Electrostatic resonances and optical responses of cylindrical clusters

C. W. Choy\textsuperscript{1}, J. J. Xiao\textsuperscript{1}, and K. W. Yu\textsuperscript{1,2}

\textsuperscript{1} Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China
\textsuperscript{2} Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China
E-mail: kwyu@phy.cuhk.edu.hk

Abstract. We developed a Green function formalism (GFF) for computing the electrostatic resonance in clusters of cylindrical particles. In the GFF, we take advantage of a surface integral equation to avoid matching the complicated boundary conditions on the surfaces of the particles. Numerical solutions of the eigenvalue equation yield a pole spectrum in the spectral representation. The pole spectrum can in turn be used to compute the optical response of these particles. For two cylindrical particles, the results are in excellent agreement with the exact results from the multiple image method and the normal mode expansion method. The results of this work can be extended to investigate the enhanced nonlinear optical responses of metal-dielectric composites, as well as optical switching in plasmonic waveguides.

1. Introduction

Electrostatic resonances (ERs) are of great interest in engineering the electromagnetic properties of metamaterials [1, 2]. Particularly they have significant implications in optical properties of composite nanomaterials, and in coupled surface plasmons of plasmonic structures [3, 4]. This is clearly reflected in the Bergman-Milton spectral representation [4, 5]. More specifically, for composites consisting of two ingredients (e.g., $\epsilon_1$ and $\epsilon_2$), by using a spectral parameter $s = (1 - \epsilon_1/\epsilon_2)^{-1}$, the material-independent eigenmodes $\{s_n, \phi_n(r)\}$ of ER are essentially determined by the microstructure of the system [4, 6, 7]. Once the electrostatic resonant eigenvalues $s_n$ and their residues $F_n$ are established, the resonant frequencies are determined by the dielectric dispersion function $\epsilon_1(\omega)$ and the macroscopic effective optical properties, e.g., bulk dielectric permittivity $\tilde{\epsilon}_{\text{eff}}$, of the system become readily known [3–5]. This theory has been extensively and successfully exploited for studies of optical random composites (e.g., see [3]), graded composites [8], periodic nanostructures [1], as well as media of various geometries [2,6]. It also facilitates studies of electrorheological fluid and electrokinetics of biological cells [9–11]. The formalism partially changes, however, when there are more than two constituent components, for example, in three-component composites [12], and in graded composites as detailed by Dong et al [13].

In this work, we utilize the recently established Green function formalism (GFF) [14] to examine ERs in metal-dielectric composites. This approach, not like traditional ones, is actually suitable for an arbitrary interface separating two media of different dielectric constants without matching of the complicated boundary conditions. We demonstrate its usage by numerically...
examine the spectral functions of a pair of nanocylinders, which yields results in good agreement with previous ones from both the multiple image method [15] and the normal-mode expansion method [16]. We then go further to extract the spectral functions of nanocylinders in a triangle which enables the investigation of particle-particle interaction as well as particle-pair interaction. The three-cylinder-in-triangle case represents a guideline for investigation on various cylinder arrays [17], which is tractable by the GFF we developed but cumbersome by traditional approaches.

2. Spectral representation using GFF: Formalism and numerical demonstration

The origin of ER is to solve potential of the whole space by Laplace’s equation subject to an applied field \( \mathbf{E}_0 = -E_0 \mathbf{y} \). According to the GFF [14], we have

\[
\left[ 1 - \frac{1}{s} G(\mathbf{r}, \mathbf{r}') \right] \phi(\mathbf{r}) = -E_0 y + \frac{1}{s} \oint_S dS' [\mathbf{n}' \cdot \nabla' G(\mathbf{r}, \mathbf{r}')] \phi(\mathbf{r}),
\]

(1)

where \( G(\mathbf{r}, \mathbf{r}') = 1/4\pi |\mathbf{r} - \mathbf{r}'| \), \( \theta(\mathbf{r}) \) the microstructure characteristic function. When \( \mathbf{r} \in S \), e.g., inside the inclusions, \( \theta(\mathbf{r}) = 0 \), equation (1) becomes \( \phi(\mathbf{r}) = -E_0 y + 1/2 \oint_S dS' [\mathbf{n}' \cdot \nabla' G(\mathbf{r}, \mathbf{r}')] \phi(\mathbf{r}) \).

