Coupled dipole method for scatterers with large permittivity

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In the coupled dipole method, a three-dimensional scattering object is discretized over a lattice into a set of polarizable units that are coupled self-consistently. Starting from the volume integral equation for the field, we show that performing the integration of the free-space field susceptibility tensor over the lattice cell dramatically improves the accuracy of the method when the permittivity of the object is large. This integration, done without any approximation, allows us to define a prescription for the polarizability used in the coupled dipole method. Our derivation is not restricted to any particular shape of the scatterer or to a cubic discretization lattice.

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I. INTRODUCTION

The scattering of an electromagnetic wave by an arbitrary, three-dimensional scatterer is a complex problem of central importance in optics and photonics. Aside from a few particular systems, the interaction of electromagnetic waves with an arbitrary object eludes an analytical representation and numerical methods are needed. Many such methods have been developed and we refer the reader to the detailed review by Kahnert [1] where the strengths and weaknesses of each method are discussed.

In this article we consider one such three-dimensional scattering approach called the coupled dipole method (CDM). This method was introduced by Purcell and Pennypacker [2] to study the scattering of light by interstellar grains with arbitrary shapes. It has been used to compute cross sections [3], optical forces [4–6], near-field light scattering [7], and spontaneous emission [8]. The theoretical foundation of the CDM relies on the fact that when an object interacts with an electromagnetic field it develops a polarization. If one considers a small enough volume inside the object, the induced polarization is uniform within this volume, and hence that small region can be represented by an electric dipole with the appropriate polarizability. Therefore, any object can be discretized as a collection of dipolar subunits. In this article we show that accounting for finite size effects for the subunits significantly improves the description of light scattering by arbitrary objects. Our formulation of the CDM is obtained through the integration of the field susceptibility tensor over the volume associated with the dipole, hence defining a different form for the polarizability. The formulation of the CDM derived here improves the accuracy of the method when dealing with scatterers with large permittivities, a situation where the conventional CDM performs poorly.

In Sec. II we describe our formulation of the CDM. In Sec. III we test the accuracy of this formulation of the polarizability and compare it to previous prescriptions. Finally, in Sec. IV we present our conclusions. The details of the computation of the integrated field susceptibility tensor are given in the Appendix.

II. THEORY

Let $\mathbf{E}^0(\omega)$ be the electric field associated with an electromagnetic wave impinging on an arbitrary object (for the sake of simplicity we will assume that the object is nonmagnetic). The incident field induces a polarization inside the object. The self-consistent electric field inside the object reads

$$\mathbf{E}(\mathbf{r},\omega) = \mathbf{E}^0(\mathbf{r},\omega) + \int_V \overleftrightarrow{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega)\chi(\mathbf{r}',\omega)\mathbf{E}(\mathbf{r}',\omega)d\mathbf{r}', \qquad (1)$$

where the integration is performed over the volume of the object. $\mathbf{E}(\mathbf{r}',\omega)$ is the macroscopic field inside the object, $\chi(\mathbf{r}',\omega)$ is the linear susceptibility of the object which we will suppose to be homogeneous, i.e.,

$$\chi(\mathbf{r}',\omega) = \chi(\omega) = \frac{\varepsilon(\omega)-1}{4\pi}, \qquad (2)$$

where $\varepsilon(\omega)$ is the relative permittivity of the object, and $\overleftrightarrow{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega)$ is the free-space electric field susceptibility tensor, which can be written as [9]

$$\overleftrightarrow{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega) = e^{(ik_0R)}\left[\left(3\frac{\mathbf{R}\otimes\mathbf{R}}{R^2} - \overleftrightarrow{\mathbf{I}}\right)\left(\frac{1}{R^3} - \frac{ik_0}{R^2}\right) + \left(\overleftrightarrow{\mathbf{I}} - \frac{\mathbf{R}\otimes\mathbf{R}}{R^2}\right)\frac{k_0^2}{R}\right] - \frac{4\pi}{3}\overleftrightarrow{\mathbf{I}}\delta(\mathbf{R}), \qquad (3)$$

with $\mathbf{R}=\mathbf{r}-\mathbf{r}'$, k_0 the modulus of the wave vector in vacuum, and $\overleftrightarrow{\mathbf{I}}$ the unit tensor. To solve Eq. (1) numerically we dis-

cretize the object into a set of N subunits arranged on a cubic lattice (for simplicity, but our approach holds for any arbitrary orthogonal lattice); hence Eq. (1) becomes

$$\mathbf{E}(\mathbf{r},\omega) = \mathbf{E}^0(\mathbf{r},\omega) + \sum_{j=1}^{N} \int_{V_j} \overleftrightarrow{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega)\chi(\omega)\mathbf{E}(\mathbf{r}',\omega)d\mathbf{r}'. \quad (4)$$

