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Spectral method for the static electric potential of a charge density in a composite medium

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A spectral representation for the static electric potential field in a two-constituent composite medium is presented. A theory is developed for calculating the quasistatic eigenstates of Maxwell's equations for such a composite. The local physical potential field produced in the system by a given source charge density is expanded in this set of orthogonal eigenstates for any position **r**. The source charges can be located anywhere, i.e., inside any of the constituents. This is shown to work even if the eigenfunctions are normalized in an infinite volume. If the microstructure consists of a cluster of separate inclusions in a uniform host medium, then the quasistatic eigenstates of all the separate isolated inclusions can be used to calculate the eigenstates of the total structure as well as the local potential field. Once the eigenstates are known for a given host and a given microstructure, then calculation of the local field only involves calculating three-dimensional integrals of known functions and solving sets of linear algebraic equations.

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I. INTRODUCTION

A spectral approach is developed for calculating the local quasistatic electric potential $\phi(\mathbf{r})$ produced in a two-constituent composite by a given charge density $\rho(\mathbf{r})$ which can be nonzero in either or both of the constituents. This is done by expanding $\phi(\mathbf{r})$ in the set of quasistatic eigenfunctions $\phi_n(\mathbf{r})$ of that structure. Those eigenfunctions depend upon the local microstructure but are independent of the actual physical parameters of the constituents, i.e., the constituent electric permittivities ϵ_1 and ϵ_2. The eigenvalues are special nonphysical values of the ratio ϵ_1/ϵ_2. Once the eigenstates are known, the calculation of $\phi(\mathbf{r})$ only requires summing a series of those eigenfunctions with coefficients which are obtained by volume integrals of the products $\phi_n^*(\mathbf{r})\rho(\mathbf{r})$.

Several spectral approaches were developed in the past. In Ref. [1] such an approach was used to calculate the macroscopic electric permittivity of a collection of spherical inclusions. In Ref. [2] a spectral approach was put forward for calculating the local monochromatic electric field $\mathbf{E}(\mathbf{r})$ produced in a two-constituent composite by a given incident field. In that case the discussion was not limited to the quasistatic regime; the field $\mathbf{E}(\mathbf{r})$ was a solution of the full Maxwell equations. The eigenvalues are still special nonphysical values of ϵ_1/ϵ_2. A different spectral approach developed more recently was introduced in Ref. [3]. In that approach a set of quasinormal modes is used to expand $\mathbf{E}(\mathbf{r})$. The eigenvalues are then special nonphysical values of the angular frequency.

The approach presented here is capable of handling any kind of given charge density in any kind of two-constituent microstructure as long as the characteristic local size scale of that microstructure is much smaller than any of the relevant physical lengths, e.g., electromagnetic (EM) wavelength or skin depth. Several preliminary versions of this approach were recently used in the context of a parallel slab type of inclusion [4,5] and in the context of a spherical inclusion [6].

The results could be useful for calculating the field produced by the emission or scattering or fluorescence of EM radiation by atoms or molecules or nanoparticles, including nonlinear processes like Raman scattering. It will work even in difficult situations like when the emitter or scatterer is in a very small gap between two metallic particles [7] or inside a nanosized particle [8,9]. Nevertheless, it should be remembered that this emission or scattering by a nanoparticle depends upon the environment. Therefore, calculating it will often be quite difficult.

Our approach works irrespective of where $\rho(\mathbf{r})$ is nonzero. This is in contrast with previous approaches where the charges had to be either outside an inclusion [4–6] or inside an inclusion [3]. Moreover, in contrast with some previous discussions [1,2,6], our approach works even if the eigenfunction normalization involves integration over an infinite volume.

The rest of this article is organized as follows. In Sec. II the basic theory of the quasistatic eigenstates is developed and it is shown how these eigenstates can be used to calculate $\phi(\mathbf{r})$ irrespective of where the charge density is nonzero. In Sec. III we develop the application of the basic theory to a microstructure composed of many ϵ_1 inclusions in an otherwise uniform ϵ_2 host. In Sec. IV we apply the basic theory to the simple example of a point charge located anywhere inside or outside a single spherical inclusion in an otherwise uniform medium. In this simple microstructure most of the results are obtained in closed form. This serves to demonstrate how simple the calculations are when based upon the spectral approach developed here. Section V summarizes our results and indicates possible future developments.

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II. BASIC THEORY OF QUASISTATIC EIGENSTATES

In the quasistatic regime, a charge density $\rho(\mathbf{r})$ produces an electric potential $\phi(\mathbf{r})$ in all space as the solution of

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi(\mathbf{r})] = -4\pi\rho(\mathbf{r}), \tag{1}$$

where $\epsilon(\mathbf{r})$ is the local electric permittivity. If the medium is a two-constituent composite then $\epsilon(\mathbf{r})$ can be represented as

$$\begin{aligned}\epsilon(\mathbf{r}) &= \theta_1(\mathbf{r})\epsilon_1 + \theta_2(\mathbf{r})\epsilon_2 = \epsilon_2 + \theta_1(\epsilon_1 - \epsilon_2)\\ &= \epsilon_2(1 - \theta_1 u), \quad u \equiv 1 - \frac{\epsilon_1}{\epsilon_2} \equiv \frac{1}{s}.\end{aligned}$$

Here θ_i, $i = 1,2$, are step functions that characterize the two constituents; $\theta_i(\mathbf{r}) = 1$ for $\mathbf{r}$ inside the subvolume V_i of the ϵ_i constituent and vanishes elsewhere. Equation (1) can now be rewritten as

$$\nabla^2\phi - u\nabla \cdot (\theta_1\nabla\phi) = -4\pi\rho/\epsilon_2. \tag{2}$$

We would like to expand the solution of this equation in a complete set of states. To that end we consider the eigenstates of the homogeneous left-hand side of Eq. (2) which satisfy

$$\nabla^2\phi_n = u_n^{(1)}\nabla \cdot (\theta_1\nabla\phi_n), \tag{3}$$

$$\phi_n(\mathbf{r}) = C/|\mathbf{r}| \quad \text{when } |\mathbf{r}| \to \infty. \tag{4}$$

The orthogonality properties of these eigenfunctions were derived previously. This was done by using a Hermitian integro-differential operator [1,6] and assuming that V_1 is a finite subvolume. That operator includes a strong singularity in its integrand, which casts some doubt regarding the possibility of changing the order of integration and differentiation [10] required to prove its Hermiticity. In the current discussion, if one of the subvolumes V_1 or V_2 is finite, then in the complementary infinite subvolume Eq. (4) is always satisfied.

