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Multiple-scattering theory for electromagnetic waves

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In this paper, a multiple-scattering formalism for electromagnetic waves is presented. Its application to the three-dimensional periodic dielectric structures is given in a form similar to the usual Korringa-Kohn-Rostoker form of scalar waves. Using this approach, the band-structure results of touching spheres of diamond structure in a dielectric medium with dielectric constant 12.96 are calculated. The application to disordered systems under the coherent-potential approximation is discussed.

I. INTRODUCTION

Recent theoretically designed periodic structures with sizable photonic band gaps and their experimental realizations[1–4] have stimulated further interest in studies of both the localization of electromagnetic (em) waves and the potential applications of the new photonic band-gap materials. While the current plane-wave-based theories can yield the photonic band structures for three-dimensional (3D) periodic dielectric structures with reasonable accuracy, an adequate treatment of 3D disordered dielectric systems is lacking even in the context of a mean-field theory, e.g., the coherent-potential approximation (CPA). Modern multiple-scattering theory (MST), through its success in the electronic structure calculations for both ordered and disordered systems, shows great promise for studies of propagation and scattering of em waves in both ordered and disordered media.

MST in its modern form has been developed mainly for studies of electronic systems, although it originated from studies of classical waves (including em waves). The scalar wave approximation to em waves, which enables the straightforward application of all the existing MST techniques, has been shown to be inadequate even qualitatively.[5] Therefore, a MST for em waves, taking into account fully their vector wave nature, will provide a unified theoretical scheme for treating both ordered and disordered dielectric systems. In this paper we present a rigorous multiple-scattering formalism and its application to both the periodic and substitutional disordered dielectric systems. We have noticed some previous works on the MST of the em waves.[6] But they only applied the theory to two-dimensional (2D) systems. There has also been some previous work[7] in the study of em waves in a disordered medium using MST. It concentrated mostly on the practical aspects of applications for some special cases such as the long-wavelength limit, rather than providing a general framework of the theory. In this paper we will present a general and rigorous framework and, through a numerical example, demonstrate that MST can be applied to study em waves with relative ease and without the need to invoke approximations. In Sec. II we first derive the MST equations for vector waves. The formalism is given in such a way that only slight modifications of existing Korringa-Kohn-Rostoker (KKR) code for electronic band calculations are necessary for photonic band calculations. The numerical results of photonic bands for touching vacuum spheres of diamond structure in a dielectric medium with dielectric constant 12.96 calculated by this approach is then reported. Finally, we discuss the Green's function in the presence of the scatterers and the prospect of applying the CPA to the em waves.

II. MULTIPLE-SCATTERING THEORY FOR em WAVES

In a medium where the dielectric constant $\epsilon(\mathbf{r})$ is position dependent, Maxwell's equations for em waves can be written as

$$\nabla\times\mathbf{E}=ik\mathbf{H},\quad \nabla\times\mathbf{H}=-ik\epsilon(\mathbf{r})\mathbf{E}\ , \tag{1}$$

which by substitution can be reduced to

$$\nabla\times[\nabla\times\mathbf{E}(\mathbf{r})]-k^2\mathbf{E}(\mathbf{r})=k^2[\epsilon(\mathbf{r})-1]\mathbf{E}(\mathbf{r}) , \tag{2}$$

where $k=\omega/c$, ω is the angular frequency and c is the speed of light in vacuum. Following the discussion given by Newton,[8] we use the free space tensor Green's function which satisfies the differential equation

$$\nabla\times[\nabla\times\mathbf{d}_0(\mathbf{r},\mathbf{r}')]-k^2\mathbf{d}_0(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')\mathbf{I} , \tag{3}$$

with the boundary condition that at large distance r it contains only outgoing spherical waves. We can combine the differential equation (2) and the scattering boundary condition into an integral equation, similar to the so-called Lippmann-Schwinger equation in the scalar wave MST:

$$\mathbf{E}(\mathbf{r})=\mathbf{E}_0(\mathbf{r})+\int d^3\mathbf{r}'\mathbf{d}_0(\mathbf{r},\mathbf{r}')k^2[\epsilon(\mathbf{r}')-1]\mathbf{E}(\mathbf{r}') . \tag{4}$$

The free space Green's function with the boundary condition specified above is given by[8]

$$\mathbf{d}_0(\mathbf{r},\mathbf{r}')=\left[\mathbf{I}+\frac{1}{k^2}\nabla\nabla\right]\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$$=\left[\mathbf{I}-\frac{1}{k^2}\nabla\nabla'\right]\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} . \tag{5}$$