To solve Eq. (1) numerically we need to make some approximations. The first one is usually to assume that the electromagnetic field is uniform over one subunit, which is a good approximation if the subunit is smaller than the wavelength inside the object. Then Eq. (4) can be written as

$$\mathbf{E}(\mathbf{r}_i,\omega) = \mathbf{E}^0(\mathbf{r}_i,\omega) + \sum_{j=1}^{N} \left(\int_{V_j} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}',\omega)d\mathbf{r}' \right) \chi(\omega)\mathbf{E}(\mathbf{r}_j,\omega). \quad (5)$$

Equation (5) is the starting point of our method. In the original form of the CDM, another approximation is made: the field susceptibility tensor is taken to be constant over any subunit. This entails that

$$\mathbf{E}(\mathbf{r}_i,\omega) = \mathbf{E}^0(\mathbf{r}_i,\omega) + \sum_{j=1,j\neq i}^{N} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}_j,\omega)\chi(\omega)\mathbf{E}(\mathbf{r}_j,\omega) - \frac{\varepsilon(\omega)-1}{3}\mathbf{E}(\mathbf{r}_i,\omega). \quad (6)$$

If we factorize the terms corresponding to the index i, we get

$$\mathbf{E}^l(\mathbf{r}_i,\omega) = \mathbf{E}^0(\mathbf{r}_i,\omega) + \sum_{j=1,j\neq i}^{N} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}_j,\omega)\alpha_j^0(\omega)\mathbf{E}^l(\mathbf{r}_j,\omega) \quad (7)$$

with

$$\alpha_j^0(\omega) = \frac{3}{4\pi}\frac{\varepsilon(\omega)-1}{\varepsilon(\omega)+2}V_j. \quad (8)$$

Equation (8) is the Clausius-Mossotti relation for the polarizability of the cubic subunit j and $\mathbf{E}^l=[(\varepsilon+2)/3]\mathbf{E}$ is the local field expressed in terms of the macroscopic field. Equation (7) is the original form of the CDM introduced by Purcell and Pennypacker [2]. The problem with this formulation is that if one computes the cross section using Eq. (8) one gets an incorrect result. This is due to the fact that the optical theorem is not satisfied. A radiation reaction term must be introduced in the expression of the polarizability to satisfy the optical theorem [3,10]:

$$\alpha_j(\omega) = \alpha_j^0(\omega)/[1-(2/3)ik_0\alpha_j^0(\omega)]. \quad (9)$$

The importance of including the radiation reaction term in the polarizability is also discussed in detail in Refs. [5,11] Several ideas have been put forward to improve the accuracy of the CDM [12–15]. These approaches have in common that they all start from the Clausius-Mossotti relation and simply add a finite-frequency correction. They also suppose that the field susceptibility tensor is constant over any given subunit. Recently, it was pointed out that the Clausius-Mossotti relation may not hold for every subunit; rather, for each subunit the polarizability should be related to its local environment [16,17]. However, so far this approach has been restricted to special geometries.

In this paper we propose a formulation of the scattering process that accounts for the geometry of the scatterer without being restricted to a particular set of shapes. Going back to Eq. (5), instead of the usual approach described previously, we compute the volume integration of the free-space susceptibility numerically. Equation (5) thus becomes

$$\mathbf{E}(\mathbf{r}_i,\omega) = \mathbf{E}^0(\mathbf{r}_i,\omega) + \sum_{j=1,j\neq i}^{N} \left(\int_{V_j} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}',\omega)d\mathbf{r}' \right) \chi(\omega)\mathbf{E}(\mathbf{r}_j,\omega) + \left(\int_{V_i} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}',\omega)d\mathbf{r}' \right) \chi(\omega)\mathbf{E}(\mathbf{r}_i,\omega). \quad (10)$$

