

## Methods of asymptotic analysis in cavity quantum electrodynamics

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(Received 28 May 2003; published 26 September 2003)

The energy-level shift of a ground-state atom in front of a nondispersive dielectric half-space is calculated by quantizing the electric field by means of a normal-mode expansion and applying second-order perturbation theory to the electric-dipole Hamiltonian  $\boldsymbol{\mu} \cdot \mathbf{E}$ . It is shown that the contributions to this shift coming from traveling and from evanescent waves can be combined into a single expression which lends itself readily to asymptotic analysis for large atom-surface separations, while in the opposite asymptotic regime when the atom is close to the surface the combined expression is less convenient. Employing a Green's-function formalism instead of the normal-mode expansion leads directly to the combined formula, and in that case it is advantageous to be able to apply the same transformation backwards and split the energy shift into a sum of distinct contributions corresponding to different physical processes. The analysis serves to shed light on common sources of error in the literature and paves the way for the study of more complicated models in cavity quantum electrodynamics.

DOI: 10.1103/PhysRevA.68.033813

PACS number(s): 42.50.Ct, 31.30.Jv, 32.70.Jz, 12.20.-m

### I. INTRODUCTION

The nature of the interaction of an atom with a surface depends on the distance between them. If the atom is close to the surface the interaction is dominated by electrostatics, i.e., the atomic dipole experiences Coulomb forces due to image charges on the other side of the surface. However, as first worked out by Casimir and Polder [1], retardation becomes important for atoms further away from the surface. This is because the electromagnetic interaction between the atom and the surface has a finite speed of propagation. Casimir and Polder considered an atom in its ground state interacting with a perfectly reflecting surface, but the analysis can be extended to excited-state atoms [2,3]. To be more realistic one needs to consider atoms interacting with imperfectly reflecting surfaces, which in the simplest case can be modeled by nondispersive dielectrics [4–6]. However, as models for the surface become more realistic, they also become more involved, which often means that crucial results for physically interesting quantities can be obtained only through numerical simulations [4,5]. While for a nondispersive surface characterized by a constant refractive index we did manage to obtain analytical results for the energy-level shifts and modified emission rates of the atom in both nonretarded and retarded limits [6], this was at the expense of having to enter into a rather involved mathematical derivation [7]. The technique devised in Ref. [7] and applied in Ref. [6] becomes too cumbersome for the more complicated problem of an atom interacting with a dispersive and absorbing dielectric surface [8]. Thus we desire to investigate easier routes to asymptotic expressions for energy-level shifts in cavity quantum electrodynamics.

In this paper we discuss an alternative approach to the problem studied in Ref. [6] where we worked with the minimal coupling Hamiltonian  $\mathbf{p} \cdot \mathbf{A}$  and applied standard first- and second-order perturbation theory. Here we calculate the energy-level shift of an atom close to a nondispersive dielectric surface by using the lowest-order multipole Hamiltonian,

i.e., the electric-dipole interaction  $\boldsymbol{\mu} \cdot \mathbf{E}$ , and we apply both second-order perturbation theory and MacLachlan's susceptibility formula obtained from linear-response theory [9]. As we wish to concentrate on the comparison of the different approaches to the problem, we shall consider only ground-state atoms and we shall work at zero temperature. For finite temperature effects we refer the reader to Ref. [10] and references therein.

The system we shall study consists of an atom in front of a nondispersive dielectric half-space; the dielectric is assumed to have a constant real, frequency-independent refractive index  $n$ . The atom is at a distance  $Z$  away from the dielectric surface, with its center fixed at the point  $\mathbf{r}_0 = (0,0,Z)$ . As mentioned above, we shall consider the atom to be in its ground state and the system to be at zero temperature, so that the fluctuations of the radiation field are solely quantum and not thermal.

In the following section we calculate the energy-level shift of the atom by quantizing the electromagnetic field through a normal-mode expansion and applying second-order perturbation theory to the dipole Hamiltonian  $\boldsymbol{\mu} \cdot \mathbf{E}$ . In Sec. II B we devise a transformation of the expression for the energy-level shift which allows us to combine the contributions from traveling and evanescent waves into a single formula. It will then be shown in Sec. II C that this makes the asymptotic analysis of the level shift rather straightforward. In Sec. III we shall make contact with Green's-function approaches based on linear-response theory (see, e.g., Refs. [9,4,5]) and compare the formulas for the level shift and the approximations for its asymptotic analysis with the previous approach. On the basis of our calculation we are able to vindicate the approximation of using the static polarizability in the retarded limit, which many previous workers have applied but often without rigorous justification. We discuss the comparison of the various approaches in Sec. IV and summarize our results. The Appendix provides details of the normal-mode functions of the electromagnetic field in the presence of a dielectric half-space.

## II. THE DIPOLE HAMILTONIAN

We consider a single-electron atom near a dielectric half-space at zero temperature; the dielectric medium is taken to be nondispersive and nondissipative, so that the dielectric permittivity of the configuration is

$$\epsilon(\mathbf{r}) = \begin{cases} n^2 & \text{for } z < 0 \\ 1 & \text{for } z > 0, \end{cases} \quad (2.1)$$

at all frequencies. We assume that the atom is in its ground state, with its center fixed at the point  $\mathbf{r}_0 = (0, 0, Z)$ . The interaction between the atom and the dielectric through the quantized electromagnetic field is described by the Hamiltonian

$$H_1 = -\boldsymbol{\mu} \cdot \mathbf{E}(\mathbf{r}, t), \quad (2.2)$$

where  $\boldsymbol{\mu} = e(\mathbf{r} - \mathbf{r}_0)$  is the electric-dipole moment operator and  $\mathbf{E}(\mathbf{r}, t)$  the transverse electric field. This Hamiltonian is the lowest order in the multipole Hamiltonian and corresponds to electric-dipole interactions [11]. In contrast to the minimal coupling Hamiltonian  $\mathbf{p} \cdot \mathbf{A}$ , the Hamiltonian in Eq. (2.2) automatically includes the electrostatic interaction between the atomic dipole and its image in the dielectric [12].

In order to quantize the electromagnetic field we need to solve Maxwell's equations in the presence of a dielectric half-space. We do this by introducing the electromagnetic potentials  $\Phi(\mathbf{r}, t)$  and  $\mathbf{A}(\mathbf{r}, t)$ . Since we are considering an overall neutral system, i.e., the net charge density in our construction is zero, we can set  $\Phi(\mathbf{r}, t) = 0$ . Furthermore, in the generalized Coulomb gauge

$$\nabla \cdot [\epsilon(\mathbf{r}) \mathbf{A}] = 0, \quad (2.3)$$

the field equations reduce to the wave equation for  $\mathbf{A}(\mathbf{r}, t)$ . Thus solutions can be obtained by taking combinations of incident, reflected, and refracted waves, and imposing continuity conditions at the vacuum-dielectric interface.

