

Multilevel Multiple Scattering Theory and Applications to Band Diagrams of Photonic Crystals

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ABSTRACT: In this study, we developed a multilevel multiple scattering theory (ML-MST) for the numerical solutions of multiple scattering equations. We formulated multiple scattering theory using vector cylindrical waves (VCW) in the MST-VCW formulation and the translational addition theorem with exciting fields in VCW. A problem with this formulation is that neighboring scatterers can have overlapping circles. In this study, multiple scattering theory is formulated using the method of moments (MoM) in the MST-MoM formulation, with the exciting field in terms of MoM unknowns. The ML-MST is developed by separating the scattering from other scatterers into neighbor and non-neighbor contributions, resulting in 2-level interactions. We then replace the MST-VCW neighbor scattering with the corresponding MST-MoM neighbor scattering. The ML-MST eliminates the issues of overlapping circles of neighbors. We apply the ML-MST formulations to the problem of band diagrams of photonic crystals by summing the scattering from non-neighbors using broadband Green's functions (BBGF). The result is the multilevel Korringa-Kohn-Rostoker (KKR) equation. Numerical illustrations were performed for the 2D case. The accuracy of the solutions was validated by comparing them with COMSOL simulations. The CPU time of the ML-MST was more than two orders of magnitude lower than that of COMSOL.

1. INTRODUCTION

There are a large number of problems in physics and engineering involving the multiple scattering of waves in scatterers. The multiple scattering theory (MST), initiated by Foldy and Lax in waves in random media and by Korringa in waves in condensed matter physics, has been an analytical method [1–3]. The numerical implementation was performed using circular cylinders and spheres [4–6]. Recently, this method has been combined in a hybrid manner with computational electromagnetic methods (CEM) to extract the T -matrix of complex structures. The hybrid method achieved a high computational efficiency. The numerical MST outperforms the computational electromagnetic methods (CEM) of finite element (FEM), finite difference in the frequency domain (FDFD), finite difference in the time domain (FDTD), and the method of moments (MoM), which is often accelerated by the multilevel fast multipole method (ML-FMM). The numerical MST approach has been applied to microwave remote sensing of corn fields, forest [7], photonic crystals [8], and metasurfaces [9].

The multiple scattering approach has been implemented with vector cylindrical waves (VCW) in the MST-VCW formulation [7], vector spherical waves (VSW) [8], and vector plane waves, including evanescent waves [9]. A problem with this formulation is that neighboring scatterers can have overlapping circles/spheres. To address this problem, we developed a multilevel multiple scattering theory (ML-MST). The ML-MST is illustrated for the case of band diagrams of photonic crystals,

showing that the ML-MST handles the problem of overlapping circles of neighboring scatterers.

Photonic crystals are periodic dielectric structures whose Bloch eigenmodes form bands and band gaps analogous to electronic bands in solids [10]. Topological photonic and acoustic crystals [11–13], in particular, exploit the topology of these bands through degeneracy lifting, gyrotropy, or symmetry breaking to support unidirectional, backscattering-immune edge states. The design of such crystals depends on the accurate and efficient calculation of the underlying band structure for many lattice geometries, scatterer shapes, and material configurations.

Several families of methods have been commonly used to compute photonic band diagrams. The plane-wave method [10, 14–16] expands fields in a Fourier basis adapted to the lattice and yields a linear eigenvalue problem; its main drawback is poor convergence for high-contrast scatterers, requiring matrices of dimensions in the thousands for two-dimensional problems and substantially more in three dimensions [10]. The finite-difference and finite-element methods [17–20], including the widely used commercial implementation in COMSOL, discretize the unit cell volumetrically and likewise produce linear eigenproblems with large numbers of unknowns. Both families discretize the entire unit cell and incur the corresponding memory and time costs at every frequency.