The integrated tensor is defined as $\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_j,\omega) = \int_{V_j} \overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}',\omega)d\mathbf{r}'$. We have isolated the diagonal term ($i=j$) as, whereas the case $i\neq j$ is easy to perform numerically, the diagonal term needs particular attention. To compute the last term of Eq. (10), $\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$, a Weyl expansion of the tensor is performed. After a tedious derivation we can write this term as

$$\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega) = \frac{16}{\pi}\overleftrightarrow{\mathbf{I}}\left\{ \int_{w_0=0}^{k_0} \frac{-k_0^2(1-e^{iw_0\Delta/2}) - w_0^2 e^{iw_0\Delta/2}}{w_0} \left[\int_{\theta=0}^{\pi/2} \frac{\sin(k_p\cos\theta\Delta/2)\sin(k_p\sin\theta\Delta/2)}{k_p^2\cos\theta\,\sin\theta} d\theta \right] dw_0 + \int_{\beta=0}^{\infty} \frac{k_0^2-(k_0^2+\beta^2)e^{-\beta\Delta/2}}{\beta} \left[\int_{\theta=0}^{\pi/2} \frac{\sin(k_e\cos\theta\Delta/2)\sin(k_e\sin\theta\Delta/2)}{k_e^2\cos\theta\,\sin\theta} d\theta \right] d\beta \right\}, \quad (11)$$

with $k_p=\sqrt{k_0^2-w_0^2}$, $k_e=\sqrt{k_0^2+\beta^2}$, and Δ the lattice spacing. Equation (11) does not contain any approximations. To our knowledge this is the first time that $\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ has been expressed in an exact form which can be computed numerically in an efficient way. Further details on the derivation of Eq. (11) are given in the Appendix.

When Δ tends toward 0, we find that $\lim_{\Delta\to 0}\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega) = -(4\pi/3)\overleftrightarrow{\mathbf{I}}$ which is the depolarization

factor computed at the center of a cube as given by Yaghjian [18]. After some work, Eq. (10) can be written in the form introduced by Purcell and Pennypacker [2]:

$$\mathbf{E}^l(\mathbf{r}_i,\omega)=\mathbf{E}^0(\mathbf{r}_i,\omega)+\sum_{j=1,j\neq i}^{N}\frac{\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_j,\omega)}{V_j}\alpha_j(\omega)\mathbf{E}^l(\mathbf{r}_j,\omega), \quad (12)$$

where the local field is defined by

$$\mathbf{E}^l(\mathbf{r}_i,\omega)=\left(\overleftrightarrow{\mathbf{I}}-\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)\frac{\varepsilon(\omega)-1}{4\pi}\right)\mathbf{E}(\mathbf{r}_i,\omega). \quad (13)$$

Notice that when $\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ reduces to $(-4\pi/3)\overleftrightarrow{\mathbf{I}}$ we recover the definition of the local field that we derived previously. The polarizability of the subunit j is now expressed as

$$\alpha_j(\omega)=\alpha_j^0(\omega)\left(1-\frac{G^{\mathrm{int}}(\mathbf{r}_j,\mathbf{r}_j,\omega)+4\pi/3}{V_j}\alpha_j^0(\omega)\right)^{-1}. \quad (14)$$

In the present study the subunit has a cubic shape and the medium is isotropic; hence the polarizability is a scalar. In Eq. (12), the quantity $\alpha_j(\omega)\mathbf{E}^l(\mathbf{r}_j,\omega)=\mathbf{p}(\mathbf{r}_j,\omega)$ is the dipole moment of subunit j induced by the incident field and the field scattered by all other subunits. Working with the local field is very convenient if one wants to evaluate the optical forces [5,6]. Yet there exist other approaches, such as the method of moments (MOM), that use the macroscopic field instead. In most three-dimensional implementations, the MOM simply amounts to solving Eq. (6), which is formally equivalent to the CDM [12,19] Eq. (7). However, only in the special case of two-dimensional objects in a stratified medium, has the integration of the field susceptibility tensor over the subunits been proposed [20].

If we perform a Taylor expansion of the imaginary part of $G^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ with respect to $k_0\Delta$, we obtain $\mathrm{Im}[G^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)/V_i]\approx(2/3)k_0^3$. Hence the radiation reaction term that is usually added to the Clausius-Mossotti polarizability appears naturally in our formulation. This radiation reaction term represents the damping of the dipole by its self-field. As the dipole oscillates, it generates an electric field $\mathbf{E}_{RR}$ at its location. The part of the electric field that is in quadrature with the dipole oscillations performs work on the dipole which dampens its oscillations. For a point dipole we have $\mathbf{E}_{RR}=i(2/3)k_0^3\mathbf{p}$ [9]. In our case, due to the finite size of the subunit, the radiation reaction field is directly connected to the integration of the imaginary part of the free-space field susceptibility: $\mathbf{E}_{RR}=i\mathrm{Im}[\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)/V_i]\mathbf{p}$.

