offers 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 as a reflecting plate can be eventually present and its presence is mathematically described by the appropriate mode functions of the field operators. In the Coulomb gauge, $\nabla \cdot \mathbf{A}(\mathbf{r}) = 0$, where $\mathbf{A}$ is the electromagnetic vector potential and $\mathbf{r}$ denotes the position vector, 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, $H_A = \sum_n E_n |\phi_n\rangle|\phi_n|$ (with E_n and $|\phi_n\rangle$, respectively, the energy and the state vector of a complete set of atomic energy eigenstates), and the field Hamiltonian, $H_F = \sum_{\mathbf{k}\lambda} \hbar\omega_k a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}$ (with $\hbar$ being the reduced Planck constant, and $\mathbf{k}$ and $\lambda = 1, 2$ representing, 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 bosonic commutation rules, and the dispersion relation $\omega_k = c|\mathbf{k}|$ holds, where c denotes the speed of light. 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]

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

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

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

where the time dependence is included in the annihilation and creation operators (here and elsewhere below, we often omit explicit indication of time dependence of the operators). $\mathbf{A}_{\mathbf{k}\lambda}(\mathbf{r})$ are the mode functions for the 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 transverse part $\mathbf{E}_{\perp}$ of the electric field operator and for the magnetic field operator $\mathbf{B}$, respectively.

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 is known, this creates still unsolved problems in determining the lineshape of the radiation emitted by spontaneous emission, because the initial state is commonly taken as an eigenstate 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 QED [38]. In the case considered here, however, there is no a problem of this kind because we consider a dressed ground state, which is an eigenstate of the total Hamiltonian, and, thus, one can safely use the minimal or the multipolar coupling Hamiltonian, according to which coupling scheme is more convenient for making simpler specific calculations (actually, in Section 3, we use the multipolar coupling Hamiltonian while in Section 4 we use the minimal coupling Hamiltonian, in both cases within the dipole approximation). The unitary equivalence between the minimal and the multipolar coupling Hamiltonians can be proved also within the dipole approximation [25,39], that is the approximation used in this paper, even if the unitary transformation can be extended also to all higher multipoles [23,40]

The minimal coupling interaction Hamiltonian, for a single one-electron atom (with electron's mass m, electric charge e and momentum $\mathbf{p}$) located at position $\mathbf{r}_A$ and in the dipole approximation, is

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

(as already noted, the explicit time dependence of the operators is omitted). 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

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

where $\boldsymbol{\mu} = e\mathbf{r}$ is the atomic electric dipole moment operator and $\boldsymbol{\mu}^{mn} = \langle\phi_m|\boldsymbol{\mu}|\phi_n\rangle$ are its matrix elements between atomic states $|\phi_m\rangle$ and $|\phi_n\rangle$ with energy E_m and E_n, respectively;

$\mathbf{D}_\perp(\mathbf{r}_A)$ is the transverse displacement field operator evaluated at $\mathbf{r}_A$. The multipolar coupling interaction Hamiltonian (5) also contains a second term of the form $2\pi \int d^3r \mathbf{P}_\perp^2(\mathbf{r})$, where $\mathbf{P}_\perp(\mathbf{r})$ is the transverse polarization field of the atom, that however is not relevant for the quantities we evaluate below and, therefore, is neglected here. Outside the atom, 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 has the same form (2) [3,39]. This is the reason why usually, when local field quantities are evaluated as in Section (3), 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 interaction Hamiltonian H_I. The true (interacting) ground state can be obtained by stationary perturbation theory; up to the second order in the atom-radiation interaction one obtains

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

where the multipolar coupling Hamiltonian (5) is used. Here, we define $E_{mn} = E_m - E_n$ and $\boldsymbol{\mu}^{mn} = \langle\phi_m|\boldsymbol{\mu}|\phi_n\rangle$ (here and in what follows, the g subscript or superscript denotes the ground state of the atom). Also, $1_{\mathbf{k}\lambda}$ denotes a state with one photon with wavevector $\mathbf{k}$ and polarization λ. In Section 3, we 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) requires adding the longitudinal electrostatic term to the quantum transverse electric field [41], 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 use in Section 4 to calculate atomic quantities in the dressed ground state,

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

where the last term originates from the $\mathbf{A}^2(\mathbf{r}_A)$ term of the interaction Hamiltonian (4), treated at first order in perturbation theory being already a second-order quantity. The sums over m and ℓ in Equations (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.