Introducing the creation and annihilation operators  $a_\nu, a_\nu^\dagger$ , one can express the field operator  $\mathbf{E}(\mathbf{r}, t)$  in terms of the normal modes  $\mathbf{f}_\nu(\mathbf{r})$

$$\mathbf{E}(\mathbf{r}, t) = i \sum_\nu \sqrt{\frac{\omega_\nu}{2}} [a_\nu e^{-i\omega_\nu t} \mathbf{f}_\nu(\mathbf{r}) - a_\nu^\dagger e^{i\omega_\nu t} \mathbf{f}_\nu^*(\mathbf{r})]. \quad (2.4)$$

The mode functions  $\mathbf{f}_\nu(\mathbf{r})$  are labeled according to the polarization and the wave vector of the incident wave, both of which are amalgamated into the greek index  $\nu$ ; their explicit form is given by Eqs. (A4)–(A7) in the Appendix.

### A. Energy-level shifts

We shall now calculate the energy-level shift by perturbation theory. Since the interaction Hamiltonian (2.2) is linear in the electron charge  $e$ , we must calculate the shift up to the second order of perturbation theory if we want to obtain it to first order in the fine-structure constant  $\alpha$ . Being linear in the electric field,  $H_1$  creates or annihilates one photon from the

state it operates on, and thus the first-order shift vanishes and only the second-order shift survives in the total shift,

$$\Delta E = - \sum_{j,\nu} \frac{|\langle j; 1_\nu | \boldsymbol{\mu} \cdot \mathbf{E}(\mathbf{r}, t) | i; 0 \rangle|^2}{E_j - E_i + \omega_\nu}.$$

Since we are interested in the change in the energy levels of the atom due to the presence of the dielectric half-space, all contributions to the level shifts due to free-space electromagnetic fluctuations should be removed. This can be implemented simply by subtracting the corresponding expressions for a transparent dielectric with  $n = 1$ . This procedure at the same time removes all divergences from the formulas [6]. In addition we make the dipole approximation and assume that the electric field at the position  $\mathbf{r}$  of the electron is roughly the same as that at the position  $\mathbf{r}_0$  of the nucleus. Using the mode expansion (2.4) and the explicit form of the mode functions  $\mathbf{f}_\nu(\mathbf{r})$  we find for the level shift

$$\begin{aligned} \Delta E(n) - \Delta E(n=1) \\ \equiv \delta E \simeq - \frac{2\alpha}{\pi m^2} \sum_j' \sum_{\sigma=\parallel, \perp} E_{ji} |\mathbf{p}_\sigma|^2 \\ \times \left[ \int_0^\infty ds \int_0^1 dt \frac{s^3}{s+1} \mathcal{T}_\sigma(t) \cos(\zeta_{ji} s t) \right. \\ \left. + \int_0^\infty ds \int_0^1 dt \frac{s^3}{s+1} \mathcal{A}_\sigma(t) \exp(-\sqrt{n^2-1} \zeta_{ji} s t) \right], \end{aligned} \quad (2.5)$$

where  $\zeta_{ji} = 2Z E_{ji} \equiv 2Z(E_j - E_i)$ . The integration variable  $s$  is effectively the photon frequency  $\omega_\nu$  in units of the frequency  $E_{ji}$  of the atomic transition, and the integration variable  $t$  originates from the integration over angles of incidence of the photon at the surface. The moduli squares of the matrix elements of the momentum between the ground state  $i$  and excited states  $j$  have been abbreviated by

$$|\mathbf{p}_\parallel|^2 \equiv |\langle j | p_x | i \rangle|^2 + |\langle j | p_y | i \rangle|^2 \quad \text{and} \quad |\mathbf{p}_\perp|^2 \equiv |\langle j | p_z | i \rangle|^2. \quad (2.6)$$

The functions  $\mathcal{T}_\sigma(t)$  and  $\mathcal{A}_\sigma(t)$  are abbreviations related to the contributions of traveling and of evanescent waves, respectively, and are given by

$$\mathcal{T}_\parallel(t) = \frac{1}{4} \left( \frac{t - \sqrt{n^2 - 1 + t^2}}{t + \sqrt{n^2 - 1 + t^2}} - t^2 \frac{n^2 t - \sqrt{n^2 - 1 + t^2}}{n^2 t + \sqrt{n^2 - 1 + t^2}} \right), \quad (2.7)$$

$$\mathcal{T}_\perp(t) = \frac{1}{2} (1 - t^2) \frac{n^2 t - \sqrt{n^2 - 1 + t^2}}{n^2 t + \sqrt{n^2 - 1 + t^2}}, \quad (2.8)$$

$$\mathcal{A}_\parallel(t) = \frac{\sqrt{n^2 - 1}}{2} \frac{(2n^2 + 1)(n^2 - 1)t^2 + 1}{(n^4 - 1)t^2 + 1} t \sqrt{1 - t^2}, \quad (2.9)$$

$$\mathcal{A}_\perp(t) = n^2 \sqrt{n^2 - 1} \frac{(n^2 - 1)t^2 + 1}{(n^4 - 1)t^2 + 1} t \sqrt{1 - t^2}. \quad (2.10)$$

We have used the identity

$$|\langle j | \boldsymbol{\mu}_\sigma | i \rangle|^2 = \frac{4\pi\alpha}{m^2 E_{ji}^2} |\langle j | \mathbf{p}_\sigma | i \rangle|^2 \quad (2.11)$$

in converting the matrix elements of the dipole-moment operator into those of the momentum operator. Since only the ground-state shift will be considered, the parameter  $\zeta_{ji}$  is positive for all intermediate states  $|j\rangle$ . Note that the parameter  $\zeta_{ji} \equiv 2ZE_{ji}$  is just the ratio of the time taken by a virtual photon to travel one round trip between the atom and the surface ( $2Z$ ) and the characteristic time scale for an atomic transition ( $1/E_{ji}$ ). Therefore, the size of  $\zeta_{ji}$  is a good criterion for the importance of retardation and serves to distinguish between the retarded and the nonretarded regimes in this problem.