With reference to equation (1), we are able to convert a volume integral differential operator \( \hat{\Gamma} \) to a surface integral-differential non-Hermitian operator \( \hat{\Gamma}' \) which reads

\[
\hat{\Gamma}' \equiv \oint_S dS' [\mathbf{n}' \cdot \nabla' G(\mathbf{r}, \mathbf{r}')].
\]

(2)

The eigen-spectrum \( \{s_n, \phi_n(\mathbf{r})\} \) of \( \hat{\Gamma}' \) is formulated in the absence of applied field (\( E_0 = 0 \)). Note that \( \hat{\Gamma}' \) is not necessarily Hermitian. We can denote \( s_n \), \( |R_n) \) and \( \langle L_n| \) as the nth eigenvalue, right eigenvector and left eigenvector of \( \hat{\Gamma}' \), respectively. The surface integral operator is easier to handle than the volume integral operator. However, we have to deal with a bi-orthogonal system due to possible non-Hermitian nature of the operator. We would like to stress that the eigenvectors only represent the potentials right on the surface but not the whole volume. According to the GFF, it is easy to find the eigenvectors of the whole volume by eigenvectors on the surface.

For illustration, we consider the case in which two identical cylinders are embedded in a homogeneous host medium. The boundaries of the first and the second cylinders satisfy \( r = f(\theta) \) and \( r = g(\theta) \) respectively. By the GFF, the potential on the surfaces (\( S_1 \) and \( S_2 \)) of the cylinders satisfies the following integral equation

\[
\phi(\mathbf{r}) = -E_0 y + \frac{1}{s} \oint_{S_1} dS' [\mathbf{n}' \cdot \nabla' G(\mathbf{r}, \mathbf{r}')] \phi(\mathbf{r}') + \frac{1}{s} \oint_{S_2} dS' [\mathbf{n}' \cdot \nabla' G(\mathbf{r}, \mathbf{r}')] \phi(\mathbf{r}').
\]

(3)

In order to solve the above integral equations, we express the potential at the surface of cylinders by step functions \( \psi_j(\theta) \)

\[
\phi_{S_1}(\theta) = \sum_n P_j \psi_j(\theta); \quad \phi_{S_2}(\theta) = \sum_n Q_j \psi_j(\theta).
\]

(4)

Then a matrix equation \( sA = -E_0 V + MA \) can be obtained, where

\[
A_i = \begin{cases} 
P_i, & \text{if } i \leq n \\
Q_{i-n}, & \text{if } i > n \end{cases},
\]

(5)

\[
M_{pq,ij} = \oint d\theta \int d\theta' \beta(\theta') [\mathbf{n} \cdot \nabla G_{pq}] \psi_i(\theta) \psi_j(\theta'),
\]

(6)

\[
V_i = \oint d\theta \psi_i(\theta) y,
\]

(7)
here \( p \) and \( q \) can be 1 or 2, while \( \beta(\theta') \) represents \( f(\theta') \) when \( q = 1 \) and \( g(\theta') \) when \( q = 2 \). Note that the diagonal elements of \( M \) cannot be evaluated directly due to the singularity of \( G \) when \( i = j \), but must be evaluated by the sum rule \( \sum_j M_{ij} = 0 \). Here \( s \) represents the eigenvalue and \( A \) represents the eigenvector, and is formulated in the absence of external field.

\[
M|R_n\rangle = s_n|R_n\rangle; \quad M^T\langle L_n| = s_n\langle L_n|. \tag{8}
\]

In this case, \( s_n, |R_n\rangle \) and \( \langle L_n| \) can be determined and hence \( F_n \) can be calculated by

\[
F_n = \frac{1}{V} \frac{\langle y|R_n\rangle\langle L_n|y\rangle}{\langle L_n|R_n\rangle}. \tag{9}
\]