Another family of methods is based on multiple scattering theory (MST) [1, 2, 21] and the closely related Korringa-Kohn-Rostoker (KKR) formulation originally developed for electron band theory [3, 22, 23]. In this approach, the periodic prob-

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lem is expressed in terms of the single-scatterer T -matrix [24] and a lattice Green's function that propagates the scattered field of one cell to the others. In our recent work, we used CEM tools to compute the single-scatterer T -matrix of complex structures, which widens the applicability of MST [7–9]. The eigenvalue equation reduces to a small matrix whose dimension is set by the number of cylindrical or spherical wave harmonics, typically 10 or fewer for the lowest bands. Because the single-scatterer T -matrix is intrinsic and independent of both the lattice and Bloch vector, it can be tabulated and reused, which makes the MST/KKR family attractive for parameter sweeps over lattice geometries and Bloch vectors. The standard MST/KKR family has been used extensively in photonic and phononic band calculations [21, 23, 25], and several open-source implementations are available [26–28].

The MST/KKR family has a structural limitation. The translation addition theorem that underlies the propagation of one scatterer's outgoing wave to the basis of another converges only when the minimum enclosing circle (in two dimensions) or sphere (in three dimensions) of one scatterer lies entirely outside that of the other [6]. When two scatterers are close enough that their enclosing circles overlap, a situation that arises generically in dense lattices, scatterers with elongated or non-convex shapes, and topological designs that pack high-permittivity inclusions tightly, the standard interaction fails to converge in the multipole basis, and the conventional KKR equation cannot be applied without modification. Several strategies have been proposed in the literature to mitigate this limitation, including plane-wave coupling formalisms that converge whenever a separating plane exists between the two scatterers [29] and assessments of the limits of the Rayleigh hypothesis for adjacent spheroids [28, 30].

In our previous studies, we focused on the broadband evaluation of the periodic lattice Green's function via the broadband Green's function (BBGF) representation [31]. The BBGF expresses the lattice sums as a frequency-independent setup, followed by a fast algebraic evaluation per frequency, and converges rapidly owing to imaginary-wavenumber extractions [32]. Combined with the KKR-MST eigenvalue equation, this yields the BBGF-KKR-MST family of methods [33], which has been applied to two-dimensional photonic crystals [31, 33], gyromagnetic topological photonic crystals [34], topological acoustics [35], and three-dimensional periodic structures [36]. Two recent extensions address the dense packing regime in 3D: irregularly shaped scatterers treated through a T -matrix obtained from a separate single-scatterer solver [37] and densely packed scatterers accommodated through higher-order T -matrix extraction from far fields [8], where the multipole order is increased to maintain the validity of the conventional spherical-wave representation as the scatterers approach each other.

In this study, we developed a multilevel multiple scattering theory (ML-MST) for numerical solutions of multiple scattering equations. Firstly, multiple scattering theory is formulated with the method of moments [38] (MST-MoM). The interior problem of each scatterer enters the formulation only through a single linear operator that maps the surface field to its outward

normal derivative. This operator is determined by the scatterer alone and is decoupled from the external environment. It can be obtained by any method suitable for the interior medium: a surface-integral equation for homogeneous scatterers, a finite element solution for complex interiors, or a volume-integral equation. The exterior MST-MoM machinery remained unchanged, regardless of the method used. The MST-MoM then has an exciting field in terms of MoM unknowns and the near-field T -matrix.

Next, we use the MST-VCW formulation with vector cylindrical waves as the basis together with the translational addition theorem. Then, the ML-MST is developed by separating the scattering from other scatterers into neighbor and non-neighbor contributions, resulting in 2-level interactions. We then replace the MST-VCW neighbor scattering with the corresponding MST-MoM neighbor scattering. The ML-MST eliminates the issues of overlapping neighbor circles. We apply the ML-MST formulations to the band diagrams of photonic crystals by summing scattering from non-neighbors using broadband Green's functions (BBGF). This modifies the previously defined D coefficients [33] to exclude the nearest neighbors. The result is a multilevel KKR equation with the new D coefficients and the near-field T -matrix. Neighbor and non-neighbor levels are truncated at different cylindrical-harmonic orders: the near-field level is retained at a higher order to capture the strong interactions of close neighbors, while the single-scatterer T -matrix is kept at a lower order to preserve its numerical stability. Numerical illustrations were performed for the 2D case. The accuracy of the solutions was validated by comparing them with COMSOL simulations. The CPU time of the ML-MST was more than two orders of magnitude lower than that of COMSOL.