It can be expanded in terms of vector spherical solid harmonics:

$$\mathbf{d}_0(\mathbf{r},\mathbf{r}')=-\sum_{lm\sigma}[|\mathbf{J}_{lm\sigma}(\mathbf{r})\rangle\langle\mathbf{H}_{lm\sigma}(\mathbf{r}')|\Theta(r'-r)+|\mathbf{H}_{lm\sigma}(\mathbf{r})\rangle\langle\mathbf{J}_{lm\sigma}(\mathbf{r}')|\Theta(r-r')] , \tag{6}$$

where l,m are angular indices, σ is either E (for electric multipole mode) or M (for magnetic multipole mode). The vector spherical solid harmonics are defined for the magnetic multipole mode as

$$|\mathbf{J}_{lmM}(\mathbf{r})\rangle=j_l(kr)|\mathbf{X}_{lm}(\hat{\mathbf{r}})\rangle ,\quad \langle\mathbf{J}_{lmM}(\mathbf{r})|=j_l(kr)\langle\mathbf{X}_{lm}(\hat{\mathbf{r}})| , \tag{7}$$

$$|\mathbf{H}_{lmM}(\mathbf{r})\rangle=-ikh_l(kr)|\mathbf{X}_{lm}(\hat{\mathbf{r}})\rangle ,\quad \langle\mathbf{H}_{lmM}(\mathbf{r})|=-ikh_l(kr)\langle\mathbf{X}_{lm}(\hat{\mathbf{r}})| , \tag{8}$$

where the vector spherical harmonics $\mathbf{X}_{lm}$ are defined as

$$\mathbf{X}_{lm}=-i\mathbf{r}\times\nabla Y_{lm}/\sqrt{l(l+1)} .$$

Note that the bra-ket notation for the magnetic multipole mode applies only on the spherical harmonics:

$$|\mathbf{X}_{lm}(\hat{\mathbf{r}})\rangle=\mathbf{X}_{lm}(\hat{\mathbf{r}}),\quad \langle\mathbf{X}_{lm}(\hat{\mathbf{r}})|=\mathbf{X}^*_{lm}(\mathbf{r}) , \tag{9}$$

and the prefactor $-i$ in Eq. (8) does not change sign. The electric multipole modes can be defined in terms of the magnetic multipole mode as follows:

$$|\mathbf{Z}_{lmE}(\mathbf{r})\rangle=-\frac{i}{k}\nabla\times|\mathbf{Z}_{lmM}\rangle , \tag{10}$$

$$\langle\mathbf{Z}_{lmE}(\mathbf{r})|=\frac{i}{k}\nabla\times\langle\mathbf{Z}_{lmM}| , \tag{11}$$

where $\mathbf{Z}$ stands for either $\mathbf{J}$ or $\mathbf{H}$.

Using Eq. (2) to substitute the factor $k^2[\epsilon(\mathbf{r})-1]\mathbf{E}$ in the integrand of Eq. (4) by $\nabla\times(\nabla\times\mathbf{E})-k^2\mathbf{E}$, integrating by parts, and making use of the equation for the free space Green's function, Eq. (3), the integral equation, Eq. (4) is transformed into

$$\mathbf{E}_0(\mathbf{r})=\oint d\mathbf{S}'_\infty\cdot\{\mathbf{d}_0(\mathbf{r},\mathbf{r}')\times[\nabla'\times\mathbf{E}(r')]+[\nabla'\times\mathbf{d}_0(\mathbf{r},\mathbf{r}')]\times\mathbf{E}(r')\} , \tag{12}$$

which is a surface integral that encloses the entire assembly of the scatterers.

Now for the treatment of MST we partition the space into nonoverlapping cells with each cell containing a single-cell scattering potential $k^2[\epsilon_j(\mathbf{r})-1]$. We have

$$\mathbf{E}_0(\mathbf{r})=\sum_j\oint d\mathbf{S}'_j\cdot\{\mathbf{d}_0(\mathbf{r},\mathbf{r}')\times[\nabla'\times\mathbf{E}(\mathbf{r}')]+[\nabla'\times\mathbf{d}_0(\mathbf{r},\mathbf{r}')]\times\mathbf{E}(\mathbf{r}')\} . \tag{13}$$

For any given $\mathbf{r}'$ inside and on the surface of cell j, we expand both $\mathbf{E}_0$ and $\mathbf{E}$ in terms of the vector spherical functions:

$$|\mathbf{E}^0(\mathbf{r})\rangle=\sum_{l'm'\sigma'}|\mathbf{J}^j_{l'm'\sigma'}(\mathbf{r})\rangle a^{(0)j}_{l'm'\sigma'} \tag{14}$$

and

$$|\mathbf{E}(\mathbf{r})\rangle=\sum_{l'm'\sigma'}|\mathbf{P}^j_{l'm'\sigma'}(\mathbf{r})\rangle a^j_{l'm'\sigma'} , \tag{15}$$

where the basis functions $\mathbf{P}^j_{lm\sigma}$ are given as

$$|\mathbf{P}^j_{lm\sigma}(\mathbf{r})\rangle=|\mathbf{J}^j_{lm\sigma}(\mathbf{r})\rangle+\int_{\text{cell } j}d\mathbf{r}'\mathbf{d}_0(\mathbf{r},\mathbf{r}')k^2[\epsilon_j(\mathbf{r}')-1]|\cdot\mathbf{P}^j_{lm\sigma}(\mathbf{r}')\rangle . \tag{16}$$