Therefore, we proceed differently in deriving those properties. To that end we consider the following integral:

$$\begin{aligned}&\int dV\theta_1(\nabla\phi_n^* \cdot \nabla\phi_m)\\ &= \int dV[\nabla \cdot (\theta_1\phi_n^*\nabla\phi_m) - \phi_n^*\nabla \cdot (\theta_1\nabla\phi_m)].\end{aligned}$$

The first term on the right-hand side transforms to a surface integral over the system envelope

$$\oint dS\,\theta_1\phi_n^*\frac{\partial\phi_m}{\partial n}.$$

When $r \equiv |\mathbf{r}| \to \infty$, the last integrand either vanishes if V_1 is finite or else behaves as $O(1/r^3)$ when V_1 is the infinite subvolume; therefore that surface integral vanishes. Using Eq. (3), the remaining term becomes

$$\begin{aligned}&-s_m^{(1)}\int dV\phi_n^*\nabla^2\phi_m\\ &= s_m^{(1)}\int dV[-\nabla \cdot (\phi_n^*\nabla\phi_m) + (\nabla\phi_n^* \cdot \nabla\phi_m)],\end{aligned}$$

where $s_n^{(1)} \equiv 1/u_n^{(1)}$. Again, the first term on the right-hand side transforms to a vanishing surface integral at ∞. We are thus left with

$$\int dV\theta_1(\nabla\phi_n^* \cdot \nabla\phi_m) = s_m^{(1)}\int dV(\nabla\phi_n^* \cdot \nabla\phi_m). \tag{5}$$

We now switch the roles of ϕ_n and ϕ_m and write

$$\begin{aligned}&\int dV\theta_1(\nabla\phi_m^* \cdot \nabla\phi_n)\\ &= \int dV[\nabla \cdot (\theta_1\phi_m^*\nabla\phi_n) - \phi_m^*\nabla \cdot (\theta_1\nabla\phi_n)]\\ &= -s_n^{(1)}\int dV\phi_m^*\nabla^2\phi_n = s_n^{(1)}\int dV(\nabla\phi_m^* \cdot \nabla\phi_n).\end{aligned}$$

It follows that

$$\left[s_n^{(1)} - \left(s_m^{(1)}\right)^*\right]\int dV(\nabla\phi_m^* \cdot \nabla\phi_n) = 0.$$

From these results we arrive at the following conclusions. (i) $(s_n^{(1)})^* = s_n^{(1)}$ is real. (ii) If $s_m^{(1)} \neq s_n^{(1)}$ then

$$\begin{aligned}&\int dV(\nabla\phi_m^* \cdot \nabla\phi_n)\\ &= \frac{1}{s_n^{(1)}}\int dV\theta_1(\nabla\phi_m^* \cdot \nabla\phi_n)\\ &= \frac{1}{1 - s_n^{(1)}}\int dV\theta_2(\nabla\phi_m^* \cdot \nabla\phi_n) = 0.\end{aligned}$$

(iii) $0 \leqslant s_n^{(1)} \leqslant 1$ since

$$\begin{aligned}0 &\leqslant \int dV\theta_1|\nabla\phi_n|^2\\ &= s_n^{(1)}\int dV|\nabla\phi_n|^2 \leqslant \int dV|\nabla\phi_n|^2.\end{aligned}$$

A V_i scalar product is now defined as

$$\langle\phi|\psi\rangle_i \equiv \int dV\theta_i(\nabla\phi^* \cdot \nabla\psi).$$

Note that all the above integrals converge, even if the integration is over all space, due to the large-$\mathbf{r}$ behavior of the eigenfunctions [see Eq. (4)].

The entire development up to this point can be repeated with Eqs. (2) and (3) replaced by

$$\nabla^2\phi - u^{(2)}\nabla \cdot (\theta_2\nabla\phi) = -4\pi\rho/\epsilon_1, \tag{6}$$

$$\nabla^2\phi_n = u_n^{(2)}\nabla \cdot (\theta_2\nabla\phi_n), \tag{7}$$

where

$$u^{(2)} = 1 - \frac{\epsilon_2}{\epsilon_1} \equiv \frac{u}{u-1} \equiv \frac{1}{s^{(2)}}, \quad s^{(2)} = 1 - s, \tag{8}$$

$$u_n^{(2)} = \frac{u_n^{(1)}}{u_n^{(1)} - 1}, \quad s_n^{(2)} \equiv \frac{1}{u_n^{(2)}} = 1 - s_n^{(1)}. \tag{9}$$

This also means that θ_1, V_1, ϵ_2, s, and $s_n^{(1)}$ are replaced by θ_2, V_2, ϵ_1, $s^{(2)}$, and $s_n^{(2)}$. We note that the V_1 and V_2 eigenfunctions are the same up to a multiplicative factor. That is due to the fact that the V_1 and V_2 normalizations differ; from Eq. (5) and its V_2 analog it follows that

$$\langle\phi_n|\phi_n\rangle_1 = s_n^{(1)}\int dV|\nabla\phi_n|^2, \tag{10}$$

$$\langle\phi_n|\phi_n\rangle_2 = s_n^{(2)}\int dV|\nabla\phi_n|^2 = \left(1 - s_n^{(1)}\right)\int dV|\nabla\phi_n|^2. \tag{11}$$

From these results it follows that if $s_n^{(1)} = 0$ then $\nabla\phi_n(\mathbf{r}) = 0$ for all $\mathbf{r} \in V_1$. Because $\phi_n(\mathbf{r})$ is continuous at the V_1-V_2 interface, it must have a constant value over that interface. From Eq. (7) it then follows that, apart from this boundary condition, that function can have an arbitrary form inside V_2. There is thus much freedom in choosing the $s_n^{(1)} = 0$ eigenfunctions inside V_2. In particular, these functions do not have to be harmonic there, and most of them are probably nonharmonic. A noteworthy exception is the $l = 0$ eigenfunction of an isolated sphere, which is harmonic in V_2 [see Eq. (33) below]. Similar properties hold for the $s_n^{(1)} = 1$ eigenfunctions: They must have a constant value in V_2 and at the V_1-V_2 interface, and there is much freedom in choosing their form in V_1. Again, these eigenfunctions are usually not harmonic there. When $s_n^{(1)}$ is neither 0 nor 1, it follows from Eqs. (3) and (7) that $\nabla^2\phi_n = 0$ inside V_1 and V_2, but not at the V_1-V_2 interface.