### B. Transformation

We wish to devise a transformation that enables us to combine the contributions of the traveling waves (the  $T$  integral) and of the evanescent waves (the  $\mathcal{A}$  integral) to the total shift (2.5) into a single integral. To save space let us define  $\mathcal{S}_\sigma$  as the sum of the two integrals in the square brackets of Eq. (2.5) and write

$$\delta E \approx -\frac{2\alpha}{\pi m^2} \sum_j' \sum_{\sigma=\parallel, \perp} E_{ji} |\mathbf{p}_\sigma|^2 \mathcal{S}_\sigma. \quad (2.12)$$

We aim to express  $\mathcal{S}_\perp$  and  $\mathcal{S}_\parallel$  each as a single integral. As the transformation we need turns out to be the same for both components, we demonstrate the calculation for the perpendicular component only.

Let us start by considering the traveling part ( $T$  integral) in  $\mathcal{S}_\perp$  which reads in full

$$\frac{1}{2} \int_0^\infty ds \int_0^1 dt \frac{s^3}{s+1} \left[ (1-t^2) \frac{n^2 t - \sqrt{n^2 - 1 + t^2}}{n^2 t + \sqrt{n^2 - 1 + t^2}} \right] \cos(\zeta_{ji} s t). \quad (2.13)$$

Making a change of variable from  $t$  to  $v = s\sqrt{1-t^2}$ , we can write the integral as

$$\text{Re} \left\{ \frac{1}{2} \int_0^\infty ds \int_0^s dv \frac{1}{s+1} \frac{v^3}{\sqrt{s^2 - v^2}} R^p \exp(i\zeta_{ji} \sqrt{s^2 - v^2}) \right\}, \quad (2.14)$$

where  $R^p$  is the Fresnel reflection coefficient of a  $p$ -polarized [13] incident wave with frequency  $s$  and the parallel component  $v$  of the wave vector, i.e.,  $v/s$  is the sine of the angle of incidence,

$$R^p(s, v) = \frac{n^2 \sqrt{s^2 - v^2} - \sqrt{n^2 s^2 - v^2}}{n^2 \sqrt{s^2 - v^2} + \sqrt{n^2 s^2 - v^2}}. \quad (2.15)$$

The evanescent part ( $\mathcal{A}$  integral) of  $\mathcal{S}_\perp$  is

$$n^2 \sqrt{n^2 - 1} \int_0^\infty ds \int_0^1 dt \frac{s^3}{s+1} \left[ \frac{(n^2 - 1)t^2 + 1}{(n^4 - 1)t^2 + 1} t \sqrt{1 - t^2} \right] \times \exp(-\sqrt{n^2 - 1} \zeta_{ji} s t). \quad (2.16)$$

By changing the variable  $t$  to  $v = s\sqrt{1 + (n^2 - 1)(1 - t^2)}$ , we obtain

$$\int_0^\infty ds \int_s^{ns} dv \frac{v^3}{s+1} \left[ \frac{n^2 \sqrt{n^2 s^2 - v^2}}{n^4 (v^2 - s^2) + n^2 s^2 - v^2} \right] \times \exp(-\zeta_{ji} \sqrt{v^2 - s^2}). \quad (2.17)$$

Since for  $s \leq v \leq ns$

$$\frac{n^2 \sqrt{n^2 s^2 - v^2}}{n^4 (v^2 - s^2) + n^2 s^2 - v^2} = \text{Re} \left\{ \frac{1}{2i \sqrt{v^2 - s^2}} \left( \frac{in^2 \sqrt{v^2 - s^2} - \sqrt{n^2 s^2 - v^2}}{in^2 \sqrt{v^2 - s^2} + \sqrt{n^2 s^2 - v^2}} \right) \right\}, \quad (2.18)$$

we can rewrite Eq. (2.17) as

$$\text{Re} \left\{ \frac{1}{2i} \int_0^\infty ds \int_s^{ns} dv \frac{1}{s+1} \frac{v^3}{\sqrt{v^2 - s^2}} \times \left( \frac{in^2 \sqrt{v^2 - s^2} - \sqrt{n^2 s^2 - v^2}}{in^2 \sqrt{v^2 - s^2} + \sqrt{n^2 s^2 - v^2}} \right) \exp(-\zeta_{ji} \sqrt{v^2 - s^2}) \right\}. \quad (2.19)$$

Moreover, because

$$\sqrt{n^2 s^2 - v^2} = i \sqrt{v^2 - n^2 s^2} \quad \forall v \in [ns, \infty), \quad (2.20)$$

the integrand of Eq. (2.19) is purely imaginary for any  $v \geq ns$ . Therefore, we can extend the range of the  $v$  integral in Eq. (2.19) to infinity without affecting the result, since we are concerned with its real part only. Hence, choosing the branch cut of the square root appropriately and writing  $\sqrt{v^2 - s^2} = -i \sqrt{s^2 - v^2}$ , we arrive at the following expression for Eq. (2.17):

$$\text{Re} \left\{ \frac{1}{2} \int_0^\infty ds \int_s^\infty dv \frac{1}{s+1} \frac{v^3}{\sqrt{s^2 - v^2}} R^p \exp(i\zeta_{ji} \sqrt{s^2 - v^2}) \right\}. \quad (2.21)$$

We note that the integrands of Eqs. (2.14) and (2.21) are exactly the same and that the ranges of their  $v$  integrals complement each other. Consequently their sum equals the integral over the whole range of  $v \in [0, \infty)$  and we can combine them in  $\mathcal{S}_\perp$ ,

$$\mathcal{S}_\perp = \text{Re} \left\{ \frac{1}{2} \int_0^\infty ds \int_0^\infty dv \frac{1}{s+1} \frac{v^3}{\sqrt{s^2-v^2}} R^p \right. \\ \left. \times \exp(i\zeta_{ji}\sqrt{s^2-v^2}) \right\}. \quad (2.22)$$

Similar manipulations for the parallel component lead to

$$\mathcal{S}_\parallel = \text{Re} \left\{ \frac{1}{4} \int_0^\infty ds \int_0^\infty dv \frac{1}{s+1} \frac{v}{\sqrt{s^2-v^2}} \right. \\ \left. \times [s^2 R^s - (s^2-v^2) R^p] \exp(i\zeta_{ji}\sqrt{s^2-v^2}) \right\} \quad (2.23)$$

with  $R^p$  given by Eq. (2.15) and  $R^s$  by

$$R^s(s, v) = \frac{\sqrt{s^2-v^2} - \sqrt{n^2 s^2 - v^2}}{\sqrt{s^2-v^2} + \sqrt{n^2 s^2 - v^2}}, \quad (2.24)$$

which is the Fresnel reflection coefficient of an  $s$ -polarized [14] incident wave with frequency  $s$  and the parallel component  $v$  of the wave vector, i.e., with an angle of incidence whose sine is  $v/s$ .