Using the expansion Eq. (6) for $\mathbf{r}$ outside the circumscribing sphere of the scattering potential in cell j, $\mathbf{P}^j_{lm\sigma}(\mathbf{r})$ can be written in terms of the spherical solid harmonics and the scattering t matrix:

$$|\mathbf{P}^j_{lm\sigma}(\mathbf{r})\rangle=|\mathbf{J}^j_{lm\sigma}(\mathbf{r})\rangle+\sum_{l'm'\sigma'}|\mathbf{H}^j_{l'm'\sigma'}(\mathbf{r})\rangle t^j_{l'm'\sigma',lm\sigma}\quad (r>r') , \tag{17}$$

where the scattering t matrix is given by

$$t^j_{l'm'\sigma',lm\sigma}=\int_{\text{cell } j}d\mathbf{r}'\langle\mathbf{J}^j_{l'm'\sigma'}(\mathbf{r}')|k^2[\epsilon_j(\mathbf{r}')-1]\cdot\mathbf{P}^j_{lm\sigma}(\mathbf{r}')\rangle . \tag{18}$$

The basis functions $\mathbf{P}^j_{lm\sigma}$ and the t matrix can be obtained either by solving a differential equation for a regular solution to the single-cell scattering problem whose boundary condition at the surface of the circumscribing sphere of that cell is specified by Eq. (17) or by solving the integral equation, Eq. (16), iteratively. In the case of dielectric spheres, the circumscribing sphere of a cell potential is identical to the dielectric sphere. The solution to the basis functions and the t matrix in this case can be obtained directly from the Mie scattering solution:[8,9]

$$t_{lm\sigma,l'm'\sigma'}=\delta_{l,l'}\delta_{m,m'}\delta_{\sigma,\sigma'}\frac{c_{lm\sigma}}{k(1+ic_{lm\sigma})},$$

and the c's are

$$c_{lmE}=\frac{-\epsilon j_l(k_i)[kaj_l(ka)]'+j_l(ka)[k_iaj_l(k_ia)]'}{\epsilon j_l(k_ia)[kan_l(ka)]'-n_l(ka)[k_iaj_l(k_ia)]'}$$

and

$$c_{lmM}=\frac{-j_l(k_ia)[kan_l(ka)]'+j_l(ka)[k_iaj_l(k_ia)]'}{j_l(k_ia)[kan_l(ka)]'-n_l(ka)[k_iaj_l(k_ia)]'}, \quad (19)$$

where n_l are spherical Neumann functions and $k_i=\sqrt{\epsilon}k$.

Substitute the expansions given by Eqs. (14) and (15), and the expansion of the free space Green's function, Eq. (6), into Eq. (13), and compare the coefficients of $|\mathbf{J}_{lm\sigma}(\mathbf{r}_i)\rangle$. We obtain

$$\sum_{j,l'm'\sigma'}[\langle\mathbf{H}^i_{lm\sigma}(\mathbf{R}_j-\mathbf{R}_i+\mathbf{r}_j)|,|\mathbf{P}^j_{l'm'\sigma'}(\mathbf{r}_j)\rangle]_{S_j}\times a^j_{l'm'\sigma'}=-a^{(0)i}_{lm\sigma}, \quad (20)$$

where S_j denotes the surface of cell j and we have used the following shorthand notation for the Wronskian-like surface integrals:

$$[\mathbf{A},\mathbf{B}]_S\equiv\oint d\mathbf{S}\cdot\{\mathbf{A}(\mathbf{r})\times[\nabla\times\mathbf{B}(\mathbf{r})]+[\nabla\times\mathbf{A}(\mathbf{r})]\times\mathbf{B}(\mathbf{r})\}. \quad (21)$$

Equation (20) is the general form of the secular equation in MST. However, the use of the cell surface integrals is often cumbersome. It can be greatly simplified for dielectric spheres, as described in the following process.

If we use the Gaussian theorem to convert the above surface integral into a volume integral, it is easy to show that if both $\mathbf{A}$ and $\mathbf{B}$ are solutions to Eq. (2) with constant dielectric constant ϵ inside the volume enclosed by the surface S, they satisfy

$$[\mathbf{A}(\mathbf{r}),\mathbf{B}(\mathbf{r})]_S=0. \quad (22)$$

This identity allows us to convert the cell surface integral in Eq. (20) to a surface integral over the circumscribing sphere of the single-cell scattering potential;

$$\sum_{j,l'm'\sigma'}[\langle\mathbf{H}^i_{lm\sigma}(\mathbf{R}_j-\mathbf{R}_i+\mathbf{r}_j)|,|\mathbf{P}^j_{l'm'\sigma'}(\mathbf{r}_j)\rangle]_{S^{\rm cir}_j}a^j_{l'm'\sigma'}=-a^{(0)i}_{lm\sigma}, \quad (23)$$

where $S^{\rm cir}_j$ denotes the surface of the circumscribing sphere of cell j.