Both expressions (6) and (7) 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 admixture of the bare ground state $|\phi_g, \{0_{\mathbf{k}\lambda}\}\rangle$ with one- and two-photon states in Equations (6) and (7), i.e., the vacuum self-dressing process, can be physically described in terms of virtual transitions occurring in the dressed ground state. Due to the counterrotating terms in the interaction Hamiltonian, the atom can make a virtual transition to an excited state $|\phi_m\rangle$ by emitting one photon of energy $\hbar\omega_k$ (as well as virtual processes involving two or more photons). This non-energy-conserving process is regulated by the energy-time uncertainty relation: the virtual state can live for a time interval of the order of $\Delta t \sim \hbar/\Delta E = (\omega_{mg} + \omega_k)^{-1}$, where $\Delta E = E_{mg} + \hbar\omega_k = \hbar(\omega_{mg} + \omega_k)$ is the energy unbalance in the virtual transition. The more the energy of the virtual excited state of the atom and/or of the virtual photon energy, the less the lifetime of the virtual state, and thus the lifetime of the virtual photon. High frequency photons have a shorter lifetime and thus they are more localized around the atom, compared to low-frequency virtual photons. This yields kind of a shell structure of the virtual photon cloud around the atom, giving information, also at large distances, on both its energy level structure and, in dynamical cases its internal structure [7,42]. These considerations also signify that in the near zone, $R \ll c/\bar{\omega}_{mg}$, where R is the distance from the atom and $\bar{\omega}_{mg}$ is an appropriate average atomic transition frequency from the ground state, the virtual photon cloud has a leading contribution from high-frequency virtual photons; on the other hand, in the far zone, $R \gg c/\bar{\omega}_{mg}$, low-frequency photons give the leading contribution to field observables. The presence of this dressing photon cloud, and its distance dependence, can be observed through the change in field observables, as we discuss in Section 3. Furthermore, the virtual photons present are responsible for various observable effects, for example the Lamb shift [43] and the van der Waals and Casimir–Polder intermolecular interactions [5,44].

The considerations given above make it quite 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.

Let us also mention that self-dressing processes can be particularly relevant in the presence of a strong atom-field coupling or of resonances. This can occur, for example, when an atom or in general a quantum emitter is inside a resonant cavity or a nanostructured electromagnetic environment such as a photonic crystal. In such cases, there may be a strong change (increase or decrease, according to the frequency) in the photonic density of states compared to the unbounded space. As a consequence, a possible relevant increase of the self-dressing processes in QED, condensed matter physics or circuit QED can occur. This can also give a strong enhancement of related physical effects, such as the Lamb shift and Casimir–Polder or resonance interatomic interactions, due to photons with frequency inside a range with modified high density of states [45–48]. Furthermore, possible conversion of virtual photons into real photons in the ultrastrong regime has been predicted [49–51].

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 from a factor of $1/(8\pi)$,

these fluctuations coincide, respectively, with the average electric and magnetic energy densities in the vacuum space around the atom in its dressed ground state (6). It can immediately be seen 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 Equations (2), (3) and (6) one finds

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

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

where $\Re$ stands to denote the real part.

The expressions (8) and (9) are general, valid for any multilevel atomic system within the dipole approximation and in the presence of perfectly conducting boundaries of arbitrary shape, provided the appropriate mode functions $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})$ and $\mathbf{g}_{\mathbf{k}\lambda}(\mathbf{r})$ are used. In the expressions (8) and (9), the energies of a complete set of atomic states are present. In the following, we explicitly consider a non-relativistic one-electron atom, where fine and hyperfine structures are sufficiently small to be neglected. However, specific cases—such as transitions involving inner-shells electrons of atoms with high nuclear charge—may yield non-negligible contributions to the energy levels and should be included. Such cases are not considered in the current study.