In some places we shall find it useful to consider the above integrals with the  $s$  integration rotated by  $\pi/2$  in the complex plane. Replacing  $s$  by  $iu$  we find

$$\mathcal{S}_\perp = \frac{1}{2} \int_0^\infty du \int_0^\infty dv \frac{1}{u^2+1} \frac{v^3}{\sqrt{u^2+v^2}} R^p \\ \times \exp(-\zeta_{ji}\sqrt{u^2+v^2}), \quad (2.25)$$

$$\mathcal{S}_\parallel = \frac{1}{4} \int_0^\infty du \int_0^\infty dv \frac{1}{u^2+1} \frac{v}{\sqrt{u^2+v^2}} \\ \times [(u^2+v^2) R^p - u^2 R^s] \exp(-\zeta_{ji}\sqrt{u^2+v^2}), \quad (2.26)$$

where  $R^{s,p}$  are now the Fresnel reflection coefficients at imaginary frequencies  $iu$ , that is,

$$R^s(iu, v) = \frac{\sqrt{u^2+v^2} - \sqrt{n^2 u^2 + v^2}}{\sqrt{u^2+v^2} + \sqrt{n^2 u^2 + v^2}}, \\ R^p(iu, v) = \frac{n^2 \sqrt{u^2+v^2} - \sqrt{n^2 u^2 + v^2}}{n^2 \sqrt{u^2+v^2} + \sqrt{n^2 u^2 + v^2}}. \quad (2.27)$$

Before proceeding to the analysis of the above equations, we would like to make a few comments. Firstly, the transformations leading from (2.13) to (2.14), and from (2.16) to (2.17) are not well behaved in some parts of the domains of integration. As one can easily check, the Jacobians of these transformations vanish for  $v=0$ , have a simple pole at  $s=0$ , and are divergent but integrable along the lines  $v=s$

and  $v=ns$ , respectively. Luckily the integrand is such that none of these points cause any problems. Secondly, the presence of the Fresnel reflection coefficients  $R^{s,p}$  and the exponential (propagation) factor  $\exp(i\zeta_{ji}\sqrt{s^2-v^2})$  in Eqs. (2.22) and (2.23) seem to suggest that one could interpret the shift as arising from interactions between the atom and virtual photons reflected from the interface. However, the exponential acquires a real negative argument when  $s < v$  and hence damps the integrands of Eqs. (2.22) and (2.23) exponentially. This corresponds to the appearance of *evanescent reflected waves* when the incident angle is above a ‘‘critical angle.’’ This is obviously unphysical since it can never take place in nature. We conclude that, although the above transformations will turn out to be advantageous for the asymptotic analysis of the level shift in Sec. II C, they distort the picture of the underlying physical processes.

### C. Asymptotic analysis

We shall now analyze the asymptotic behavior of the level shift in the nonretarded and retarded limits, when the atom is close to or far from, respectively, the surface of the dielectric. The length scale on which to measure this distance is given by the wavelengths of typical transitions in the atom. Thus the parameter  $\zeta_{ji} \equiv 2ZE_{ji}$  provides a suitable criterion for characterizing these two asymptotic regimes: we have  $\zeta_{ji} \ll 1$  in the nonretarded limit, and  $\zeta_{ji} \gg 1$  in the retarded limit. According to Eq. (2.12) the dependence of the energy shift on the distance from the surface is all contained in the two integrals  $\mathcal{S}_\sigma$ , so that we will concentrate on examining the asymptotic behavior of  $\mathcal{S}_\sigma$ .

#### 1. The nonretarded regime

Since the analysis for the parallel and the perpendicular components of  $\mathcal{S}_\sigma$  is very similar, we demonstrate the calculation for just one of them and choose  $\mathcal{S}_\perp$ .

For  $\zeta_{ji} \ll 1$  the exponential in Eq. (2.25) damps the integrand only very weakly. However, one cannot approximate the exponential as its presence is essential for the convergence of the integral. An alternative strategy is to rescale the integral by making the change of variables  $u=x/\zeta_{ji}$ ,  $v=y/\zeta_{ji}$ , which gives

$$\mathcal{S}_\perp = \frac{1}{2\zeta_{ji}^2} \int_0^\infty dx \int_0^\infty dy \frac{1}{x^2 + \zeta_{ji}^2} \frac{y^3}{\sqrt{x^2 + y^2}} R^p \\ \times \exp(-\sqrt{x^2 + y^2}). \quad (2.28)$$

But this integral is also not convergent in the limit  $\zeta_{ji} \rightarrow 0$  and thus does not lend itself to easy asymptotic analysis. The same would be true if we had rescaled the integral (2.22), although its degree of divergence for  $\zeta_{ji} \rightarrow 0$  would be less.

In contrast, if we go back to the original expression (2.5) before the transformation of Sec. II B, the asymptotic analysis for small  $\zeta_{ji}$  is very simple. Scaling the  $s$  integration in Eq. (2.5) by introducing the new variable  $w = \zeta_{ji}s$  we find

$$\begin{aligned} \delta E = & -\frac{2\alpha}{\pi m^2} \sum_j' \sum_{\sigma=\parallel,\perp} \frac{E_{ji} |\mathbf{p}_\sigma|^2}{\zeta_{ji}^3} \\ & \times \left[ \int_0^\infty dw \int_0^1 dt \frac{w^3}{w+\zeta_{ji}} \mathcal{T}_\sigma(t) \cos(wt) \right. \\ & \left. + \int_0^\infty dw \int_0^1 dt \frac{w^3}{w+\zeta_{ji}} \mathcal{A}_\sigma(t) \exp(-\sqrt{n^2-1}wt) \right]. \end{aligned} \quad (2.29)$$

In this integral the limit  $\zeta_{ji} \rightarrow 0$  is without problems. Simply replacing  $w + \zeta_{ji}$  by  $w$  in the denominator of the integrand and straightforward integration yield for the level shift in the nonretarded limit:

$$\delta E^{(\text{nonret})} \sim -\left(\frac{n^2-1}{n^2+1}\right) \frac{\alpha}{16m^2 \mathcal{Z}^3} \sum_j' \frac{|\mathbf{p}_\parallel|^2 + 2|\mathbf{p}_\perp|^2}{E_{ji}^2}. \quad (2.30)$$

One could also easily derive the next-to-leading order by approximating  $1/(w + \zeta_{ji}) \approx 1/w - \zeta_{ji}/w^2$  in Eq. (2.29).