To convert Eq. (23) into a more usable form, we use the identities Eqs. (A14)–(A16) in Appendix A and obtain the following Wronskian relations:

$$[\langle\mathbf{Z}_{lm\sigma}|,|\mathbf{Z}_{l'm'\sigma'}\rangle]_S=0, \quad (24)$$

where $\mathbf{Z}$ stands for either $\mathbf{J}$ or $\mathbf{H}$, and

$$\begin{aligned}&[\langle\mathbf{J}_{lm\sigma}|,|\mathbf{H}_{l'm'\sigma'}\rangle]_S=\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'},\\&[\langle\mathbf{H}_{lm\sigma}|,|\mathbf{J}_{l'm'\sigma'}\rangle]_S=-\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}.\end{aligned} \quad (25)$$

The above equations can be regarded as normalization conditions for the spherical solid harmonics.

Similar to the case of the scalar solid harmonic, the regular and irregular vector solid harmonics can also be expanded in terms of "structure constants." In Appendix B, we derive the following expansion:

$$\langle\mathbf{H}_{lm\sigma}(\mathbf{r}-\mathbf{R})|=\sum_{l'm'\sigma'}G_{lm\sigma;l'm'\sigma'}(\mathbf{R})\langle\mathbf{J}_{l'm'\sigma'}(\mathbf{r})|, \quad (26)$$

where the structure constants $G_{lm\sigma;l'm'\sigma'}(\mathbf{R})$ are given by

$$G_{lm\sigma;l'm'\sigma'}(\mathbf{R})=\begin{cases}\sum_\mu C(l1l;m-\mu\mu)g_{lm-\mu;l'm'-\mu}(\mathbf{R})C(l'1l';m'-\mu\mu), & \sigma=\sigma'\\ \left[\frac{2l'+1}{l'+1}\right]^{1/2}\sum_\mu C(l1l;m-\mu\mu)g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})C(l'-11l';m'-\mu\mu), & \\ \sigma=M,\sigma'=E & \\ -\left[\frac{2l'+1}{l'+1}\right]^{1/2}\sum_\mu C(l1l;m-\mu\mu)g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})C(l'-11l';m'-\mu\mu), & \\ \sigma=E,\ \sigma'=M & \end{cases} \quad (27)$$

and the $g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})$'s are the structure constants for the scalar waves. Applying the above equations (24), (25), and (26) to Eq. (23), we finally obtain

$$-a^{(0)i}_{lm\sigma}=\sum_{j,lm\sigma}\left[\delta_{ij}\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}-\sum_{l''m''\sigma''}G^{ik}_{lm\sigma,l''m''\sigma''}t_{l''km''\sigma'',l'm'\sigma'}\right]a^j_{l'm'\sigma'}. \quad (28)$$

Equation (28) is the MST equation for photon scattering problems. Except for the additional matrix indices σ and σ', it is in exactly the same form as the MST equation for a scalar wave.

For stationary-state solutions, i.e., solutions to Eq. (4) without the incident wave $\mathbf{E}_0$, the problem becomes to solve the following secular equation:

$$\det\left|\delta_{ij}\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}-\sum_{l''m''\sigma''}G^{ik}_{lm\sigma,l''m''\sigma''}t_{l''km''\sigma'',l'm'\sigma'}\right|=0. \quad (29)$$

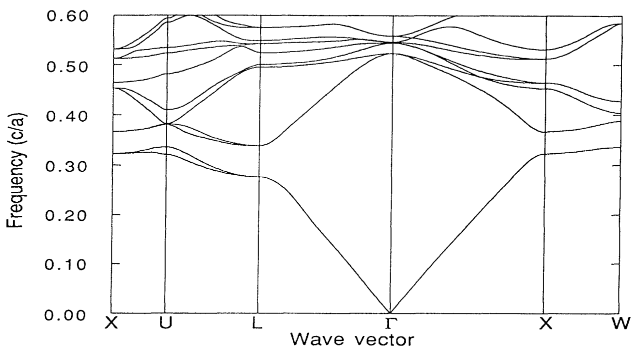

FIG. 1. Calculated photonic band structure for a diamond dielectric structure consisting of touching vacuum spheres in a material of dielectric constant 12.96. The frequency is given in units of c/a, where a is the cubic lattice constant of the diamond lattice and c is the speed of light in vacuum.