We would like to use the eigenfunctions $\phi_n(\mathbf{r})$ to expand the solution $\phi(\mathbf{r})$ of Eq. (2). To this end we first assume that $\rho(\mathbf{r})$ is nonzero only in V_2. In that case $\phi(\mathbf{r})$ is harmonic in V_1. Therefore, we can expand it using only the eigenfunctions that are harmonic there. In fact, it is easy to show that if V_1 has a finite spatial extent, then any field $\psi(\mathbf{r})$ that is harmonic there will always be V_1 orthogonal to any eigenfunction $\phi_n(\mathbf{r})$ that has $u_n^{(1)} = 1$ as its V_1 eigenvalue and has a constant value $\phi_{n,\text{const}}$ outside V_1,

$$\begin{aligned}
\langle\phi_n|\psi\rangle_1 &= \int_{V_1} dV(\nabla\phi_n^* \cdot \nabla\psi)\\
&= \int_{V_1} dV[\nabla\cdot(\phi_n^*\nabla\psi) - \phi_n^*\nabla^2\psi]\\
&= \phi_{n,\text{const}} \oint_{\partial V_1} dS\frac{\partial\psi}{\partial n} = \phi_{n,\text{const}} \int_{V_1} dV\,\nabla^2\psi = 0,
\end{aligned}$$

where ∂V_1 denotes the V_1-V_2 interface and we used the fact that $\phi_n(\mathbf{r}) = \phi_{n,\text{const}}$ on that interface in order to take it outside the interface integral.

To determine the expansion of $\phi(\mathbf{r})$ when $\rho(\mathbf{r})$ is nonzero only outside V_1 we write

$$\phi = \phi_0 + \phi_{\text{sc}}, \tag{12}$$

where $\phi_0(\mathbf{r})$, to be called the incident field, is the solution of Eq. (2) in the uniform medium ϵ_2:

$$\nabla^2\phi_0 = -\frac{4\pi\rho}{\epsilon_2}. \tag{13}$$

We will assume that the total charge $\int d^3r\rho(\mathbf{r})$ is finite; therefore $\phi_0(\mathbf{r})$ will decrease as $1/r$ at large distances. The scattered field $\phi_{\text{sc}}(\mathbf{r})$ satisfies

$$\nabla^2\phi_{\text{sc}} = u\nabla\cdot[\theta_1\nabla(\phi_0 + \phi_{\text{sc}})]. \tag{14}$$

Inside V_1 both $\phi_0(\mathbf{r})$ and $\phi_{\text{sc}}(\mathbf{r})$ are harmonic functions; therefore they can both be expanded there, using only the harmonic eigenfunctions, as

$$\theta_1\phi_0 = \theta_1\sum_n A_n\phi_n, \quad \theta_1\phi_{\text{sc}} = \theta_1\sum_n B_n\phi_n. \tag{15}$$

In order to calculate A_n we consider the scalar product $\langle\phi_n|\phi_0\rangle_1 = A_n\langle\phi_n|\phi_n\rangle_1$:

$$\begin{aligned}
\langle\phi_n|\phi_0\rangle_1 &\equiv \int dV\theta_1(\nabla\phi_n^*\cdot\nabla\phi_0)\\
&= \int dV[\nabla\cdot(\phi_0\theta_1\nabla\phi_n^*) - \phi_0\nabla\cdot(\theta_1\nabla\phi_n^*)]\\
&= -s_n^{(1)}\int dV\phi_0\nabla^2\phi_n^* = s_n^{(1)}\int dV(\nabla\phi_0\cdot\nabla\phi_n^*)\\
&= -s_n^{(1)}\int dV\phi_n^*\nabla^2\phi_0 = \frac{4\pi s_n^{(1)}}{\epsilon_2}\int dV\phi_n^*(\mathbf{r})\rho(\mathbf{r})
\end{aligned} \tag{16}$$

$$\Rightarrow A_n = \frac{4\pi s_n^{(1)}}{\epsilon_2}\frac{\int dV\phi_n^*\rho}{\langle\phi_n|\phi_n\rangle_1}. \tag{17}$$

Because we have assumed that $\rho(\mathbf{r}) \neq 0$ only outside V_1, in practice the integration in the last expression is only over the complementary subvolume V_2.

Inside V_1 the incident field can be represented as

$$\theta_1\phi_0(\mathbf{r}) = \theta_1\frac{4\pi}{\epsilon_2}\sum_n s_n^{(1)}\frac{\int dV\phi_n^*\rho}{\langle\phi_n|\phi_n\rangle_1}\phi_n(\mathbf{r}).$$

Note that, although each term in this expansion depends on the microstructure via $s_n^{(1)}$, ϕ_n, and $\langle\phi_n|\phi_n\rangle_1$, the final result for $\phi_0(\mathbf{r})$ should be independent of that. Therefore, we can use a simplified artificial microstructure (e.g., a single spherical inclusion) to calculate ϕ_0 in the artificial V_1. This can sometimes be easier than computing ϕ_0 by numerical solution of Eq. (13). However, in order to use ϕ_0 of Eq. (13), or ϕ_0 of Eq. (22) below, in Eq. (12) we will need to know it also outside V_1 or outside V_2, respectively.

Multiplying Eq. (14) by ϕ_n^* and integrating over all space, we get

$$\begin{aligned}
\int dV\phi_n^*\nabla^2\phi_{\text{sc}} &= u\int dV\phi_n^*\nabla\cdot[\theta_1\nabla(\phi_0 + \phi_{\text{sc}})]\\
&= u\int dV\,\nabla\cdot[\phi_n^*\theta_1\nabla(\phi_0 + \phi_{\text{sc}})]\\
&\quad - u\int dV\theta_1[\nabla\phi_n^*\cdot\nabla(\phi_0 + \phi_{\text{sc}})]\\
&= -u(A_n + B_n)\langle\phi_n|\phi_n\rangle_1,
\end{aligned} \tag{18}$$

but also

$$\begin{aligned}
&\int dV\phi_n^*\nabla^2\phi_{\text{sc}}\\
&= \int dV[\nabla\cdot(\phi_n^*\nabla\phi_{\text{sc}}) - (\nabla\phi_n^*\cdot\nabla\phi_{\text{sc}})]\\
&= \int dV[-\nabla\cdot(\phi_{\text{sc}}\nabla\phi_n^*) + (\phi_{\text{sc}}\nabla^2\phi_n^*)]\\
&= u_n^{(1)}\int dV\phi_{\text{sc}}\nabla\cdot(\theta_1\nabla\phi_n^*)\\
&= u_n^{(1)}\int dV[\nabla\cdot(\phi_{\text{sc}}\theta_1\nabla\phi_n^*) - \theta_1(\nabla\phi_{\text{sc}}\cdot\nabla\phi_n^*)]\\
&= -u_n^{(1)}\langle\phi_n|\phi_{\text{sc}}\rangle_1 = -u_n^{(1)}B_n\langle\phi_n|\phi_n\rangle_1.
\end{aligned} \tag{19}$$