The energy shift (2.30) in the nonretarded limit is of course exactly the electrostatic shift, which is a separate contribution right from the start if one works in  $\mathbf{p} \cdot \mathbf{A}$  coupling [cf. Eq. (4.9) in Ref. [6]].

## 2. The retarded regime

In the retarded regime, when  $\zeta_{ji} \gg 1$ , the exponential in Eq. (2.25) strongly damps the integrand. If  $\zeta_{ji}$  is large then the only significant contributions to the integral come from small  $\sqrt{u^2 + v^2}$ , i.e., from a region close to the origin in the  $(u, v)$  plane where both  $u$  and  $v$  are small. Thus we can apply Watson's lemma [15] and approximate the integrand by Taylor expanding its denominator around  $u=0$ ,

$$\frac{1}{u^2+1} \approx 1 - u^2 + u^4 - \dots \quad (2.31)$$

With this approximation we can calculate the double integral in Eq. (2.25) by changing variables into polar coordinates ( $u = r \cos \phi$  and  $v = r \sin \phi$ ). The result is

$$\mathcal{S}_\perp \sim \frac{c_4^\perp}{\zeta_{ji}^4} = \frac{c_4^\perp}{16\mathcal{Z}^4 E_{ji}^4} \quad (2.32)$$

with  $c_4^\perp$  given by

$$\begin{aligned} c_4^\perp = & -\frac{1}{2} \left\{ \frac{2n^2+3n-8}{n^2-1} - 3 \frac{2n^4-2n^2-1}{(n^2-1)^{3/2}} \ln(n + \sqrt{n^2-1}) \right. \\ & \left. - \frac{6n^4}{(n^2-1)\sqrt{n^2+1}} \ln \left[ \frac{\sqrt{n^2+1}+1}{n(\sqrt{n^2+1}+n)} \right] \right\}. \end{aligned} \quad (2.33)$$

In the same way, using the first term of the expansion (2.31) in (2.26), we can compute the leading order of  $\mathcal{S}_\parallel$ . We obtain

$$\mathcal{S}_\parallel \sim \frac{c_4^\parallel}{\zeta_{ji}^4} = \frac{c_4^\parallel}{16\mathcal{Z}^4 E_{ji}^4} \quad (2.34)$$

with  $c_4^\parallel$  given by

$$\begin{aligned} c_4^\parallel = & \frac{6n^4-3n^3-2n^2+2}{n^2-1} - \frac{3n^2(2n^4-2n^2+1)}{(n^2-1)^{3/2}} \ln(n \\ & + \sqrt{n^2-1}) - \frac{6n^6}{(n^2-1)\sqrt{n^2+1}} \ln \left[ \frac{\sqrt{n^2+1}+1}{n(\sqrt{n^2+1}+n)} \right]. \end{aligned} \quad (2.35)$$

Substituting these results into Eq. (2.12), we find for the energy-level shift in the retarded regime

$$\delta E^{(\text{ret})} \sim -\frac{\alpha}{8\pi m^2 \mathcal{Z}^4} \sum_j' \frac{c_4^\parallel |\mathbf{p}_\parallel|^2 + c_4^\perp |\mathbf{p}_\perp|^2}{E_{ji}^3}, \quad (2.36)$$

which agrees with what we found in Ref. [6], Eqs. (4.14) and (4.18), but only after a great deal more effort and with the help of the mathematical techniques devised in Ref. [7].

Although in Ref. [6] we worked in  $\mathbf{p} \cdot \mathbf{A}$  coupling which gives slightly different expressions, we can see what the nature of the problem is by inspecting the expression for the energy-level shift in Eq. (2.5) before the transformation. There Watson's lemma cannot be applied since all one can say is that for large  $\zeta_{ji}$  the contributions to the integrals come from regions where the product  $st$  is small. The fact that the product of the two integration variables  $s$  and  $t$  is small does not let one draw any conclusions about each of them individually. In particular, it is fallacious to conclude that  $s$  must be small, since  $t$  can be zero, which would make the product  $st$  small even if  $s$  is large. The same applies vice versa.

Alternatively, one could attempt to derive an asymptotic expression for Eq. (2.5) for large  $\zeta_{ji}$  by repeated integration by parts, either in one or the other variable, or two dimensionally by applying Stokes' theorem in the  $(s, t)$  plane. However, this method fails, too, because integration by parts with respect to one variable generates inverse powers of the other which cause the integral over that variable to diverge at the lower limit. Similar problems beset the two-dimensional equivalent of integration by parts. The underlying cause of all these problems is that the arguments of the cosine and the exponential in Eq. (2.5) have a stationary point at  $(s, t) = (0, 0)$  in the corner of the domain of integration. The only way of deriving a correct asymptotic expression for Eq. (2.5) for large  $\zeta_{ji}$  is to subtract this problematic point and treat it separately. We refer the reader to Ref. [7] for the details of how to do this. In the present context it suffices to note that the asymptotic analysis in the retarded regime is very simple in the transformed expressions (2.25) and (2.26), but highly complicated in the expressions for the level shift (2.5) before the transformation. This is just the reverse of the situation in the nonretarded limit.

### III. LINEAR-RESPONSE THEORY AND GREEN'S-FUNCTION FORMALISM

In this section we compare the formulas obtained in Sec. II with those based on linear-response theory. We shall see that using just the first term of the expansion in Eq. (2.31) is equivalent to approximating the polarizability in the retarded regime by its static value, which is an approximation that has been widely adopted in the literature, though often without rigorous justification.