Using the Bloch's theorem for a periodic system, we can Fourier-transform Eq. (29) and obtain

$$\det\left|\delta_{s,s'}\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}-\sum_{l''m''\sigma''}G^{(s,s')}_{lm\sigma,l''m''\sigma''}(\mathbf{k})t^{s'}_{l''m''\sigma'',l'm'\sigma'}\right|=0\ , \quad (30)$$

where the indices s and s' are site indices within each unit cell and $G(\mathbf{k})$'s are the structure constants

$$G^{(s,s')}_{lm\sigma,l'm'\sigma'}(\mathbf{k})=\sum_{\mathbf{R}_i}e^{i\mathbf{k}\cdot\mathbf{R}_i}G^{(s,s')}_{lm\sigma,l'm'\sigma'}(\mathbf{R}_j-\mathbf{R}_i) \quad (31)$$

and can be calculated similarly as those for scalar waves.[10]

In order to test our formalism and its convergence properties, we have carried out a band-structure calculation for touching spheres in a diamond structure in a dielectric medium with dielectric constant 12.96. Calculations were carried out with the angular momentum truncated at various values. We found little change in the results beyond $l_{max}=3$. In addition, the results for $l_{max}=3$ agree with those obtained using plane waves[11] within a half percent. The results of our calculation using $l_{max}=3$ are shown in Fig. 1.

We note that, for the same level of accuracy, MST needs far fewer basis functions than plane-wave-based methods. In our case, $l_{max}=3$ means 2×15 basis functions each in the electric and the magnetic multipole modes, for a total of a 60×60 size matrix.

III. THE GREEN'S FUNCTION AND THE CPA

The main advantage of MST compared to other approaches is its direct calculation of the Green's function and its capability of dealing with defects and disorder. A Green's-function formalism is the prerequisite for the application of the coherent-potential approximation[12] to a disordered system. MST in this regard provides the natural framework,[13] in addition to the less sophisticated case of that of a tight-binding model.

A general derivation of the scalar Green's function with the MST framework for an arbitrary space-filling scattering potential is given in recent works.[14,15] In this section we outline the generalization to the vector Green's function. As in the scalar wave case, to apply KKR-CPA,[16] we assume in this section that all cell scattering potentials are spherically symmetric. The generalization of the Green's function to nonspherical potentials follows exactly as in the case of scalar waves.

The Green's function $\mathbf{d}(\mathbf{r},\mathbf{r}')$ satisfies the differential equation

$$\nabla\times[\nabla\times\mathbf{d}(\mathbf{r},\mathbf{r}')]-k^2\mathbf{d}(\mathbf{r},\mathbf{r}')-k^2[\epsilon(\mathbf{r})-1]\mathbf{d}(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')\mathbf{I}\ . \quad (32)$$

Under the boundary condition that the Green's function becomes an outgoing spherical wave at infinity, we can obtain the Dyson equation for the Green's function in a form similar to that for the wave function:

$$\mathbf{d}(\mathbf{r},\mathbf{r}')=\mathbf{d}_0(\mathbf{r},\mathbf{r}')+\int d^3\mathbf{r}''k[\epsilon(\mathbf{r}'')-1]\mathbf{d}_0(\mathbf{r},\mathbf{r}'')\mathbf{d}(\mathbf{r}'',\mathbf{r}')\ . \quad (33)$$

Similar to the scalar case, the Green's function can be expressed in terms of the regular and irregular solutions within each cell (for $|\mathbf{r}|>|\mathbf{r}'|$):

$$\mathbf{d}(\mathbf{r},\mathbf{r}')=-\sum_{lm\sigma,l'm'\sigma'}|\boldsymbol{\eta}^i_{lm\sigma}(\mathbf{r})\rangle\tau^{ij}_{lm\sigma,l'm'\sigma'}\langle\boldsymbol{\eta}^j_{l'm'\sigma'}(\mathbf{r}')|+\sum_{lm\sigma}|\boldsymbol{\xi}^i_{lm\sigma}(\mathbf{r})\rangle\langle\boldsymbol{\eta}^i_{lm\sigma}(\mathbf{r}')|\delta_{ij}\ , \quad (34)$$

where $\boldsymbol{\eta}^i$ is the regular solution inside cell i,

$$|\boldsymbol{\eta}^i_{lm\sigma}(\mathbf{r})\rangle=(t^i_{lm\sigma})^{-1}|\mathbf{P}^i_{lm\sigma}(\mathbf{r})\rangle$$

and ξ^i is the irregular solution in cell i which matches continuously and smoothly to the solid harmonic $\mathbf{J}$ on the circumscribing sphere. Note that in the above equation the t matrix has only diagonal elements due to the spherical symmetry. It is easy to verify that the expansion of the Green's function in the form of Eq. (34) satisfies the differential equation, Eq. (32), for any $\mathbf{r}\neq\mathbf{r}'$. The proper singular behavior at $\mathbf{r}=\mathbf{r}'$ and the normalization are determined by the matrix τ, which is the generalization of the scattering path operator in the scalar MST.[17] By substituting the expansion Eq. (34) into the Dyson equation, Eq. (33), and using the expansion of the free space Green's function in terms of the structure constants, also noting that the regular solution satisfies the integral equation