The paper is organized as follows. Section 2 formulates the MST-MoM and introduces the near-field T -matrix. In Section 3, we summarize the MST-VCW formulation with the translational addition theorem. In Section 4, the multilevel MST is formulated with the neighbor contributions of MST-VCW replaced by those of MST-MoM. In Section 5, the ML-MST formulation is applied to a photonic crystal by summing the non-neighbor contributions using the broadband Green's function. The ML-KKR equation is derived. Section 6 presents the numerical results, comparisons with COMSOL, and CPU benchmarks.

2. MULTIPLE SCATTERING THEORY WITH MOM

Previously, multiple scattering theory equations were rigorously derived from integral equations using vector spherical waves (VSW) and spheres [6, 39]. In this section, we rigorously derive the multiple scattering theory using the MoM. These equations are useful because, in the MoM formulation, distances between neighbors can be close, and neighbors can be within the circumscribing circles. The 2D problem is considered for a simple illustration, and the methodology can be readily extended to vector 3D problems. For 2D, $\bar{\rho} = (x, y) = (\rho, \phi)$. Consider the scattering by a single scatterer with surface S , as shown in Fig. 1. The exterior problem has μ, ε and

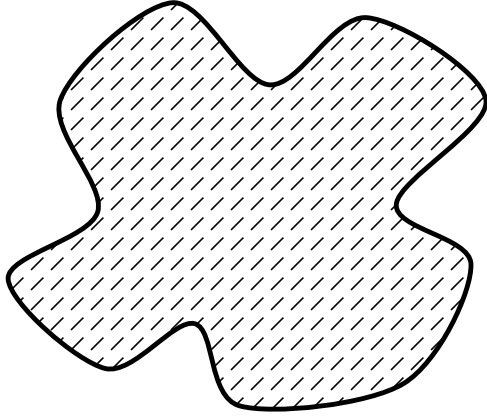


FIGURE 1. A single two-dimensional scatterer.

$k = \omega\sqrt{\mu\varepsilon}$. The Green's function is

$$g(\bar{\rho}, \bar{\rho}') = \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{\rho}'|). \quad (1)$$

Let $\bar{r}$ be outside S but near the scatterer boundary. The surface integral equation is [6], for $\bar{r} \in S^+$,

$$\begin{aligned} \psi_{\text{inc}}(\bar{\rho}) + \int_S d\ell' [\psi(\bar{\rho}') \hat{n}' \cdot \nabla' g(\bar{\rho}, \bar{\rho}') \\ - g(\bar{\rho}, \bar{\rho}') \hat{n}' \cdot \nabla' \psi(\bar{\rho}')] = \psi(\bar{\rho}), \end{aligned} \quad (2)$$

where $\hat{n}$ is the outward normal to S , and $d\ell'$ is the line integration over S . Let the boundary values be $\hat{n}' \cdot \nabla' \psi(\bar{\rho}') = J(t')$ and $\psi(\bar{\rho}') = \psi(t')$. We divide the circumference into N small intervals σ_n , $n = 1, \dots, N$, of size Δt , with the center point t_n corresponding to (x_n, y_n) . Because each interval is small, $J(t')$ and $\psi(t')$ are assumed to be constant over σ_n as follows:

$$J(t') = \sum_{n=1}^N J_n f_n(t), \quad \psi(t') = \sum_{n=1}^N \psi_n f_n(t), \quad (3)$$

where $f_n(t)$ is the pulse basis function, which is equal to 1 for $t \in \sigma_n$ and 0 otherwise. Point matching at $\bar{r}_m = (x_m, y_m)$ on $S_q^{(+)}$ gives

$$\begin{aligned} \psi_{\text{inc}}(\bar{\rho}_m) - \sum_n J_n \int_{\sigma_n} d\ell' g(\bar{\rho}_m, \bar{\rho}') \\ + \sum_n \psi_n \int_{\sigma_n} d\ell' \hat{n}' \cdot \nabla' g(\bar{\rho}_m^+, \bar{\rho}') = \psi(\bar{\rho}_m). \end{aligned} \quad (4)$$