In linear-response theory, the response of a system to an external perturbation is described by its susceptibility. If the external perturbation is weak then one can assume the response of the system to be linear and apply the superposition principle. For two weakly interacting systems, McLachlan showed that the interaction energy between them can be expressed in terms of the product of their susceptibility at imaginary frequencies [9]. Applying this formalism to the problem at hand, one finds that the level shift of a ground-state atom is given by (cf., e.g., [4])

$$\delta E = -\frac{1}{2\pi} \sum_{l,m} \int_0^\infty d\xi G_{lm}^R(\mathbf{r}_0, \mathbf{r}_0; i\xi) \Pi_{lm}(i\xi). \quad (3.1)$$

The indices  $l, m$  refer to Cartesian tensor components, and  $\Pi_{lm}(i\xi)$  is the atomic polarizability tensor of the ground state at imaginary frequencies

$$\begin{aligned} \Pi_{lm}(i\xi) &= 2 \sum_j' E_{ji} \frac{\langle i | \mu_l | j \rangle \langle j | \mu_m | i \rangle}{E_{ji}^2 + \xi^2} \\ &= \frac{8\pi\alpha}{m^2} \sum_j' \frac{1}{E_{ji}} \frac{\langle i | p_l | j \rangle \langle j | p_m | i \rangle}{E_{ji}^2 + \xi^2}. \end{aligned} \quad (3.2)$$

The susceptibility  $G_{lm}$  of the electric field is the same as the field's retarded Green's function [9], which can be easily worked out from classical electromagnetism by considering the Sommerfeld problem of the radiation by an oscillating electric dipole near a semi-infinite dielectric [16]. Since we are not interested in the full interaction energy of the atom with the electromagnetic field, which would be the Lamb shift in free space, but only in the part that is due to the presence of the dielectric half-space, we can drop the free-space contribution from the Green's function and consider only the part that corresponds to the classical dipole field that is reflected by the dielectric. The reflected part  $G_{lm}^R$  of the retarded Green's function at coinciding spatial points and for frequencies along the positive imaginary axis reads

$$G_{lm}^R(\mathbf{r}_0, \mathbf{r}_0; i\xi) = 0 \quad \forall l \neq m, \quad (3.3)$$

$$\begin{aligned} G_{xx}^R(\mathbf{r}_0, \mathbf{r}_0; i\xi) &= G_{yy}^R(\mathbf{r}_0, \mathbf{r}_0; i\xi) \\ &= \frac{1}{8\pi} \int_0^\infty d\kappa \frac{\kappa}{\sqrt{\xi^2 + \kappa^2}} [(\xi^2 + \kappa^2)R^p - \xi^2 R^s] \\ &\quad \times \exp(-2\mathcal{Z}\sqrt{\xi^2 + \kappa^2}), \end{aligned} \quad (3.4)$$

$$\begin{aligned} G_{zz}^R(\mathbf{r}_0, \mathbf{r}_0; i\xi) &= \frac{1}{4\pi} \int_0^\infty d\kappa \frac{\kappa^3}{\sqrt{\xi^2 + \kappa^2}} R^p \\ &\quad \times \exp(-2\mathcal{Z}\sqrt{\xi^2 + \kappa^2}), \end{aligned} \quad (3.5)$$

where the Fresnel reflection coefficients  $R^{s,p}$  are the same as in Eq. (2.27) except for the replacement of  $u$  by  $\xi$  and  $v$  by  $\kappa$ . We use the expression for the atomic polarizability (3.2) and write the energy shift as

$$\begin{aligned} \delta E &= -\frac{4\alpha}{m^2} \sum_j' \frac{1}{E_{ji}} \left( |\mathbf{p}_\parallel|^2 \int_0^\infty d\xi \frac{G_{xx}^R(i\xi)}{E_{ji}^2 + \xi^2} \right. \\ &\quad \left. + |\mathbf{p}_\perp|^2 \int_0^\infty d\xi \frac{G_{zz}^R(i\xi)}{E_{ji}^2 + \xi^2} \right). \end{aligned} \quad (3.6)$$

If we rescale the integration variables in Eq. (3.4), (3.5), and (3.6) by the atomic transition energy  $E_{ji}$  such that  $\xi = E_{ji} u$  and  $\kappa = E_{ji} v$ , it becomes obvious that the expression for the energy shift (3.6) derived from linear-response theory is indeed identical to the one of Eq. (2.12) obtained through normal mode expansion and standard perturbation theory once one has applied the transformation of Sec. II B and cast it into the form (2.25) and (2.26).

Having made contact between the results of the two approaches, we are in the position to examine the approximations made in the asymptotic analysis of the energy shift. In particular, applying Watson's lemma in the retarded regime and using just the first term of the expansion (2.31) is equivalent to approximating

$$\frac{1}{E_{ji}^2 + \xi^2} \sim \frac{1}{E_{ji}^2} \quad (3.7)$$

in Eq. (3.6). This amounts to replacing the atomic polarizability by its value at zero frequency, i.e.,

$$\begin{aligned} \Pi_{lm}(i\xi) &= \frac{8\pi\alpha}{m^2} \sum_j' \frac{1}{E_{ji}} \frac{\langle i | p_l | j \rangle \langle j | p_m | i \rangle}{E_{ji}^2 + \xi^2} \\ &\sim \frac{8\pi\alpha}{m^2} \sum_j' \frac{1}{E_{ji}^3} \langle i | p_l | j \rangle \langle j | p_m | i \rangle \\ &\equiv \Pi_{lm}(0). \end{aligned} \quad (3.8)$$

According to Eqs. (3.1) and (3.6), the shift in the retarded regime is thus given by

$$\begin{aligned} \delta E^{(\text{ret})} &\sim -\frac{1}{2\pi} \Pi_{lm}(0) \int_0^\infty d\xi G_{lm}^R(i\xi) \\ &= -\frac{4\alpha}{m^2} \sum_j' \frac{1}{E_{ji}^3} \left( |\mathbf{p}_\parallel|^2 \int_0^\infty d\xi G_{xx}^R(i\xi) \right. \\ &\quad \left. + |\mathbf{p}_\perp|^2 \int_0^\infty d\xi G_{zz}^R(i\xi) \right). \end{aligned} \quad (3.9)$$

As in Sec. II C 2, the integrals in Eq. (3.9) can be calculated exactly by changing variables into polar coordinates,  $\xi = r \cos \phi$  and  $\kappa = r \sin \phi$ ; one finds

$$\int_0^\infty d\xi G_{xx}^R(i\xi) = \frac{c_4^\parallel}{32\pi Z^4}$$

and

$$\int_0^\infty d\xi G_{zz}^R(i\xi) = \frac{c_4^\perp}{32\pi Z^4}. \quad (3.10)$$

Substituting these formulas into Eq. (3.9) we recover our previous result (2.36).

Thus, in the retarded regime ( $\zeta_{ji} \gg 1$ ) the leading order of the ground-state shift is determined by the static value of the atomic polarizability [9]. In other words, in the retarded regime it is the contribution of virtual photons with frequencies much lower than the atomic transition frequency ( $\xi \ll E_{ji}$ ) that dominates the level shift. The atom is “static” in its electromagnetic response because the time scale  $1/E_{ji}$  of the internal evolution of the atom is much shorter than a typical oscillation period of the relevant virtual photons, so that the fields as seen by the atom are in effect static.