Comparing the last results of Eqs. (18) and (19), we now get

$$B_n = \frac{s_n^{(1)}}{s - s_n^{(1)}} A_n = \frac{4\pi}{\epsilon_2} \frac{\left(s_n^{(1)}\right)^2}{s - s_n^{(1)}} \frac{\int dV \phi_n^*(\mathbf{r})\rho(\mathbf{r})}{\langle \phi_n | \phi_n \rangle_1}. \tag{20}$$

In order to extend the V_1 expansion of $\phi_{\mathrm{sc}}(\mathbf{r})$ also to $\mathbf{r} \in V_2$ we write

$$\begin{aligned} \nabla^2 \phi_{\mathrm{sc}} &= u \sum_n (A_n + B_n) \nabla \cdot (\theta_1 \nabla \phi_n) \\ &= \sum_n \frac{u}{u_n^{(1)}} (A_n + B_n) \nabla^2 \phi_n \\ &\Rightarrow \nabla^2 \left[\phi_{sc} - \frac{4\pi}{\epsilon_2} \sum_n \frac{\left(s_n^{(1)}\right)^2}{s - s_n^{(1)}} \frac{\int dV \phi_n^*(\mathbf{r})\rho(\mathbf{r})}{\langle \phi_n | \phi_n \rangle_1} \phi_n(\mathbf{r}) \right] \\ &= 0. \end{aligned}$$

Because $\phi_{\mathrm{sc}}(\mathbf{r})$ and $\phi_n(\mathbf{r})$ behave as $1/|\mathbf{r}|$ when $\mathbf{r} \to \infty$ the expression in the square brackets must vanish. Thus we get

$$\begin{aligned} \phi_{\mathrm{sc}} &= \frac{4\pi}{\epsilon_2} \sum_n \frac{\left(s_n^{(1)}\right)^2}{s - s_n^{(1)}} \frac{\int dV \phi_n^*(\mathbf{r})\rho(\mathbf{r})}{\langle \phi_n | \phi_n \rangle_1} \phi_n(\mathbf{r}) \\ &= \sum_n B_n \phi_n(\mathbf{r}), \end{aligned} \tag{21}$$

which must hold in all space. This looks just like the expansion of $\phi_{\mathrm{sc}}(\mathbf{r})$ inside V_1 in Eq. (15). However, we have now shown that this expansion is valid both inside and outside V_1. The last expansion was already obtained previously [6]. However, we will now show how it can be recast so as to apply to situations where $\rho(\mathbf{r})$ is not limited to being nonzero only outside V_1. This will work even in cases where V_2 is infinite.

We would like to point out that the extension of the expansion of $\theta_1 \phi_{\mathrm{sc}}$ for $\mathbf{r} \in V_1$ in Eq. (15) to the expansion of ϕ_{sc} for all $\mathbf{r}$ in Eq. (21) could also have been obtained by noting that Eq. (15) determines the values of $\phi_{\mathrm{sc}}(\mathbf{r})$ also at the V_1-V_2 interface, where that function is continuous. Therefore, the expression $\theta_2 \sum_n B_n \phi_n(\mathbf{r})$, which is a sum of states that are harmonic in V_2 and decrease to 0 when $r \to \infty$, satisfies the correct boundary conditions on $\phi_{\mathrm{sc}}(\mathbf{r})$ in V_2. Therefore, it must represent $\phi_{\mathrm{sc}}(\mathbf{r})$ there.

It is also worth pointing out that, since ϕ_{sc} is harmonic inside both V_1 and V_2, though not at the V_1-V_2 interface, it can be expanded there using eigenstates that are also harmonic inside both V_1 and V_2. Thus we do not need any nonharmonic eigenstates for these expansions.

If $\rho(\mathbf{r})$ is nonzero only inside V_1 then $\phi(\mathbf{r})$ and $\phi_0(\mathbf{r})$ are not harmonic functions there. We might consider expanding these fields there by using, besides the harmonic eigenfunctions, also the $u_n^{(1)} = 1$ nonharmonic eigenfunctions. However, in this case $\phi(\mathbf{r})$ and $\phi_0(\mathbf{r})$ are often so singular in V_1 (e.g., $1/r$) that their gradients are not square integrable there. In that case they usually cannot be expanded in this way. We therefore proceed in a different fashion by switching the roles of the two constituents: We repeat all of the above discussion with V_1, s, $s_n^{(1)}$, and $\langle \phi_n | \phi_n \rangle_1$ replaced by V_2, $s^{(2)}$, $s_n^{(2)}$, and $\langle \phi_n | \phi_n \rangle_2 = (1 - s_n^{(1)}) \langle \phi_n | \phi_n \rangle_1 / s_n^{(1)}$ [see Eqs. (10) and (11)]. In that case Eqs. (3), (13)–(15), (17), (20), and (21) will be replaced, respectively, by Eq. (7) and

$$\nabla^2 \phi_0 = -\frac{4\pi\rho}{\epsilon_1}, \tag{22}$$

$$\begin{aligned} \nabla^2 \phi_{\mathrm{sc}} &= u^{(2)} \nabla \cdot [\theta_2 \nabla(\phi_0 + \phi_{\mathrm{sc}})], \\ \theta_2 \phi_0 &= \theta_2 \sum_n A_n^{(2)} \phi_n, \quad \theta_2 \phi_{\mathrm{sc}} = \theta_2 \sum_n B_n^{(2)} \phi_n, \\ A_n^{(2)} &= \frac{4\pi s_n^{(2)}}{\epsilon_1} \frac{\int dV \phi_n^* \rho}{\langle \phi_n | \phi_n \rangle_2}, \\ B_n^{(2)} &= \frac{s_n^{(2)}}{s^{(2)} - s_n^{(2)}} A_n^{(2)} = \frac{4\pi}{\epsilon_1} \frac{\left(s_n^{(2)}\right)^2}{s^{(2)} - s_n^{(2)}} \frac{\int dV \phi_n^*(\mathbf{r})\rho(\mathbf{r})}{\langle \phi_n | \phi_n \rangle_2}, \end{aligned}$$

$$\phi_{\mathrm{sc}} = \frac{4\pi}{\epsilon_1} \sum_n \frac{\left(s_n^{(2)}\right)^2}{s^{(2)} - s_n^{(2)}} \frac{\int dV \phi_n^* \rho}{\langle \phi_n | \phi_n \rangle_2} \phi_n(\mathbf{r}) \tag{23}$$

$$= \frac{4\pi}{\epsilon_1} \sum_n \frac{s_n^{(1)}\left(1 - s_n^{(1)}\right)}{s_n^{(1)} - s} \frac{\int dV \phi_n^* \rho}{\langle \phi_n | \phi_n \rangle_1} \phi_n(\mathbf{r}). \tag{24}$$

Note that in the last form of the expansion for ϕ_{sc} we have used Eqs. (8), (9), and (11) to substitute for $s^{(2)}$, $s_n^{(2)}$, and $\langle \phi_n | \phi_n \rangle_2$. Thus, if one of the constituents has an infinite volume and the other has a finite volume, we can expand the field created by a charge located in the finite volume constituent using the normalization over this constituent.