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 term in both Equations (8) and (9) represents the bare position-independent zero-point term (z.p.t.), present even in the absence of the atom and given by

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

Both of expressions in Equation (11), as is known, contain an ultraviolet divergence [3].

The other terms on the right-hand side of Equations (8) and (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), one obtains for the renormalized fluctuations, i.e., the fluctuations obtained after subtraction of the bare vacuum ones,

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

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

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

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

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

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

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

Equations (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 (14) and (15), the contribution from the first term in the square brackets is factorized in k and k' and can be evaluated analytically, while the second term is not factorized. We give here the approximated expressions valid in the near and far zones as defined in Section 2. 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 considered here, this length scale should be intended as an appropriate average of $k_{\ell g}^{-1}$ over all atomic states ℓ, similarly to what is done in the Bethe nonrelativistic calculation of the Lamb shift [22,52].

Let us start with the electric field fluctuations (14).

In the near zone, $R \ll k_{\ell g}^{-1}$, one may 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 in Equation (14) above 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', one finds

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

After some algebra, using the relations given in Appendix A, one finally obtains

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

where $\hat{\mathbf{R}} = \mathbf{R}/R$ is the unit vector along the direction of $\mathbf{R}$. The result (17) shows that in the near zone the renormalized electric field fluctuations scale as R^{-6}, and the fluctuations are essentially given by the longitudinal field contribution (the transverse field contribution is negligible at short distances, as indeed expected) [41]. Both one- and two-photon components of the dressed ground state (6) contribute in this region.

In the far zone, $R \gg k_{\ell g}^{-1}$, one may 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 then

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

The spatial dependence obtained from the two terms in the square brackets inside the k, k'-integrals in the second row of Equation (18) can be immediately obtained from a dimensional analysis, and the dependences behave as R^{-8} for the first term and as R^{-7} for the second term. Thus, in the far zone, the first term can be neglected. After some algebra and using the relations given in Appendix A, one finally finds

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

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

The expressions (16)–(19) obtained are valid for a generic multilevel atomic system and highlight a decay law for the renormalized electric field fluctuations as R^{-6} in the near zone and R^{-7} in the far zone. Let us 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 the retardation effects given by the transverse component of the electric field.

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

In the near zone, $R \ll k_{\ell g}^{-1}$, which yields $k \gg k_{\ell g}$, if the denominators in the square brackets of Equation (15) were approximated at the zeroth order in $k_{\ell g}/k$ as done for the electric case in this Section just above, the explicit calculation shows that one gets zero because the contributions from the two terms in the square brackets cancel each other. Thus, one needs to consider the first order in $k_{\ell g}/k$, so to use

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

After some algebra one obtains

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

Factorizing the integrals over k and k' in Equation (21) by using $\int_0^\infty du\exp[-u(k+k')] = (k+k')^{-1}$ as was done for the electric case above, exploiting the relations from Appendix A, one finally finds

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

The result (22) yields 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 Equation (17).

In the far zone, $R \gg k_{\ell g}^{-1}$, one has $k, k' \ll k_{\ell g}$ and Equation (15) can be approximated to

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

Using the relations from Appendix A and factorizing the k, k' as in the cases just above, one finally obtains

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

Similarly to the electric case analyzed above in this Section, the far-zone magnetic field fluctuations scale as R^{-7} and are 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 those states are referred 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 $\omega_{eg} = ck_{eg} = (E_e - E_g)/\hbar c$ and a well-defined direction of the transition dipole moment, for example, along the z-axis, from the expressions (17), (19), (22) and (24), one recovers the earlier results in the literature [3,53,54]. One also recovers the earlier results for the energy density of the virtual photon cloud obtained in the framework of relativistic quantum field theory in the ground state of the hydrogen atom [55], as well as the results obtained with different Hamiltonian schemes [41,56]; an extension to an excited atom can be found in Ref. [57].

In the near zone, $R \ll k_{eg}^{-1}$, one obtains

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

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

In the far zone, $R \gg k_{eg}^{-1}$, one obtains

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

The near- and far-zone expressions (25) and (26), respectively, for the two-level case reveal 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 to have a spherical symmetry, provided a sum over the relevant intermediate atomic states (specifically, the sum over ℓ in the previous expressions) is taken. Let us now address explicitly this point.