$$\langle\boldsymbol{\eta}^i_{lm\sigma}(\mathbf{r})|=\langle\mathbf{J}^i_{lm\sigma}(\mathbf{r})|(t^i_{lm\sigma})^{-1}+\int d^3\mathbf{r}'\mathbf{d}_0(\mathbf{r},\mathbf{r}')[\epsilon(r)-1]\langle\boldsymbol{\eta}^i_{lm\sigma}(\mathbf{r}')|\ ,$$

and it matches to

$$\langle\mathbf{J}^i_{lm\sigma}(\mathbf{r})|(t^i_{lm\sigma})^{-1}+\langle\mathbf{H}^i_{lm\sigma}(\mathbf{r})|$$

at the boundary of the sphere, we obtain the equation for the scattering path operator:

$$\tau^{ij}_{lm\sigma,l'm'\sigma'}=t^{i}_{lm\sigma}\delta_{ij}\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}+t^{i}_{lm\sigma}\sum_{\substack{k\neq i\\ l''m''\sigma''}}G^{ik}_{lm\sigma,l''m''\sigma''}\tau^{ku}_{l''m''\sigma'',l'm'\sigma'}\ . \tag{35}$$

Clearly, the matrix τ can be calculated by inverting the secular matrix given in Eq. (29).

If two different scattering potentials, described by the t matrixes $t^{A}_{lm\sigma}$ and $t^{B}_{lm\sigma}$, are randomly distributed on a given lattice, the CPA can be used to treat the system within a mean-field context. Following the approach of KKR-CPA, we define an effective mean-field medium represented by a t matrix $t^{C}_{lm\sigma}$, whose values are determined self-consistently, and the scattering path operator for the effective medium is given by

$$\tau^{C,ij}_{lm\sigma,l'm'\sigma'}=t^{C}_{lm\sigma}\delta_{ij}\delta_{ll'}\delta_{mm'}\delta_{\sigma\sigma'}+t^{C}_{lm\sigma}\sum_{\substack{k!=i\\ l''m''\sigma''}}G^{ik}_{lm\sigma,l''m''\sigma''}\tau_{l''C,kj_{m''\sigma'',l',m'\sigma'}}\ . \tag{36}$$

The scattering effect of an A- or B-type sphere on site 0 is described by the impurity problem

$$\tau^{\alpha,00^{-1}}=t^{\alpha-1}-t^{C-1}+\tau^{C,00^{-1}}\ ,\quad \alpha=A,B\ , \tag{37}$$

where the quantities in the above equation are matrices in l, m, and σ. The CPA self-consistent condition can then be expressed as

$$\tau^{C,00}_{lm\sigma,l'm'\sigma'}=\sum_{\alpha=A,B}c_{\alpha}\tau^{\alpha,00}_{lm\sigma,l'm'\sigma'}\ , \tag{38}$$

where c_α is the concentration of type-α potential cells. Equations (36), (37), and (38) are used to determine the quantities τ^C, t^C, and $\tau^{A,00}$ and $\tau^{B,00}$.[18]

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APPENDIX A: USEFUL RELATIONS OF VECTOR SPHERICAL HARMONICS

We follow the convention of Ref. 19 and define the functions

$$T_{Jlm}(\hat{\mathbf{r}})=\sum_{\mu}C(l1J;m-\mu\mu)Y_{lm-\mu}(\hat{\mathbf{r}})\hat{\zeta}_{\mu}\ , \tag{A1}$$

where the vectors $\hat{\zeta}$ are defined as

$$\hat{\zeta}_1=-\frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_1+i\hat{\mathbf{e}}_2),\quad \hat{\zeta}_{-1}=\frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_1-i\hat{\mathbf{e}}_2),\quad \hat{\zeta}_0=\hat{\mathbf{e}}_3\ , \tag{A2}$$

and $\hat{\mathbf{e}}_i$ are unit vectors along the Cartesian coordinate axes.

$T_{Jlm}(\hat{\mathbf{r}})$ are related to the vector harmonics by the following equations:

$$T_{llm}(\hat{\mathbf{r}})=\mathbf{X}_{lm}(\hat{\mathbf{r}})\ , \tag{A3}$$

$$T_{ll+1m}(\hat{\mathbf{r}})=-\left[\frac{l+1}{2l+1}\right]^{1/2}\mathbf{X}^{(o)}_{lm}(\hat{\mathbf{r}})+\left[\frac{l}{2l+1}\right]^{1/2}\mathbf{X}^{(e)}_{lm}(\hat{\mathbf{r}})\ , \tag{A4}$$