If $\rho(\mathbf{r})$ is nonzero in both V_1 and V_2 then we can separate it into a sum $\rho = \rho_1 + \rho_2$ where ρ_i is nonzero only in V_i. Equations (2) and (6) are then solved for $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$, produced, respectively, by $\rho_1(\mathbf{r})$ and $\rho_2(\mathbf{r})$. The total potential field is then $\phi(\mathbf{r}) = \phi_1(\mathbf{r}) + \phi_2(\mathbf{r})$.

If $\rho(\mathbf{r})$ represents a surface charge density at the V_1-V_2 interface then it must be proportional to a one-dimensional Dirac δ function at that surface. That two-dimensional or one-dimensional charge density can be assigned either to V_1 or to V_2. A particular example of this is described in Sec. IV below, after Eqs. (40) and (41).

III. CLUSTERS OF NONOVERLAPPING INCLUSIONS

When the microstructure is an array of finite inclusions we can start by calculating the eigenstates $\phi_{a\alpha}$ and $s_{a\alpha}$ of the isolated inclusions, where a denotes the inclusion and α its eigenstate. For $\mathbf{r} \in V_1$ an eigenfunction ϕ_n of the total array can be expanded in the $\phi_{a\alpha}$ as

$$\theta_1 \phi_n = \sum_{a\alpha} A_{a\alpha}^{(n)} \theta_a \phi_{a\alpha}, \tag{25}$$

where $\theta_a(\mathbf{r})$ is the analog of $\theta_1(\mathbf{r})$ for the inclusion a, i.e., $\theta_a(\mathbf{r}) = 1$ for $\mathbf{r}$ inside that inclusion but vanishes elsewhere. In order to calculate the expansion coefficients $A_{a\alpha}^{(n)}$ we calculate the integral

$$\begin{aligned} &\int dV \phi_{a\alpha}^* \nabla^2 \phi_n \\ &= \int dV [\nabla \cdot (\phi_{a\alpha}^* \nabla \phi_n) - (\nabla \phi_{a\alpha}^* \cdot \nabla \phi_n)] \\ &= \int dV [-\nabla \cdot (\phi_n \nabla \phi_{a\alpha}^*) + \phi_n \nabla^2 \phi_{a\alpha}^*] \end{aligned}$$

$$\begin{aligned} &= u_{a\alpha}\int dV\phi_n\nabla\cdot(\theta_a\nabla\phi^*_{a\alpha})\\ &= u_{a\alpha}\int dV[\nabla\cdot(\phi_n\theta_a\nabla\phi^*_{a\alpha}) - \theta_a(\nabla\phi^*_{a\alpha}\cdot\nabla\phi_n)]\\ &= -u_{a\alpha}\langle\phi_{a\alpha}|\phi_n\rangle_a = -u_{a\alpha}A^{(n)}_{a\alpha}\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a, \end{aligned} \tag{26}$$

where the isolated inclusion scalar product is defined by

$$\langle\phi|\psi\rangle_a \equiv \int dV\theta_a(\nabla\phi^*\cdot\nabla\psi).$$

To get the final result in Eq. (26) we have used the fact that $\langle\phi_{a\alpha}|\phi_{a\beta}\rangle_a = 0$ for $\alpha \neq \beta$.

We can also write

$$\begin{aligned} \int dV\phi^*_{a\alpha}\nabla^2\phi_n &= u^{(1)}_n\int dV\phi^*_{a\alpha}\nabla\cdot(\theta_1\nabla\phi_n)\\ &= -u^{(1)}_n\int dV\theta_1(\nabla\phi^*_{a\alpha}\cdot\nabla\phi_n) = -u^{(1)}_n\langle\phi_{a\alpha}|\phi_n\rangle_1\\ &= -u^{(1)}_n\sum_{b\beta}A^{(n)}_{b\beta}\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b. \end{aligned} \tag{27}$$

Comparing the results of Eqs. (26) and (27) we get

$$u_{a\alpha}A^{(n)}_{a\alpha}\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a = u^{(1)}_n\sum_{b\beta}A^{(n)}_{b\beta}\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b.$$

Note that $\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b$ is a scalar product of eigenfunctions of inclusions a and b that are different in general, but taken over the volume of just one of them, namely, b. Therefore, even if the inclusions have the same shape and volume, and therefore have the same isolated inclusion eigenstates, this scalar product is usually nonzero even if $\alpha = \beta$.

The preceding equation can be rewritten as

$$s^{(1)}_n A^{(n)}_{a\alpha} = \sum_{b\beta}M_{a\alpha,b\beta}A^{(n)}_{b\beta}, \tag{28}$$

$$M_{a\alpha,b\beta} \equiv s_{a\alpha}\frac{\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b}{\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a},\quad M_{b\beta,a\alpha} = s_{b\beta}\frac{\langle\phi_{b\beta}|\phi_{a\alpha}\rangle_a}{\langle\phi_{b\beta}|\phi_{b\beta}\rangle_b}. \tag{29}$$

If we normalize all the isolated inclusion eigenfunctions to 1, i.e., $\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a = 1$, then the matrix $\hat{M}$, the elements of which are $M_{a\alpha,b\beta}$, is a Hermitian matrix:

$$\begin{aligned} \langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b &= \int dV\theta_b(\nabla\phi^*_{a\alpha}\cdot\nabla\phi_{b\beta})\\ &= \int dV[\nabla\cdot(\phi^*_{a\alpha}\theta_b\nabla\phi_{b\beta}) - \phi^*_{a\alpha}\nabla\cdot(\theta_b\nabla\phi_{b\beta})]\\ &= -s_{b\beta}\int dV\phi^*_{a\alpha}\nabla^2\phi_{b\beta}\\ &= -s_{b\beta}\int dV[\nabla\cdot(\phi^*_{a\alpha}\nabla\phi_{b\beta}) - (\nabla\phi^*_{a\alpha}\cdot\nabla\phi_{b\beta})]\\ &= s_{b\beta}\int dV[\nabla\cdot(\phi_{b\beta}\nabla\phi^*_{a\alpha}) - \phi_{b\beta}\nabla^2\phi^*_{a\alpha}]\\ &= -\frac{s_{b\beta}}{s_{a\alpha}}\int dV\phi_{b\beta}\nabla\cdot(\theta_a\nabla\phi^*_{a\alpha}) = \frac{s_{b\beta}}{s_{a\alpha}}\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_a. \end{aligned}$$

From this it follows that $M_{b\beta,a\alpha} = (M_{a\alpha,b\beta})^*$.