The exterior impedance matrix elements are

$$Z_{mn}^D = \int_{\sigma_n} d\ell' g(\bar{\rho}_m, \bar{\rho}'), \quad (5)$$

$$Z_{mn}^N = - \int_{\sigma_n} d\ell' \hat{n}' \cdot \nabla' g(\bar{\rho}_m, \bar{\rho}'), \quad n \neq m, \quad (6)$$

$$Z_{mm}^N = \frac{1}{2}, \quad (7)$$

and the interior impedance matrix elements are

$$Z_{mn}^{D,\text{int}} = - \int_{\sigma_n} d\ell' g_{\text{int}}(\bar{\rho}_m, \bar{\rho}'), \quad (8)$$

$$Z_{mn}^{N,\text{int}} = \int_{\sigma_n} d\ell' \hat{n}' \cdot \nabla' g_{\text{int}}(\bar{\rho}_m, \bar{\rho}'), \quad n \neq m, \quad (9)$$

$$Z_{mm}^{N,\text{int}} = \frac{1}{2}. \quad (10)$$

The cross terms between scatterers q and p are

$$Z_{mqn_p}^{D(qp)} = \int_{\sigma_n^{(p)}} d\ell' g(\bar{\rho}_m^{(q)}, \bar{\rho}'), \quad (11)$$

$$Z_{mqn_p}^{N(qp)} = - \int_{\sigma_n^{(p)}} d\ell' \hat{n}' \cdot \nabla' g(\bar{\rho}_m^{(q)}, \bar{\rho}'). \quad (12)$$

Then, the MoM equation becomes [6]

$$\sum_n Z_{mn}^D J_n + \sum_n Z_{mn}^N \psi_n = \psi_{\text{inc},m}, \quad (13)$$

or, in matrix notation, $\bar{\bar{Z}}^D \bar{J} + \bar{\bar{Z}}^N \bar{\psi} = \bar{\psi}_{\text{inc}}$.

For the interior problem, with μ_{int} , ε_{int} and $k_{\text{int}} = \omega\sqrt{\mu_{\text{int}}\varepsilon_{\text{int}}}$,

the Green's function is $g_{\text{int}}(\bar{r}, \bar{r}') = \frac{i}{4} H_0^{(1)}(k_{\text{int}}|\bar{\rho} - \bar{\rho}'|)$. Using Green's theorem with the interior wave function ψ_{int} ,

$$\begin{aligned} \int_S d\ell' \hat{n}' \cdot [\psi_{\text{int}}(\bar{\rho}') \nabla' g_{\text{int}}(\bar{\rho}, \bar{\rho}') \\ - g_{\text{int}}(\bar{\rho}, \bar{\rho}') \nabla' \psi_{\text{int}}(\bar{\rho}')] = 0 \end{aligned} \quad (14)$$

if $\bar{\rho}$ is outside S . Applying pulse basis functions with $\psi_{\text{int}}(\bar{\rho}') = \psi_{\text{int},n}$ and $\hat{n}' \cdot \nabla' \psi_{\text{int}}(\bar{\rho}') = J_{\text{int},n}$ over σ_n , and point matching at $\bar{r}_m^+$,

$$\sum_n J_{\text{int},n} Z_{mn}^{D,\text{int}} + \sum_n \psi_{\text{int},n} Z_{mn}^{N,\text{int}} = 0, \quad (15)$$

or $\bar{\bar{Z}}^{D,\text{int}} \bar{J}_{\text{int}} + \bar{\bar{Z}}^{N,\text{int}} \bar{\psi}_{\text{int}} = 0$. The boundary conditions at S give $\bar{\psi}_{\text{int}} = \bar{\psi}$ and $\bar{J}_{\text{int}} = \rho \bar{J}$, with

$$\rho = \begin{cases} \varepsilon_{\text{int}}/\varepsilon & \text{for TE,} \\ \mu_{\text{int}}/\mu & \text{for TM.} \end{cases} \quad (16)$$

Then, $\bar{\bar{Z}}^{D,\text{int}} \rho \bar{J} + \bar{\bar{Z}}^{N,\text{int}} \bar{\psi} = 0$, so that $\bar{J} = \bar{Q} \bar{\psi}$ with

$$\bar{Q} = -\frac{1}{\rho} \left(\bar{\bar{Z}}^{D,\text{int}} \right)^{-1} \bar{\bar{Z}}^{N,\text{int}}. \quad (17)$$