We have performed the quadrature over a cubic subunit, but the quadrature can be done over a parallelepiped (see the Appendix). In that case $\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ would always be a diagonal tensor but the elements of the diagonal can be different [see Eq. (A8) of the Appendix]. Such a lattice geometry would, for instance, be useful to study the scattering of light by an object with significantly different extensions in the three directions of space.

III. RESULTS

To test the accuracy resulting from the integration of the tensor we study the scattering of light by a homogeneous sphere, as an analytic solution is known in the form of a Mie series, but we emphasize that the method presented here does not depend on the shape of the scatterer. We will compare our results to the extinction, absorption, and scattering efficiencies computed after using the Mie solution. The computation of the cross sections with the CDM is performed using Eq. (3.01) of Ref. [3] for the extinction, and Eq. (3.06) of Ref. [3] for the absorption, i.e.,

$$C_{\mathrm{ext}}=\frac{4\pi k_0}{|\mathbf{E}^0|^2}\sum_{j=1}^{N}\mathrm{Im}[\mathbf{E}^0(\mathbf{r}_j,\omega)\cdot\mathbf{p}^*(\mathbf{r}_j,\omega)], \quad (15)$$

$$C_{\mathrm{abs}}=\frac{4\pi k_0}{|\mathbf{E}^0|^2}\sum_{j=1}^{N}|\mathbf{p}(\mathbf{r}_j,\omega)|^2\left[\mathrm{Im}\left(\frac{1}{\alpha_j(\omega)}\right)-\frac{2}{3}k_0^3\right]. \quad (16)$$

The scattering cross section is obtained as the difference between the extinction and absorption cross sections [3]. If we use the polarizability defined by Eq. (14), Eq. (15) is always used for obtaining the extinction cross section, but the absorption cross section is now computed as

$$C_{\mathrm{abs}}=\frac{4\pi k_0}{|E_0|^2}\sum_{j=1}^{N}|\mathbf{E}^l(\mathbf{r}_j,\omega)|^2\{\mathrm{Im}[\alpha_j(\omega)] - \mathrm{Im}[G^{\mathrm{int}}(\mathbf{r}_j,\mathbf{r}_j,\omega)]|\alpha_j(\omega)|^2\}, \quad (17)$$

where $\mathrm{Im}[G^{\mathrm{int}}(\mathbf{r}_j,\mathbf{r}_j,\omega)]$ represents the energy lost by a radiating dipole. We will compare the present formulation (IT for integrated tensor) of the polarizability to other known prescriptions. We will consider the usual CDM with radiation reaction (RR) correction [Eq. (9)], the lattice dispersion relation (LDR) [15], and the polarizability defined by Lakhtakia (LAK) [12]. Lakhtakia defines the polarizability by integrating the field susceptibility over a spherical region of the same volume as the cubic subunit [19]. In that case the polarizability is analytical. To check the validity of the approximation done by Lakhtakia, we will compute the cross sections with Eq. (14) for the definition of the polarizability, i.e., by integrating only the diagonal elements of the tensor (IDT).

The sphere is discretized into $N=2320$ subunits. We present in Figs. 1 and 2 the relative error in percent between Mie and the different method used versus $|n|k_0\Delta$, where n is the refractive index of the object: $n=\sqrt{\varepsilon}$ ($|n|k_0\Delta$ large corresponds to a large value of Δ).

In Fig. 1 we have taken $\varepsilon=2.25+i$. We first observe that the integration of the diagonal term only (IDT) leads to a result very close to that obtained with the polarizability of Lakhtakia. Thus, the approximation made by Lakhtakia by replacing the cube by a sphere is valid. Then, we notice that the integration of the field susceptibility tensor for all terms (IT) yields an overall slightly more accurate cross section.