Here $s^{(1)}_n$ and $A^{(n)}_{a\alpha}$ are the eigenvalues and eigenvectors of the Hermitian matrix $\hat{M}$. They can be found by solving numerically the matrix eigenvalue problem of Eq. (28). From Eq. (29) it follows that the nonzero off-diagonal elements of that matrix are proportional to overlap integrals of pairs of eigenfunctions from different inclusions. When a and b denote the same inclusion the elements of $\hat{M}$ are

$$M_{a\alpha,a\beta} \equiv s_{a\alpha}\langle\phi_{a\alpha}|\phi_{a\beta}\rangle_a = s_{a\alpha}\delta_{\alpha\beta}.$$

In order to extend Eq. (25) to a representation of ϕ_n everywhere we consider the following equation:

$$\begin{aligned} \nabla^2\phi_n &= u^{(1)}_n\nabla\cdot(\theta_1\nabla\phi_n) = u^{(1)}_n\nabla\cdot\left(\sum_{a\alpha}\theta_a A^{(n)}_{a\alpha}\nabla\phi_{a\alpha}\right)\\ &= \sum_{a\alpha}\frac{u^{(1)}_n}{u_{a\alpha}}A^{(n)}_{a\alpha}\nabla^2\phi_{a\alpha}\\ &\Rightarrow \nabla^2\left(\phi_n - \sum_{a\alpha}\frac{s_{a\alpha}}{s^{(1)}_n}A^{(n)}_{a\alpha}\phi_{a\alpha}\right) = 0. \end{aligned}$$

From this it follows that the last term in large parentheses must vanish. Thus we get

$$s^{(1)}_n\phi_n(\mathbf{r}) = \sum_{a\alpha}s_{a\alpha}A^{(n)}_{a\alpha}\phi_{a\alpha}(\mathbf{r}), \tag{30}$$

which is valid for *all* **r**. We note that the form of this expansion differs from that of Eq. (25). We also note that each of the isolated inclusion eigenfunctions $\phi_{a\alpha}(\mathbf{r})$ is used everywhere, i.e., not only inside its inclusion a. This is in contrast with Eq. (25), where each eigenfunction is used only inside its own inclusion. The importance of Eq. (30) is that it provides an expression for $\phi_n(\mathbf{r})$ which is valid also outside V_1. This can be used to expand the physical field $\phi(\mathbf{r})$ using Eqs. (12), (13), and (21)–(24). In this way we will get expansions for $\phi(\mathbf{r})$ in both V_1 and V_2, irrespective of where $\rho(\mathbf{r})$ is nonzero. We note that if all the isolated inclusion eigenfunctions $\phi_{a\alpha}$ are normalized to 1, namely, $\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a = 1$ for all a and α, and if all the eigenvectors $A^{(n)}_{a\alpha}$ are also normalized to 1, namely, $\sum_{a\alpha}|A^{(n)}_{a\alpha}|^2 = 1$, then $\phi_n(\mathbf{r})$ is also normalized to 1 in V_1, namely, $\langle\phi_n|\phi_n\rangle_1 = 1$.

An alternative procedure for calculating the scattered potential ϕ_{sc} when $\rho(\mathbf{r})$ is nonzero only outside the inclusions is as follows. We first expand ϕ_0 and ϕ_{sc} in the $\phi_{a\alpha}$ eigenfunctions inside V_1:

$$\theta_1\phi_0 = \sum_{a\alpha}A_{a\alpha}\theta_a\phi_{a\alpha},\quad \theta_1\phi_{\text{sc}} = \sum_{a\alpha}B_{a\alpha}\theta_a\phi_{a\alpha}. \tag{31}$$

In order to determine the coefficients $A_{a\alpha}$ we calculate the following integral in two ways:

$$\begin{aligned} \int dV\phi^*_{a\alpha}\nabla^2\phi_0 &= \int dV\phi_0\nabla^2\phi^*_{a\alpha}\\ &= u_{a\alpha}\int dV\phi_0\nabla\cdot(\theta_a\nabla\phi^*_{a\alpha})\\ &= -u_{a\alpha}\int dV\theta_a(\nabla\phi^*_{a\alpha}\cdot\nabla\phi_0)\\ &= -u_{a\alpha}\langle\phi_{a\alpha}|\phi_0\rangle_a = -u_{a\alpha}A_{a\alpha}\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a, \end{aligned}$$

but also

$$\int dV\phi^*_{a\alpha}\nabla^2\phi_0 = -\frac{4\pi}{\epsilon_2}\int dV\phi^*_{a\alpha}\rho.$$

From these results it follows that

$$A_{a\alpha} = \frac{4\pi s_{a\alpha}}{\epsilon_2}\frac{\int dV\phi^*_{a\alpha}\rho}{\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a}.$$

In order to determine the coefficients $B_{a\alpha}$ we now calculate the following integral in two ways:

$$\begin{aligned}\int dV\phi^*_{a\alpha}\nabla^2\phi_{\rm sc} &= \int dV\phi_{\rm sc}\nabla^2\phi^*_{a\alpha}\\ &= u_{a\alpha}\int dV\phi_{\rm sc}\nabla\cdot(\theta_a\nabla\phi^*_{a\alpha})\\ &= -u_{a\alpha}\int dV\theta_a(\nabla\phi_{\rm sc}\cdot\nabla\phi^*_{a\alpha})\\ &= -u_{a\alpha}\langle\phi_{a\alpha}|\phi_{\rm sc}\rangle_a = -u_{a\alpha}B_{a\alpha}\langle\phi_{a\alpha}|\phi_{a\alpha}\rangle_a,\end{aligned}$$

but also

$$\begin{aligned}\int dV\phi^*_{a\alpha}\nabla^2\phi_{\rm sc} &= u\int dV\phi^*_{a\alpha}\nabla\cdot[\theta_1\nabla(\phi_0+\phi_{\rm sc})]\\ &= -u\int dV\theta_1[\nabla\phi^*_{a\alpha}\cdot\nabla(\phi_0+\phi_{\rm sc})]\\ &= -u\langle\phi_{a\alpha}|(\phi_0+\phi_{\rm sc})\rangle_1\\ &= -u\sum_{b\beta}(A_{b\beta}+B_{b\beta})\langle\phi_{a\alpha}|\phi_{b\beta}\rangle_b.\end{aligned}$$