$$T_{ll-1m}(\hat{\mathbf{r}})=\left[\frac{l}{2l+1}\right]^{1/2}\mathbf{X}^{(o)}_{lm}(\hat{\mathbf{r}})+\left[\frac{l+1}{2l+1}\right]^{1/2}\mathbf{X}^{(e)}_{lm}(\hat{\mathbf{r}})\ , \tag{A5}$$

where

$$\mathbf{X}_{lm}(\hat{\mathbf{r}})=\frac{-i\mathbf{r}\times\nabla Y_{lm}(\hat{\mathbf{r}})}{\sqrt{l(l+1)}}\ , \tag{A6}$$

$$\mathbf{X}^{(o)}_{lm}(\hat{\mathbf{r}})=\hat{\mathbf{r}}Y_{lm}(\hat{\mathbf{r}})\ , \tag{A7}$$

and

$$\mathbf{X}^{(e)}_{lm}(\hat{\mathbf{r}})=\frac{r\nabla Y_{lm}(\hat{\mathbf{r}})}{\sqrt{l(l+1)}}\ . \tag{A8}$$

The vector harmonics $\mathbf{X}$ can be shown to have the following properties:

$$\mathbf{X}^{(e)}_{lm}(\hat{\mathbf{r}})=-i\hat{\mathbf{r}}\times\mathbf{X}_{lm}(\hat{\mathbf{r}})\ , \tag{A9}$$

$$\mathbf{X}_{lm}(\hat{\mathbf{r}})=-i\hat{\mathbf{r}}\times X^{(e)}_{lm}(\hat{\mathbf{r}})=-ir\nabla\times\mathbf{X}^{(e)}_{lm}(\hat{\mathbf{r}})\ , \tag{A10}$$

$$\mathbf{X}^{(o)}_{lm}(\hat{\mathbf{r}})=-i\frac{r^2}{\sqrt{l(l+1)}}\nabla\times\left[\frac{1}{r}\mathbf{X}_{lm}(\hat{\mathbf{r}})\right]\ . \tag{A11}$$

From the definition of the harmonic functions for the electric multipole mode, Eq. (10), and the relations given above, we have

$$\mathbf{J}_{lmE}(\mathbf{r})=\left[\frac{l+1}{2l+1}\right]^{1/2}j_{l-1}(kr)\mathbf{T}_{ll-1m}(\hat{\mathbf{r}})-\left[\frac{l}{2l+1}\right]^{1/2}j_{l+1}(kr)\mathbf{T}_{ll+1m}(\hat{\mathbf{r}})\ , \tag{A12}$$

$$\mathbf{H}_{lmE}(\mathbf{r})=\left[\frac{l+1}{2l+1}\right]^{1/2}h_{l-1}(kr)\mathbf{T}_{ll-1m}(\hat{\mathbf{r}})-\left[\frac{l}{2l+1}\right]^{1/2}h_{l+1}(kr)\mathbf{T}_{ll+1m}(\hat{\mathbf{r}})\ . \tag{A13}$$

Using these results and the orthogonality of the vector spherical harmonics, we can obtain the following equalities:

$$\oint d\mathbf{S}\cdot\langle\mathbf{Z}_{lm\sigma}(\mathbf{r})|\times|\mathbf{Z}_{l'm'\sigma}(\mathbf{r})\rangle=0\ , \tag{A14}$$

$$\oint d\mathbf{S}\cdot[\langle \mathbf{Z}_{lmM}(\mathbf{r})|\times|\mathbf{Z}_{l'm'E}(\mathbf{r})\rangle + \langle \mathbf{Z}_{lmE}(\mathbf{r})|\times|\mathbf{Z}_{l'm'M}(\mathbf{r})\rangle]=0 \ , \tag{A15}$$

$$\oint d\mathbf{S}\cdot[\langle \mathbf{J}_{lmM}(\mathbf{r})|\times|\mathbf{H}_{l'm'E}(\mathbf{r})\rangle + \langle \mathbf{J}_{lmE}(\mathbf{r})|\times|\mathbf{H}_{l'm'M}(\mathbf{r})\rangle]=-\frac{i}{k}\delta_{ll'}\delta_{mm'} \ , \tag{A16}$$

where the integration is over the surface $\mathbf{S}$ of a sphere. These equalities are useful in deriving the Wronskian relations involving wave functions.

APPENDIX B: EXPANSION OF IRREGULAR VECTOR HARMONICS

The structure constants can be defined as the coefficients of expansion of the irregular solid harmonics. In this appendix we use the expansion of the irregular vector harmonics to derive an expression for the structure constants.