#### IV. SUMMARY AND DISCUSSION

The main achievement of this paper is the discovery of a transformation between the integral expressions for the energy-level shift as obtained from a normal-mode expansion of the field and the application of standard perturbation theory, on the one hand, and that resulting from linear-response theory and employing the retarded Green’s function, on the other hand. This is of value since it helps greatly or, for more complicated systems, even makes possible the asymptotic analysis of the energy-level shift, which is the only way to extract physically meaningful information from a calculation otherwise amenable only to full-scale numerical analysis in a multidimensional parameter space. It turns out that the result of the normal-mode approach lends itself to easy asymptotic analysis in the nonretarded regime when the atom is close to the wall but is very awkward to deal with in the retarded regime when the atom is far from the wall, whereas the opposite applies to the result of the Green’s-function approach—asymptotic analysis is uncomplicated in the retarded regime but difficult in the nonretarded. The example system investigated here, an atom close to a nondispersive dielectric half-space, is simple enough to allow the explicit demonstration of the various approaches. However, for instance, the same system but with absorption and dispersion in the dielectric included is orders of magnitude more difficult to treat [8], and the knowledge of the transformation devised in this paper is essential for extracting useful asymptotic expressions from otherwise unmanageably complicated expressions.

The two approaches differ also in other aspects. In the normal-mode approach the contributions from traveling and evanescent waves are readily identifiable and separate, whereas they appear combined in one expression in the

Green’s-function approach. Thus the underlying physical processes of the emission, propagation, reflection, and reabsorption of virtual photons in the interaction of an atom with a dielectric wall are transparent and easy to understand in the normal-mode approach. By contrast, the Green’s-function approach hides such microscopic processes from view and just considers macroscopic subsystems and their response to perturbations. While one point of view need not *a priori* be any more advantageous than the other, the artificial separation of the system into two subsystem has the drawback of inviting errors in the asymptotic analysis: both atom and field susceptibilities depend on the frequency  $i\xi$  which is integrated from 0 to  $i\infty$  in the expression for the level shift (3.1) and it is thus ill advised to make approximations in either of the two susceptibilities without considering carefully the whole integral [17].

Furthermore, care must be taken when rescaling two-dimensional integrals. Besides the integral over the frequency  $s$  in Eq. (2.5) or  $i\xi$  in Eq. (3.1), the expressions for the level shifts also involve an integral over another variable,  $t$  in Eq. (2.5) and  $\kappa$  in Eqs. (3.4) and (3.5), which in the mode-expansion approach can be seen to stem from a summation over angles of incidence. Simply scaling one variable with the other [17] is tempting but incorrect if the scaling variable ranges to either 0 or  $\infty$ , or even both. In this case one must consider the rescaling as a variable transformation of both variables and carefully examine the behavior of the Jacobian throughout the domain of integration. For the integrals appearing in  $S_{\parallel,\perp}$  the zeros and singularities of the Jacobian pose no threats, as we saw in Sec. II B. However, that there is an issue and that it may be subtle, one can see, for example, by looking at the electrostatic shift. When working in  $\boldsymbol{\mu} \cdot \mathbf{E}$  coupling the electrostatic shift is part of the result of second-order perturbation theory, but the minimal coupling Hamiltonian  $\mathbf{p} \cdot \mathbf{A}$  does not include the electrostatic interaction which must be taken into account separately in that approach [12]. Thus taking the difference of the perturbative shift due to the  $\boldsymbol{\mu} \cdot \mathbf{E}$  Hamiltonian and that due to the  $\mathbf{p} \cdot \mathbf{A}$  Hamiltonian up to second order in  $e$ , given by Eqs. (2.5) and [6], respectively, should give the electrostatic shift. Using the same notations as in Eqs. (2.6)–(2.10) we find that the electrostatic shift can be written [18]

$$\begin{aligned} & -\frac{2\alpha}{\pi m^2} \sum_j' \sum_{\sigma=\parallel,\perp} E_{ji} |\mathbf{p}_\sigma|^2 \left[ \int_0^\infty du \int_0^1 dt u^2 \mathcal{T}_\sigma(t) \right. \\ & \quad \times \cos(\zeta_{ji} ut) + \int_0^\infty du \int_0^1 dt u^2 \mathcal{A}_\sigma(t) \\ & \quad \left. \times \exp(-\sqrt{n^2-1} \zeta_{ji} ut) \right]. \end{aligned} \quad (4.1)$$

This expression can be evaluated directly, though one has to take care not to separate the two summands since each taken by itself is divergent ([6], Appendix C). The result is the well-known expression for the electrostatic shift, namely,

$$-\left(\frac{n^2-1}{n^2+1}\right)\frac{\alpha}{16m^2\mathcal{Z}^3}\sum_j', \frac{|\mathbf{p}_{\parallel}|^2+2|\mathbf{p}_{\perp}|^2}{E_{ji}^2}, \quad (4.2)$$

plus some ‘‘contact terms,’’ i.e., terms that contribute only when the atom is sitting directly on the surface of the dielectric where  $\mathcal{Z}=0$ . These are physically irrelevant because the macroscopic model is inapplicable anyway for atom-surface distances of the order of the Bohr radius and below. Alternatively, one could analyze Eq. (4.1) by applying the transformation devised in Sec. II B, which greatly simplifies the calculation and leads to elementary integrals. Surprisingly, though, this approach yields just the electrostatic shift (4.2) but no ‘‘contact terms.’’ The only possible cause for the mysterious disappearance of the contact terms is the singular behavior of the transformation at a few places in the domain of integration.

Finally, we would like to comment on the difference between dipole and minimal-coupling Hamiltonians when applied in cavity QED. We have seen in this paper and in comparison with the analysis of [6] that there is no great advantage or disadvantage to either. Both lead to similar expressions when the field has been quantized by a normal-mode expansion. Depending on the particular problem at hand, it may or may not be convenient to have the electrostatic interaction included in the dipole Hamiltonian or handle it separately when working in minimal coupling. What makes a great deal of difference, however, is whether one works with a mode expansion or with linear-response theory and the Green’s function of the field. The mode-expansion approach permits easy asymptotic analysis in the near zone, and the Green’s-function approach greatly simplifies the asymptotic analysis in the far zone. The transformation devised in this paper lets one have the best of both worlds without duplicating a calculation, which for complicated systems may not even be possible.

#### ACKNOWLEDGMENTS

It is a pleasure to acknowledge financial support for S.T.W. from the National Science Council of Taiwan, and for C.E. from the Royal Society and through a grant from the U.K. Engineering and Physical Sciences Research Council.