From these results we get the following set of linear algebraic equations for $B_{a\alpha}$:

$$sB_{a\alpha} = \sum_{b\beta}M_{a\alpha,a\beta}(A_{b\beta}+B_{b\beta}).$$

In order to extend the expansion of $\phi_{sc}(\mathbf{r})$ to values of $\mathbf{r}$ that are outside V_1 we proceed as follows:

$$\begin{aligned}\nabla^2\phi_{\rm sc} &= u\nabla\cdot[\theta_1\nabla(\phi_0+\phi_{\rm sc})]\\ &= u\nabla\cdot\sum_{a\alpha}(A_{a\alpha}+B_{a\alpha})\theta_a\nabla\phi_{a\alpha}\\ &= \sum_{a\alpha}\frac{u}{u_{a\alpha}}(A_{a\alpha}+B_{a\alpha})\nabla^2\phi_{a\alpha}\\ &\Rightarrow \nabla^2\left(\phi_{\rm sc}-\sum_{a\alpha}\frac{s_{a\alpha}}{s}(A_{a\alpha}+B_{a\alpha})\phi_{a\alpha}\right) = 0.\end{aligned}$$

From this it follows that

$$\phi_{\rm sc} = \sum_{a\alpha}\frac{s_{a\alpha}}{s}(A_{a\alpha}+B_{a\alpha})\phi_{a\alpha}, \tag{32}$$

which is valid for *all* $\mathbf{r}$. This differs from the expansion in Eq. (31), even for $\mathbf{r}\in V_1$. The reason for this is that, whereas in Eq. (31) each eigenfunction $\phi_{a\alpha}$ is used only inside its own inclusion a, in Eq. (32) each of those eigenfunctions is used everywhere, including the insides of all the other inclusions as well as the complementary volume V_2. This is similar to the remarks made following Eq. (30) above.

If $\rho(\mathbf{r})$ is nonzero only inside some of the inclusions then we will need to use values of the eigenfunctions of the cluster outside the inclusions. The eigenfunctions will still be given by Eq. (30), but the relevant eigenvalues will be the V_2 eigenvalues $s^{(2)}_n = 1 - s^{(1)}_n$. Equation (21) will now be replaced by Eqs. (23) and (24).

IV. APPLICATION TO A PARTICULAR MICROSTRUCTURE

A simple example of the situation where $\rho(\mathbf{r})$ is nonzero is when there is a point charge q inside or outside a radius-R spherical inclusion in an otherwise uniform host medium. The inside of the sphere is V_1, where $\epsilon = \epsilon_1$, while its outside is V_2, where $\epsilon = \epsilon_2$. The function $\phi_0(\mathbf{r})$ is now the simple Coulomb potential of a point charge q located at $\mathbf{r}_0$ in a uniform medium, namely,

$$\phi_0(\mathbf{r}) = \frac{q}{\epsilon_i|\mathbf{r}-\mathbf{r}_0|} \quad \text{for } \mathbf{r}_0\in V_i.$$

The eigenstates are then ($l = 0,1,2,\ldots, -l\leqslant m\leqslant l$)

$$\phi_{lm}(\mathbf{r}) = \begin{cases} r^l Y_{lm}(\Omega) & \text{in } V_1,\ r<R\\ R^{2l+1}\frac{1}{r^{l+1}}Y_{lm}(\Omega) & \text{in } V_2,\ r>R,\end{cases} \tag{33}$$

$$(2l+1)s^{(1)}_{lm} = l,\quad (2l+1)s^{(2)}_{lm} = (l+1), \tag{34}$$

$$\langle\phi_{lm}|\phi_{lm}\rangle_1 = lR^{2l+1},\quad \langle\phi_{lm}|\phi_{lm}\rangle_2 = (l+1)R^{2l+1}, \tag{35}$$

where $Y_{lm}(\Omega)$ is a normalized spherical harmonic, i.e., $\int d\Omega\, Y^*_{lm}Y_{l'm'} = \delta_{ll'}\delta_{mm'}$.

As shown in Sec. II for the general case, these eigenfunctions are the same, irrespective of whether we choose to normalize them in the $r<R$ or $r>R$ regions. Equation (35) exemplifies the general relation $\langle\psi_n|\psi_n\rangle_2 = [(1-s^{(1)}_n)/s^{(1)}_n]\langle\psi_n|\psi_n\rangle_1$, which follows from Eqs. (10) and (11), between the normalizations in these two regions. Equation (34) exemplifies the general relation of Eq. (9) between the $s^{(1)}_n$ and $s^{(2)}_n$ eigenvalues. We note that the infinite sequences of these eigenvalues have a single accumulation point, namely, $s^{(i)}_{lm}\to 1/2$ when $l\to\infty$. This is in agreement with a general theorem proved in Ref. [11]. We also note that there is now an isotropic eigenfunction, namely, ϕ_{00}, which has the eigenvalues $s^{(1)}_{00} = 0$, $s^{(2)}_{00} = 1$. The electric field of that eigenfunction vanishes when $r<R$; this is why that eigenfunction did not appear in Ref. [1].