The irregular vector harmonic for the magnetic multipole mode is given by

$$\begin{aligned}\langle \mathbf{H}_{lmM}(\mathbf{r}-\mathbf{R})| &= -ikh_l(k|\mathbf{r}-\mathbf{R}|)\mathbf{X}^*_{lm}(\widehat{\mathbf{r}-\mathbf{R}}) \\ &= -ik\sum_{\mu} C(l1L;m-\mu\mu)h_l(k|\mathbf{r}-\mathbf{R}|) \\ &\quad \times Y^*_{lm-\mu}(\widehat{\mathbf{r}-\mathbf{R}})\hat{\xi}^*_{\mu} \ .\end{aligned} \tag{B1}$$

Expanding the scalar solid harmonics on the right-hand side in terms of the scalar structure constants,

$$\begin{aligned} g_{lm;l'm'}(\mathbf{R}) &= -4\pi ik\sum_{l''m''} i^{l-l'+l''}C_{lm;l'm';l''m''}h_{l''}(kR) \\ &\quad \times Y_{l''m''}(-\hat{\mathbf{R}}) \ , \end{aligned} \tag{B2}$$

we obtain

$$\begin{aligned}\langle \mathbf{H}_{lmM}(\mathbf{r}-\mathbf{R})| &= \sum_{\mu l'm'} C(l1l;m-\mu\mu)g_{lm;l'm'}(\mathbf{R})j_{l'}(kr)Y^*_{l'm'-\mu}(\hat{\mathbf{r}})\hat{\xi}^*_{\mu} \\ &= \sum_{\mu l'm'} C(l1l;m-\mu\mu)g_{lm;l'm'}(\mathbf{R})j_{l'}(kr)\sum_J C(l'1J;m'-\mu\mu)\mathbf{T}^*_{Jl'm'}(\hat{\mathbf{r}}) \ .\end{aligned} \tag{B3}$$

Interchange l' and J, and note that the summation over J goes through $l'-1$, l', and $l'+1$. We obtain

$$\begin{aligned}\langle \mathbf{H}_{lmM}(\mathbf{r}-\mathbf{R})| = \sum_{\mu l'm'} C(l1l;m-\mu\mu)[&g_{lm-\mu;l'm'-\mu}(\mathbf{R})j_{l'}(kr)C(l'1l';m'-\mu\mu)T^*_{l'l'm'}(\hat{\mathbf{r}}) \\ &+g_{lm-\mu;l'+1m'-\mu}(\mathbf{R})j_{l'+1}(kr)C(l'+11l';m'-\mu\mu)\mathbf{T}^*_{l'l'+1m'}(\hat{\mathbf{r}}) \\ &+g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})j_{l'-1}(kr)C(l'-11l';m'-\mu\mu)\mathbf{T}^*_{l'l'-1m'}(\hat{\mathbf{r}})] \ .\end{aligned} \tag{B4}$$

Using the relation

$$\begin{aligned}&\sum_{\mu} C(l1l;m-\mu\mu)\left[\frac{l'}{l'+1}\right]^{1/2} g_{lm-\mu;l'+1m'-\mu}(\mathbf{R})j_{l'-1}(kr)C(l'+11l';m'-\mu\mu) \\ &\qquad = -\sum_{\mu} C(l1l;m-\mu\mu)\left[\frac{l'}{l'+1}\right]^{1/2} g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})j'_{l'-1}(kr)C(l'-11l';m'-\mu\mu) \ ,\end{aligned} \tag{B5}$$

we finally obtain for the magnetic multipole mode,

$$\begin{aligned}\langle \mathbf{H}_{lmM}(\mathbf{r}-\mathbf{R})| = \sum_{\mu l'm'} C(l1l;m-\mu\mu)\Bigg\{&g_{lm-\mu;l'm'-\mu}(\mathbf{R})C(l'1l';m'-\mu\mu)\langle \mathbf{J}_{l'm'M}(\mathbf{r})| \\ &+\left[\frac{2l'+1}{l'+1}\right]^{1/2} g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})C(l'-11l';m'-\mu\mu)\langle \mathbf{J}_{l'm'E}(\mathbf{r})|\Bigg\} \ .\end{aligned} \tag{B6}$$

For the electric multipole mode, we apply $\nabla\times$ to the above equation and use the relation between the E-mode and the M-mode wave functions, noting that both $\mathbf{H}$ and $\mathbf{J}$ are solutions in free space, and obtain

$$\begin{aligned}\langle \mathbf{H}_{lmE}(\mathbf{r}-\mathbf{R})| = \sum_{\mu l'm'} C(l1L;m-\mu\mu)\Bigg\{&g_{lm-\mu;l'm'-\mu}(\mathbf{R})C(l'1l';m'-\mu\mu)\langle \mathbf{J}_{l'm'E}(\mathbf{r})| \\ &-\left[\frac{2l'+1}{l'+1}\right]^{1/2} g_{lm-\mu;l'-1m'-\mu}(\mathbf{R})C(l'-11l';m'-\mu\mu)\langle \mathbf{J}_{l'm'M}(\mathbf{r})|\Bigg\} \ .\end{aligned} \tag{B7}$$

The above two equations are equivalent to Eqs. (26) and (27), where the structure constants are defined.

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