In Equations (14) and (15), the sum over the atomic intermediate states $|\phi_\ell\rangle$ involves, in general, 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 and m are the 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 $|\phi_g\rangle = |\phi_{100}\rangle = |R_{10}\rangle|Y_0^0\rangle$. Let us point out that the atomic model considered here consists of a nonrelativistic spinless one-electron atom and the atomic states identified by the quantum numbers n, l and m used constitute a basis set of the atomic Hamiltonian H_A, as requested by the perturbative expansion (6) for the dressed interacting ground state obtained in Section 2.

Due to the dipole approximation used here, dipole selection rules impose that only intermediate atomic states with $l = 1$ contribute. Thus, the sum over ℓ reduces to a sum 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 was seen in the two-level case in this Section. However, it is straightforward to show that when the sum is taken over the three allowed values of m, the result is spherically symmetric and the angular dependence disappears, also yielding a more compact expression. Let us first apply these considerations to the general expressions (14) and (15), for the electric and magnetic field fluctuations and then in more detail for the approximations (19) and (24), in the near and far zones. The indices p and q in the expressions (19) and (24) represent 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, one straightforwardly obtains

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

Substituting Equation (27) into Equation (19) and (24) and using the relations (A7) and (A8), it can be shown that the summation over m yields, as expected, a dependence of the expressions (19) and (24) only on R but not on spherical angles. We give here only the final results in the near- and far-zone limits, starting from the results (17) and (19) for the

electric component and the results (22) and (24) for the magnetic component. After some straightforward algebra, one gets

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

for the electric field fluctuations, and

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

for the magnetic field fluctuations (here, $\mu = |\boldsymbol{\mu}|$). In the expressions (28) and (29), the sum over n, as already stated, includes both the discrete and continuous parts of the energy spectrum of the atom.

The field fluctuations (28) and (29) extend over a large distance from the atom, and these fluctuations 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 Waals or Casimir–Polder interaction between atoms/molecules [3,22]. This gives a direct and transparent physical interpretation to the origin of such quantum interactions between atoms or molecules.

Thus, the electric and magnetic field fluctuations are directly observable through the 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 nanometers. For example, if a second (test) isotropic atom is placed in the space around our (source) atom in the far zone, when the distance between those (test and source) atoms R is larger than $k_{\ell g}^{-1}$ and low-frequency virtual photons are involved in the renormalized field fluctuations, the test atom responds to electric and magnetic fluctuations through its static electric and magnetic polarizability, α_T^E and α_T^M, respectively, yielding an interaction energy given by [3,5,22,41,58,59]

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

where the far-zone expressions of (28) and (29) are used and the static ground-state electric polarizability of atom A, $\alpha_A^E = 2/(3\hbar c)\sum_n \frac{|\langle R_{10}|\mu|R_{n1}\rangle|^2}{k_{n1}}$, is introduced. The expressions in Equation (30) coincide with the Casimir–Polder interaction between the two atoms as obtained from fourth-order perturbation theory [39,60]. An analogous relationship exists in the near zone too, even being more complicated because the dynamical polarizability of the test atom, $\alpha_T(\omega)$, involved , as well as an integration over the frequency ω, since high-frequency virtual photons play a main role in this case [61,62]. Furthermore, to stress is that the non-additive three-body Casimir–Polder dispersion interaction allows to probe other properties of dressed vacuum-field fluctuations and field energy densities. Actually, if one considers the self-dressing of two atoms, kind of an interference effect is obtained at the fourth order in the atom-field coupling, yielding a sixth-order three-body component of the Casimir–Polder interaction energy between the two atoms and a third test atom [63].

All this shows relevant indirect methods to measure dressed field fluctuations around a quantum emitter; at the end of this Section we discuss direct experimental ways to measure such fluctuations as well as their spatial correlations.