In Fig. 2 we perform the same calculation but for a large relative permittivity: $\varepsilon=10+10i$. The IDT result is still close to the one given by the Lakhtakia method. We see that the IT method is better for all the cross sections from small values of $|n|k_0\Delta$ until $|n|k_0\Delta\approx 0.3$. The fact that the IT method is better for small $|n|k_0\Delta$ is always true irrespective of the value of the relative permittivity (in Fig. 1 due to the small

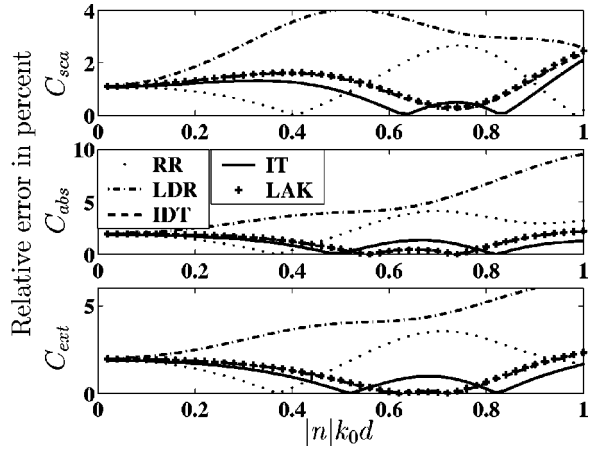

FIG. 1. Scattering properties of a pseudosphere with $N=2320$ and $\varepsilon=n^2=2.25+i$. Relative error (in percent) for the extinction, absorption, and scattering cross sections between different methods and the exact Mie result. The relative error is plotted versus the normalized lattice spacing $|n|k_0\Delta$, where k_0 is the free-space wave vector of the incident light. Dotted line, radiation reaction correction (RR); dash-dotted line, lattice dispersion relation (LDR); dashed line, polarizability is defined by integrating only the diagonal element of the tensor (IDT); solid line, computation is done by integrating all the elements of the field susceptibilities tensor (IT). The curves with the symbol + pertain to calculations using the polarizability defined by Lakhtakia.

value of the relative permittivity this is true only until $|n|k_0\Delta=0.1$). When the size of the subunit is very small compared to the wavelength, the field susceptibility tensor $\overleftrightarrow{\mathbf{G}}(\mathbf{r}_j,\mathbf{r}_j,\omega)$ for $\mathbf{r}_j$ in the vicinity of $\mathbf{r}_i$ varies as $1/|\mathbf{r}_j-\mathbf{r}_i|^3$; hence the approximation of a uniform field susceptibility tensor over the subunit does not hold. Therefore, the integration of $\overleftrightarrow{\mathbf{G}}(\mathbf{r}_j,\mathbf{r}_j,\omega)$ allows us to go beyond this approximation. For any given value of $|n|k_0\Delta$, different relative permittivities correspond to different sizes of the subunit, the size decreasing when the relative permittivity increases. This is the reason why the difference between the IT and the other results is more visible in Fig. 2 where the relative permittivity is larger.

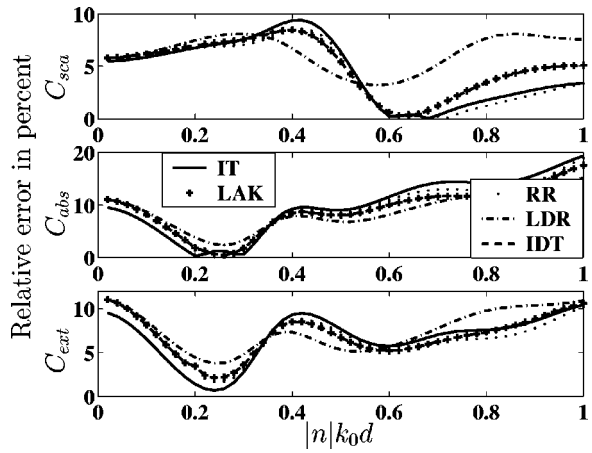

FIG. 2. Same as Fig. 1 but for $\varepsilon=n^2=10+10i$.