Figure 1 shows the major poles \( s_1^{(L)} \) and \( s_1^{(T)} \) against separation ratio \( \sigma = \rho/2r \). The previous spectral poles from multiple image method [15] are also plotted. It can be seen that our numerical results match perfectly with the analytic solution. Figures 2(a)–2(d) shows the pole spectra of two approaching cylinders with different separation ratio \( \sigma \). These agree well with the results by the normal-mode expansion method [16]. Clearly, only modes with \( s_n > 0.5 \) are excited in the transverse case while only modes with \( s_n < 0.5 \) are excited in the longitudinal case. Moreover, the spectra for the longitudinal case are symmetric with that for the transverse case about \( s = 0.5 \). When the two cylinders are far away from each other, modes are concentrated at \( s = 0.5 \) and this is corresponding to the isolated cylinder case. Figures 2(e)–2(h) show the pole spectra of three cylinders arranging in an isosceles triangle with different height to base ratio \( \rho = H/\sigma \). In figure 2(e), the three cylinders are arranged in an equilateral triangle. The locations of the poles are the same for the transverse and longitudinal cases. When we move the cylinder at the upper vertex away from the base cylinder pair, fewer poles are excited. We can also compare the pole spectrum in figures 2(g) and 2(a). It can be seen that figure 2(g) is similar to figure 2(a), except for the enhancement of the poles near 0.5. We can understand the situation as follows. In the case of figure 2(g), the upper cylinder is quite far away from the base cylinders. As a result, there is less interaction between them and we can regard the system as a simple superposition of the isolated cylinder (monomer) and the two base cylinders (dimer) at a separation \( \sigma = 1.1 \).

3. Summary and conclusions
Based on a recently established Green function formalism, we have developed an exact method for the study of spectral representation of two electromagnetic media separated by arbitrary
Figure 2. Pole spectra of two approaching cylinders with separation ratio: (a) $\sigma = 1.1$, (b) $\sigma = 1.5$, (c) $\sigma = 3$, and (d) $\sigma = 10$, and pole spectra of three cylinders arranging in an isosceles triangle with base separation ratio $\sigma = 1.1$ and different height to base ratio $\rho = H/\sigma$: (e) $\rho = 0.866$ (equilateral triangle), (f) $\rho = 1$, (g) $\rho = 1.5$, and (h) $\rho = 3$. Note that black solid lines and red dotted lines correspond to the transverse case and longitudinal case respectively.

Acknowledgments

This work was supported by the RGC Earmarked Grant of the Hong Kong SAR Government.

References

[1] Shvets G and Urzhumov Y A 2003 Phys. Rev. Lett. 93 243902
[2] Fredkin D R and Mayergoyz I D 2003 Phys. Rev. Lett. 91 253902
[3] Stockman M I, Faleev S V and Bergman D J 2001 Phys. Rev. Lett. 87 167401; and references therein.
[4] Bergman D J 1978 Phys. Rep. 43 377; Bergman D J 1979 Phys. Rev. B 19 2359; Bergman D J and Stroud D 1992 Solid State Physics vol 46, eds Ehrenreich H and Turnbull D (New York: Academic Press) p 147
[5] McPhedran R C and Milton G W 1981 Appl. Phys. A: Solids Surf. 26 207
[6] Milton G W 2002 The Theory of Composites (New York: Cambridge University Press)
[7] Gu Y, Yu K W, and Sun H 1999 Phys. Rev. B 59 12847
[8] Huang J P and Yu K W 2006 Phys. Rep. 431 87
[9] Kim K, Stroud D, Li X and Bergman D J 2005 Phys. Rev. E 71 031503
[10] Huang J P, Yu K W and Gu G Q 2002 Phys. Rev. E 65 021401
[11] Huang J P, Karttunen M, Yu K W, and Dong L 2003 Phys. Rev. E 67 021403
[12] Gu Y and Gong Q H 2003 Phys. Rev. B 67, 014209; Gu Y and Gong Q H 2004 Phys. Rev. B 69 035105
[13] Dong L, Karttunen M and Yu K W 2005 Phys. Rev. E 72 016613
[14] Yu K W, Sun H and Wan J T K 2000 Physica B 279 78; Yu K W and Wan J T K 2001 Comput. Phys. Commun. 142 368
[15] Yu K W and Wan J T K 2000 Comput. Phys. Commun. 129 177
[16] Rojas R, Claro F and Proetto C R 2000 Phys. Rev. E 62 5688
[17] Ng M Y and Liu W C 2006 Opt. Express 14 4504