Another essential consequence of the self-dressing of an atom is the change in 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 Equations (2) and (A2) one has [17,64]

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

where $\mathbf{R}=\mathbf{r}-\mathbf{r}'$. Equation (31) shows that quantum vacuum fluctuations have relevant nonlocal features and vacuum field correlations scale as R^{-4} with the distance. This is quite an essential point with a fundamental interest, also in view of the recent experimental measurements of vacuum fluctuations and their correlations including the nonlocal properties of vacuum field correlations, exploiting electro-optic sampling techniques [65–68]. The presence of such vacuum field correlations is directly related to two-body dispersion interactions between atoms or molecules because such field correlations induce and correlate dipole moments in them [69–72].

In the presence of the atom, also vacuum field correlations are modified. A direct calculation shows that, in the unbounded space [64],

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

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, [73]. In the far zone, that is $R,R'\gg c/\omega_{\ell g}$, one has $f(\omega_{\ell g}(R+R')/c)\simeq(\omega_{\ell g}(R+R')/c)^{-1}$ [73]; thus, the renormalized field correlation (32) asymptotically scales with the seventh inverse 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 (31). This scaling can be related to the distance dependence in the far zone of the three-body component of the dispersion Casimir–Polder interaction energy between three-atoms [64,74,75]; in other words, three-body Casimir–Polder interactions allow probing the change in 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 noticing from the equations obtained, specifically from Equations (28) and (29), that, in both the near and far zones, the renormalized field fluctuations (or, equivalently, the related field energy densities) obtained in this Section are positive for the electric part while is negative for the magnetic part. This signifies that the presence of the atom increases the electric field fluctuations and decreases the magnetic field fluctuations, with respect to those fluctuations present even in the absence of any field source and given by Equation (11). This feature, in our opinion, is an essential 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 [76,77], a negative energy density of the magnetic field would be obtained when an electric dipolar field source is present. This feature 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, often considered as a proof of the

existence of vacuum fluctuations, can be indeed obtained also without mentioning the vacuum energy [78].

Finally, let us mention recent measurement setups for a direct measure of vacuum field fluctuations and their correlations, in addition to their indirect measurement through dispersion interactions as already mentioned in this Section. These experimental techniques, based on femtosecond electro-optic detection in a cryogenic nonlinear crystal, have allowed to measure the fluctuating electric vacuum field in the free space in the Terahertz frequency range and its temporal and spatial coherence [65,66,79]. Furthermore, possibility of using electric-optic sampling experiments for separately probing vacuum and source field fluctuations has been recently proposed in the literature [68,80]. These techniques could also possibly be exploited to directly measure the changes in the vacuum fluctuations and their spatial correlations due to the presence of an atom or a generic quantum emitter, as investigated in this paper.

4. Effect of the Self-Dressing on Atomic Observables

In Section 3, we analyzed in detail the effects of the ground-state self-dressing of the atom, that is 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, certainly, an energy shift leading, after mass renormalization, to the Lamb shift [3,43,52]. A new aspect that we investigate here is the change in the average atomic radius due to the virtual processes when the virtual photon is emitted, and the consequent change in average value of the electron–nucleus potential energy. Actually, 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 known Welton interpretation of the Lamb shift, ascribed to a change in the average electron–nucleus electrostatic energy due to the fluctuating motion of the electron caused by its interaction with the electric vacuum fluctuations [81–83].

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

We now evaluate the average value of the operator r^q, 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. One obtains

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

Using the 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 Equation (10), one finds

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

Equation (34) shows that the virtual processes of emission/absorption of photons continuously occurring in the dressed ground state of the interacting system also yield a change in the average value of r^q, 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 already mentioned Welton model for the ground-state Lamb shift of the hydrogen atom will be a subject of future work. Here, let us only stress some relevant conceptual aspects obtained exploiting some reasonable approximations. In particular, including only the contribution of intermediate atomic levels with principal quantum number $n = 2$, one obtains