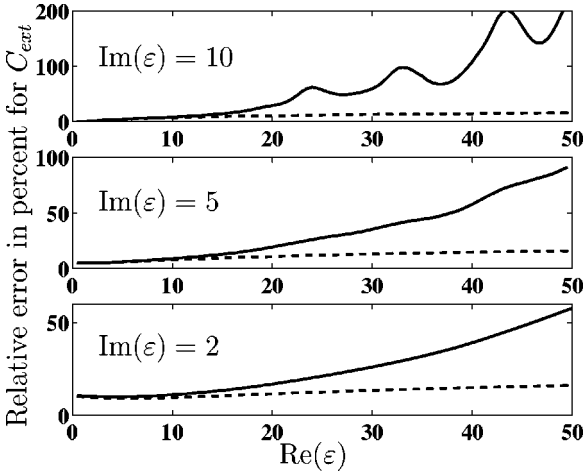

FIG. 3. Relative error (in percent) for the extinction cross section for $|n|k_0\Delta=0.02$ versus $\mathrm{Re}(\varepsilon)$ for three different values of $\mathrm{Im}(\varepsilon)$. Solid line, radiation reaction correction (RR); dashed line, computation done by integrating all the elements of the field susceptibility tensor (IT).

To be more general, Fig. 3 presents the error on the extinction cross section for a given $|n|k_0\Delta=0.02$, versus the real part of the relative permittivity for three different imaginary part of the relative permittivity: $\mathrm{Im}(\varepsilon)=2$, 5, and 10. We compare the IT result to the standard calculation accounting only for the radiation reaction term (RR). Note that all the other prescriptions of the polarizability are equivalent to RR for this small value of $|n|k_0\Delta$. Figure 3 shows clearly that the IT method leads to a better estimate of the cross section. This is particularly true when the polarizability has a small imaginary part (2) and a large real part (50). In that case the relative error is about 200% for RR whereas the IT calculation gives a relative error below 15%. We can even see some oscillations in the RR method due to morphological resonances, which are usually hard to describe with the CDM when the imaginary part of the permittivity is small. These oscillations are not present in the IT calculation, which demonstrates the robustness of our present prescription for the polarizability. In fact, irrespective of $\mathrm{Im}(\varepsilon)$, the IT method gives the same relative error for $\mathrm{Re}(\varepsilon)=50$, less than 15%. Notice that for the sake of computation time we use a small number N of subunits; however, increasing N would decrease the relative error.

IV. CONCLUSION

In conclusion we have derived a prescription for the polarizability in which the interaction of each subunit with itself is treated by accounting for its finite volume, through the integration of the full field susceptibility tensor over the subunit. This integration is performed without any approximation. In doing this we validate the approximations used by Lakhtakia in his derivation of a polarizability with finite-size effects. Our derivation is, however, more general and can be applied to a formulation of the coupled dipole method with a noncubic orthogonal lattice. It should be possible to extend our approach to a case where the subunits have arbitrary

shapes; however, in such a case the polarizability tensor may not be diagonal. We showed that integrating the full field susceptibility tensor increases the accuracy of the CDM when the size of the subunit is small compared to the wavelength in the medium. These results are particularly dramatic when the relative permittivity becomes large, a situation where the conventional formulation of the CDM performs very poorly. Finally, we emphasize that the approach presented here is not restricted to any particular geometry of the scatterer.

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APPENDIX: COMPUTATION OF THE DIAGONAL TERM OF THE FREE-SPACE FIELD SUSCEPTIBILITY

A Weyl expansion of the tensor $\overleftrightarrow{\mathbf{G}}$ yields [21]

$$\overleftrightarrow{\mathbf{G}}(\mathbf{r}_i,\mathbf{r}',\omega)=\frac{i}{2\pi}\left[\int_{\mathbf{k}}\frac{dk_x dk_y}{w_0}\overleftrightarrow{\mathbf{M}}\times e^{\{i[k_x(x_i-x')+k_y(y_i-y')+iw_0|z_i-z'|]\}}\right]-4\pi\delta(\mathbf{r}_i-\mathbf{r}') \tag{A1}$$

with

$$\overleftrightarrow{\mathbf{M}}=\begin{pmatrix} k_0^2-k_x^2 & -k_xk_y & -\gamma w_0 k_x \\ k_xk_y & k_0^2-k_y^2 & -\gamma w_0 k_y \\ -\gamma w_0 k_x & -\gamma w_0 k_y & k^2 \end{pmatrix}, \tag{A2}$$

where $\gamma=\mathrm{sgn}(z_i-z')$, $w_0=\sqrt{k_0^2-k^2}$, and $k^2=k_x^2+k_y^2$. Using Eq. (A1), the integrated tensor over a subunit is defined as