From Eq. (16) we can conclude that, when $\rho(\mathbf{r}) = q\delta^3(\mathbf{r}-\mathbf{r}_0)$ and $\mathbf{r}_0\in V_2$,

$$\langle\phi_n|\phi_0\rangle_1 = \frac{4\pi q s^{(1)}_n}{\epsilon_2}\phi^*_n(\mathbf{r}_0). \tag{36}$$

Similarly, when $\mathbf{r}_0\in V_1$,

$$\langle\phi_n|\phi_0\rangle_2 = \frac{4\pi q s^{(2)}_n}{\epsilon_1}\phi^*_n(\mathbf{r}_0). \tag{37}$$

Using Eqs. (21) and (23) we now get a series for $\phi(\mathbf{r})$ of a point charge at $\mathbf{r}_0$ in a radius-R sphere structure. For $|\mathbf{r}_0|<R$,

$$\phi(\mathbf{r}) = \frac{q}{\epsilon_1|\mathbf{r}-\mathbf{r}_0|} + \frac{4\pi q}{\epsilon_1}\sum_{lm}\frac{\left(s^{(2)}_l\right)^2}{s^{(2)}-s^{(2)}_l}\frac{\phi^*_{lm}(\mathbf{r}_0)\phi_{lm}(\mathbf{r})}{\langle\phi_{lm}|\phi_{lm}\rangle_2}, \tag{38}$$

and for $|\mathbf{r}_0| > R$,

$$\phi(\mathbf{r}) = \frac{q}{\epsilon_2|\mathbf{r}-\mathbf{r}_0|} + \frac{4\pi q}{\epsilon_2}\sum_{lm}\frac{\left(s_l^{(1)}\right)^2}{s-s_l^{(1)}}\frac{\phi_{lm}^*(\mathbf{r}_0)\phi_{lm}(\mathbf{r})}{\langle\phi_{lm}|\phi_{lm}\rangle_1}. \tag{39}$$

The normalization scalar product, which appears in the denominators of the above equations, allows the use of the unnormalized eigenfunctions $\phi_{lm}(\mathbf{r})$ everywhere. This may be useful because, except for the normalization, these eigenfunctions are the same in both cases. We note that when $\mathbf{r}_0$ or $\mathbf{r}$ lies along the z axis, only the $m = 0$ terms in these series are nonzero. In order to get a more explicit form for the series of Eqs. (38) and (39) we use Eqs. (33)–(35), as well as the equality [see, e.g., Eq. (B.98) in Ref. [12]]

$$\sum_{m=-l}^{l} Y_{lm}^*(\Omega_0)Y_{lm}(\Omega) = \frac{2l+1}{4\pi}P_l(\cos\alpha),$$

where α is the angle between Ω and Ω_0 and P_l is the order-l Legendre polynomial. In this way we get, for $r_0 < R$,

$$\phi(\mathbf{r}) - \frac{q}{\epsilon_1|\mathbf{r}-\mathbf{r}_0|} = \frac{q}{\epsilon_1}\sum_{l=0}^{\infty}\frac{l+1}{2l+1}\frac{r_0^l P_l(\cos\alpha)}{\frac{l}{2l+1}-s} \times\begin{cases}\frac{r^l}{R^{2l+1}}, & r < R\\ \frac{1}{r^{l+1}}, & r > R.\end{cases} \tag{40}$$

and for $r_0 > R$,

$$\phi(\mathbf{r}) - \frac{q}{\epsilon_2|\mathbf{r}-\mathbf{r}_0|} = \frac{q}{\epsilon_2}\sum_{l=1}^{\infty}\frac{l}{2l+1}\frac{P_l(\cos\alpha)}{s-\frac{l}{2l+1}}\frac{1}{r_0^{l+1}} \times\begin{cases}r^l, & r < R\\ \frac{R^{2l+1}}{r^{l+1}}, & r > R.\end{cases} \tag{41}$$

It is useful to note here that, although these expressions may look like power series in r or $1/r$, they are in fact series in a set of mutually orthogonal states in a Hilbert space. Therefore, there is no question that these series always converge to the right answers.

When $r_0 = R$, Eqs. (40) and (41) lead to the same values for $\phi(\mathbf{r})$: In order to see this we can use the well known expansion of $1/|\mathbf{r}-\mathbf{R}|$ in a series of Legendre polynomials—see Eq. (B.99) of Ref. [12]. This is a special example of the remarks in the final paragraph of Sec. II.

When the point charge is at the sphere center, it is clear that only the isotropic eigenfunction $\phi_{00}(\mathbf{r})$ has a nonzero scalar product with the above forms of $\phi_0(\mathbf{r})$. It is then easy to use Eq. (40) to get that

$$\phi(\mathbf{r}) = \begin{cases}\frac{q}{\epsilon_1 r} + \frac{q}{\epsilon_1 R}\frac{\epsilon_1-\epsilon_2}{\epsilon_2}, & r < R\\ \frac{q}{\epsilon_2 r}, & r > R,\end{cases}$$

which is the well known correct result. Note that the constant added to the $1/r$ potential in the first line makes no contribution to the electric field but ensures that $\phi(\mathbf{r})$ is continuous at the sphere surface $r = R$.

Clearly, the approach used here provides a much simpler way to get an infinite series representation for $\phi(\mathbf{r})$ than other methods, e.g., approaches based on image charges (see Ref. [13]) or approaches based on expanding in quasinormal modes (see, e.g., Ref. [3]).

V. SUMMARY AND DISCUSSION

A spectral approach to the calculation of a local electrostatic or quasistatic electric field in a two-constituent composite medium was developed which applies to cases where that field is produced by a given charge density that can exist anywhere in the system. This is relevant for studies where that field is produced by the decay of an excited atom or molecule, or by the scattering of electromagnetic radiation by an atom or molecule or nanoparticle, when these particles are much smaller than the relevant wavelength and are closer than that wavelength to the V_1-V_2 interface. In these cases $\rho(\mathbf{r})$ should usually be calculated using quantum mechanics and will depend upon the heterogeneous environment. In some cases a higher-frequency field can be generated by a strong local physical field via the nonlinear polarization, which can be produced either by the local field induced by an incident plane wave or by a basic radiation emitter within the system. That induced nonlinear polarization can be used as the source term in the linear differential equation for the higher-frequency field in the same composite structure.

The examples treated in Sec. IV have often been solved previously for the case where the point charge is outside the sphere (see, e.g., Ref. [14]). However, the case where that charge is at an arbitrary point inside the sphere is much more complicated using traditional methods. By contrast, our approach is equally simple in both cases. Our treatment shows that the spectral method presented here is much simpler and easier to use than traditional methods. Even in the case of a general microstructure, the most computationally difficult step is the calculation of the quasistatic eigenstates which are harmonic in both V_1 and V_2. Once those are known, the calculation of the physical field resulting from any given source only requires calculating integrals and summing a series. While the series is infinite in principle and each term requires the calculation of a three-dimensional integral, in practice only a small number of terms and integrals are important. This is especially true if the system is close to a resonance, i.e., if the physical value of s is close to one of the eigenvalues $s_n^{(1)}$, or if the point source is far from the V_1-V_2 interface (see Ref. [6]).

In the future this approach should be extended to deal with composite structures of more than two constituents. It should also be extended beyond the quasistatic regime, so as to apply to the solution of the full Maxwell equations in a composite medium, without any restrictions on the size of the inclusions vs the electromagnetic wavelengths or skin depths.

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