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

where $\mathbf{r}^{gm} = \langle\phi_{100}|\mathbf{r}|\phi_{21m}\rangle$. From Equation (35), one concludes 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, one has: $\langle R_{10}|r|R_{10}\rangle = 3a_0/2$, $\langle R_{21}|r|R_{21}\rangle = 5a_0$, $\langle R_{10}|r^2|R_{10}\rangle = 3a_0^2$, $\langle R_{21}|r^2|R_{21}\rangle = 30a_0^2$, where a_0 is the Bohr's radius [84]. Substitution into Equation (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 $\langle R_{21}|r^{-1}|R_{21}\rangle = (4a_0)^{-1}$ [84]: thus, the 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, well consistent with the Welton model and interpretation for the ground-state Lamb shift [11,81],

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

The summation over $\mathbf{k}$ in Equation (35), and present in the potential energy shift (37), can be straightforwardly evaluated in the continuum limit, $V \to \infty$. After polarization sum evaluated using Equation (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 $k_M \gg k_{21}$, one obtains

$$\frac{1}{V}\sum_{\mathbf{k}\lambda}\frac{|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{r}^{gm}|^2k_{21}^2}{k(k_{21}+k)^2} \simeq \frac{|\mathbf{r}^{gm}|^2k_{21}^2}{3\pi^2}\log\left(\frac{k_M}{k_{21}}\right). \tag{38}$$

Therefore, the shift in the average value of $V(r)$ in the dressed ground state has only a logarithmic ultraviolet divergence, with no need for renormalization (actually, there is no linearly divergent term in $\langle V(r)\rangle$, as also found in the Welton model [81]). This seems to

be related to the fact that nonrelativistic linearly diverging terms appear in the electron's kinetic energy only [22,52].

The new results obtained in this Section quantitatively show, as expected from a qualitative 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 ground-state Lamb shift of an hydrogen atom [22,81,85]. 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 in the average electron's potential energy in the nucleus Coulomb field. In the case considered here, the fluctuating motion of the electron is related to quantum processes due to interaction of the electron 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 this point in more detail, including the summation over all intermediate atomic states, in a future study.

5. Conclusions

In this paper, we have examined the self-dressing of a multilevel atom, such as a hydrogen atom, interacting with the quantum electromagnetic field within dipole approximation, in the interacting ground state of the atom. We have evaluated the dressed ground state of the atom up to the second order in perturbation theory, both in the minimal and in the multipolar coupling schemes, and assessed several relevant field and atomic quantities. We have first investigated the modifications in the quantum fluctuations of the electric and magnetic fields around the atom, relative to the bare field fluctuations present in the bare vacuum state. General expressions are obtained, valid at any distance greater than the Bohr radius; we then have approximated those expressions in the so-called near (nonretarded) and far (retarded) zones. We have discussed the distance scaling of the formulas obtained, stressing that the presence of the atom enhances electric field fluctuations and reduces magnetic field fluctuations, with respect to the fluctuations 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. Furthermore, we have investigated the structure of the equal-time spatial correlations of the electric field in the dressed ground state and discussed nonlocal features of the correlations and their direct connection with non-additive three-body Casimir–Polder interactions.

Finally, we have explored the influence of self-dressing on atomic observables, such as the average electron–nucleus distance and the average squared distance, as well as the change in average potential energy of the atomic electron in the nuclear electric field. These changes, driven by virtual processes related to the self-dressing, enabled us to provide a fundamental quantum basis for the Welton interpretation of the ground-state Lamb shift of the hydrogen atom, framed in terms of atomic self-dressing mechanisms.

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Appendix A

We list here some helpful formulas for handling polarization sums and angular integrations, often used in this paper [3,23,39].

Polarization sums:

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

where $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$ are polarization unit vectors ($\lambda = 1, 2$), orthogonal to each other and to the wavevector $\mathbf{k}$, $\hat{\mathbf{b}}_{\mathbf{k}\lambda} = \hat{\mathbf{k}} \times \hat{\mathbf{e}}_{\mathbf{k}\lambda}$, δ_{mn} is the Kronecker delta, 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.

Other helpful formulas, used in this paper:

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

where i, j indicate Cartesian components and the unit vector $\hat{\mathbf{R}} = \mathbf{R}/R$ is introduced. Specific 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 Equation (A5), one then obtains

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

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

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

where the differential operator

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

is defined acting on the coordinate R.

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