$$\overleftrightarrow{\mathbf{G}}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)=\left[\int_{V_i}d^3\mathbf{r}'\frac{i}{2\pi}\int_{\mathbf{k}}\frac{dk_x dk_y}{w_0}\overleftrightarrow{\mathbf{M}}\times e^{\{i[k_x(x_i-x')+k_y(y_i-y')+iw_0|z_i-z'|]\}}\right]-4\pi \tag{A3}$$

$$=\frac{i}{2\pi}\left[\int_{\mathbf{k}}\frac{dk_x dk_y}{w_0}\overleftrightarrow{\mathbf{M}}\int_{V_i}d^3\mathbf{r}'\times e^{\{i[k_x(x_i-x')+k_y(y_i-y')+iw_0|z_i-z'|]\}}\right]-4\pi.$$

It is easy to perform the integration over the spatial coordinates using Δ as the spacing lattice of the subunit ($V_i=\Delta^3$). Incidentally, one can note that the nondiagonal terms of the integrated tensor vanish, and that the components xx, yy, and zz are physically identical. Hence, with $M_{zz}=k^2$, we obtain

$$G_{zz}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)=\frac{4}{\pi}\left[\int_{\mathbf{k}}dk_x dk_y\frac{\sin(k_x\Delta/2)\sin(k_y\Delta/2)}{k_xk_y}\times\frac{k^2}{w_0^2}(-1+e^{iw_0\Delta/2})\right]-4\pi. \tag{A4}$$

The problem in computing this integral numerically is that the integral converges very slowly, as the integrand varies as $1/k$ when k_x,k_y tend to infinity. To solve this problem of convergence we use the following relation:

$$I=-\frac{4}{\pi}\int_{\mathbf{k}}dk_x dk_y\frac{\sin(k_x\Delta/2)\sin(k_y\Delta/2)}{k_xk_y}=-4\pi. \tag{A5}$$

Now if we move to polar coordinates ($dk_xdk_y=kdkd\theta$), we have

$$G_{zz}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)=\frac{4}{\pi}\int_{k=0}^{\infty}\int_{\theta=0}^{2\pi}\frac{kdkd\theta}{w_0^2}(-k_0^2+k^2e^{iw_0\Delta/2})\times\frac{\sin(k\cos\theta\Delta/2)\sin(k\sin\theta\Delta/2)}{k^2\cos\theta\sin\theta}. \tag{A6}$$

This new integrand converges as $1/k^3$ when k tends to infinity; hence a fast convergence is obtained. However, when $k=k_0$ we have $w_0=0$ and the integrand is not defined. This value corresponds to the transition from propagating to evanescent modes ($k>k_0$). We change the variable of integration to w_0 and use $kdk=-w_0dw_0$. Using parity considerations we finally get

$$G_{zz}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)=\frac{16}{\pi}\left(\int_{w_0=k_0}^{0}+\int_{w_0=0}^{i\infty}\right)\times\left[\int_{\theta=0}^{\pi/2}d\theta\frac{\sin(k\cos\theta\Delta/2)\sin(k\sin\theta\Delta/2)}{k^2\cos\theta\sin\theta}\right]\times\frac{k_0^2-k^2e^{iw_0\Delta/2}}{w_0}dw_0. \tag{A7}$$

Equation (A7) is the sum of two integrals. The first one is the integration over the propagating mode ($w_0=0,\ldots,k_0$) and the second one that over the evanescent mode ($w_0=0,\ldots,i\infty$). Therefore Eq. (A7) is defined irrespective of the values of w_0, k, and θ. With a little algebra, Eq. (A7) can be written as Eq. (11) where for the sake of clarity we have separated the two integrals.

If the subunit is not a cube but a parallelepiped ($\Delta_x\times\Delta_y\times\Delta_z$), a similar derivation yields

$$G_{zz}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)=\frac{16}{\pi}\left(\int_{w_0=k_0}^{0}+\int_{w_0=0}^{i\infty}\right)\times\left[\int_{\theta=0}^{\pi/2}d\theta\frac{\sin(k\cos\theta\Delta_x/2)\sin(k\sin\theta\Delta_y/2)}{k^2\cos\theta\sin\theta}\right]\times\frac{k_0^2-k^2e^{iw_0\Delta_z/2}}{w_0}dw_0, \tag{A8}$$

where $G_{xx}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ and $G_{yy}^{\mathrm{int}}(\mathbf{r}_i,\mathbf{r}_i,\omega)$ are obtained by permutation of the indices x,y,z.

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