#### APPENDIX: NORMAL MODES

In this appendix we provide details about the notations used in the text, and also explicit expressions for the normal modes  $\mathbf{f}_{\nu}(\mathbf{r})$  in the mode expansion (2.4). We label each normal mode by its incident wave. For instance, the normal mode with the incident wave vector  $\mathcal{K}$  and the polarization  $\varrho$  is described by the mode function  $\mathbf{f}_{\nu}(\mathbf{r}, t)$  with  $\nu = (\varrho, \mathcal{K})$ . It is helpful to introduce a notation which distinguishes wave vectors that belong to different sides of the interface. We follow the convention of Carniglia and Mandel [19] and use  $\mathbf{K}$  for wave vectors belonging to the side  $z > 0$ , and  $\mathbf{k}$  for those belonging to the other side,  $z < 0$ . In our geometry, this means that the incident wave vector is

$$\mathcal{K} = \begin{cases} \mathbf{K} & \text{for right-incident modes} \\ \mathbf{k} & \text{for left-incident modes,} \end{cases} \quad (A1)$$

and the sum over modes is

$$\begin{aligned} \sum_{\nu} &\equiv \sum_{\varrho} \int \frac{d^3\mathcal{K}}{(2\pi)^3} \\ &= \sum_{\varrho} \left[ \int_{K_z < 0} \frac{d^3\mathbf{K}}{(2\pi)^3} + \int_{k_z > 0} \frac{d^3\mathbf{k}}{(2\pi)^3} \right]. \end{aligned} \quad (A2)$$

The normal modes  $\mathbf{f}_{\nu}(\mathbf{r})$  form an orthogonal, complete set [20]. For comparison with previous workers [19,21,22] we point out that we have chosen a slightly different normalization; in our case the orthonormality relation is

$$\int d^3\mathbf{r} \epsilon(\mathbf{r}) \mathbf{f}_{\varrho, \mathcal{K}}^*(\mathbf{r}) \cdot \mathbf{f}_{\varrho', \mathcal{K}'}(\mathbf{r}) = (2\pi)^3 \delta_{\varrho\varrho'} \delta^{(3)}(\mathcal{K} - \mathcal{K}'). \quad (A3)$$

The two polarizations of the modes are widely known as transverse electric (‘‘TE’’) and transverse magnetic (‘‘TM’’), or, in the language of Ref. [17],  $s$  and  $p$  wave modes (see also [13,14]). The explicit form of the  $\mathbf{f}_{\nu}(\mathbf{r})$  is

$$\begin{aligned} \mathbf{f}_{s, \mathbf{K}}(\mathbf{r}) &= \hat{\boldsymbol{\epsilon}} \left( e^{i\mathbf{K}\cdot\mathbf{r}} \Theta(z) + \frac{K_z - k_z}{K_z + k_z} e^{i\mathbf{K}^{(R)}\cdot\mathbf{r}} \Theta(z) \right. \\ &\quad \left. + \frac{2K_z}{K_z + k_z} e^{i\mathbf{k}\cdot\mathbf{r}} \Theta(-z) \right), \end{aligned} \quad (A4)$$

$$\begin{aligned} \mathbf{f}_{s, \mathbf{k}}(\mathbf{r}) &= \frac{\hat{\boldsymbol{\epsilon}}}{n} \left( e^{i\mathbf{k}\cdot\mathbf{r}} \Theta(-z) + \frac{k_z - K_z}{k_z + K_z} e^{i\mathbf{K}^{(R)}\cdot\mathbf{r}} \Theta(-z) \right. \\ &\quad \left. + \frac{2k_z}{k_z + K_z} e^{i\mathbf{K}\cdot\mathbf{r}} \Theta(z) \right), \end{aligned} \quad (A5)$$

$$\begin{aligned} \mathbf{f}_{p, \mathbf{K}}(\mathbf{r}) &= - \left( (\hat{\mathbf{K}} \times \hat{\boldsymbol{\epsilon}}) e^{i\mathbf{K}\cdot\mathbf{r}} \Theta(z) \right. \\ &\quad + (\hat{\mathbf{K}}^{(R)} \times \hat{\boldsymbol{\epsilon}}) \frac{n^2 K_z - k_z}{n^2 K_z + k_z} e^{i\mathbf{K}^{(R)}\cdot\mathbf{r}} \Theta(z) \\ &\quad \left. + (\hat{\mathbf{k}} \times \hat{\boldsymbol{\epsilon}}) \frac{2nK_z}{n^2 K_z + k_z} e^{i\mathbf{k}\cdot\mathbf{r}} \Theta(-z) \right), \end{aligned} \quad (A6)$$

$$\begin{aligned} \mathbf{f}_{p, \mathbf{k}}(\mathbf{r}) &= - \frac{1}{n} \left( (\hat{\mathbf{k}} \times \hat{\boldsymbol{\epsilon}}) e^{i\mathbf{k}\cdot\mathbf{r}} \Theta(-z) \right. \\ &\quad + (\hat{\mathbf{k}}^{(R)} \times \hat{\boldsymbol{\epsilon}}) \frac{k_z - n^2 K_z}{k_z + n^2 K_z} e^{i\mathbf{K}^{(R)}\cdot\mathbf{r}} \Theta(-z) \\ &\quad \left. + (\hat{\mathbf{K}} \times \hat{\boldsymbol{\epsilon}}) \frac{2nk_z}{k_z + n^2 K_z} e^{i\mathbf{K}\cdot\mathbf{r}} \Theta(z) \right), \end{aligned} \quad (A7)$$

where



$$k_z = -\sqrt{n^2 K^2 - K_x^2 - K_y^2} \quad (\text{A8})$$

in Eqs. (A4) and (A6), and

$$K_z = \sqrt{k^2/n^2 - k_x^2 - k_y^2} \quad (\text{A9})$$

in Eqs. (A5) and (A7).  $\mathbf{K}^{(R)} = (K_x, K_y, -K_z)$  is the reflected

wave vector of  $\mathbf{K}$ , and similarly  $\mathbf{k}^{(R)}$  is of  $\mathbf{k}$ ;  $\hat{\mathbf{K}}$  is the unit vector of  $\mathbf{K}$ , and similarly for the other vectors.  $\Theta(z)$  is the Heaviside step function.

A convenient choice for the unit polarization vector  $\hat{\boldsymbol{\epsilon}}$  is

$$\hat{\boldsymbol{\epsilon}} = (\boldsymbol{\kappa} \times \hat{\mathbf{z}}) / |\boldsymbol{\kappa} \times \hat{\mathbf{z}}|. \quad (\text{A10})$$

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