Substituting into the exterior problem gives $\bar{\psi}$ in terms of $\bar{\psi}_{\text{inc}}$,

$$\bar{\psi} = \left(\bar{\bar{Z}}^D \bar{Q} + \bar{\bar{Z}}^N \right)^{-1} \bar{\psi}_{\text{inc}}. \quad (18)$$

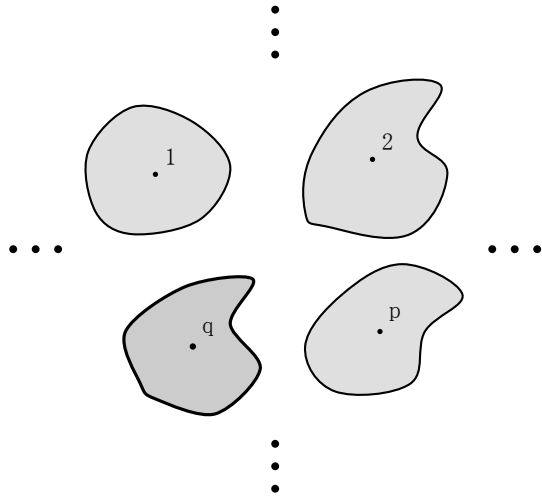


FIGURE 2. The illustration of N scatterers where the shown scatterers are indexed as 1, 2, q , p .

Next, we consider multiple scattering by N discrete scatterers with boundaries S_p , $p = 1, \dots, N$ (Fig. 2); the shape of each scatterer can be different. Isolating scatterer q ,

$$\begin{aligned} \psi_{\text{inc}}(\bar{\rho}) + \int_{S_q} d\ell' [\psi(\bar{\rho}') \hat{n}' \cdot \nabla' g(\bar{\rho}, \bar{\rho}') \\ - g(\bar{\rho}, \bar{\rho}') \hat{n}' \cdot \nabla' \psi(\bar{\rho}')] \\ + \sum_{p \neq q} \int_{S_p} d\ell' [\psi(\bar{\rho}') \hat{n}' \cdot \nabla' g(\bar{\rho}, \bar{\rho}') \\ - g(\bar{\rho}, \bar{\rho}') \hat{n}' \cdot \nabla' \psi(\bar{\rho}')] = \psi(\bar{\rho}) \end{aligned} \quad (19)$$

if $\bar{\rho}$ is outside the scatterers. We use point matching on S_q .

Using the matrix elements $Z_{m_q n_p}^{D(qp)}$ and $Z_{m_q n_p}^{N(qp)}$,

$$\begin{aligned} \bar{Z}^{N(qq)} \bar{\psi}(q) + \bar{Z}^{D(qq)} \bar{J}(q) \\ + \sum_{p \neq q} \left(\bar{Z}^{N(qp)} \bar{\psi}(p) + \bar{Z}^{D(qp)} \bar{J}(p) \right) = \bar{\psi}^{\text{inc}}(q). \end{aligned} \quad (20)$$

For each scatterer, the interior problem gives $\bar{J}(p) = \bar{Q}^{(p)} \bar{\psi}(p)$ with $\bar{Q}^{(p)} = -\frac{1}{\rho_p} (\bar{Z}^{D, \text{int}, (p)})^{-1} \bar{Z}^{N, \text{int}, (p)}$. Then

$$\begin{aligned} \left(\bar{Z}^{N(qq)} + \bar{Z}^{D(qq)} \bar{Q}^{(q)} \right) \bar{\psi}(q) \\ + \sum_{p \neq q} \left(\bar{Z}^{N(qp)} + \bar{Z}^{D(qp)} \bar{Q}^{(p)} \right) \bar{\psi}(p) = \bar{\psi}^{\text{inc}}(q). \end{aligned} \quad (21)$$

Let the exciting field $\bar{\psi}^{\text{ex}}(q)$ of scatterer q be

$$\bar{\psi}^{\text{ex}}(q) = \bar{\psi}^{\text{inc}}(q) - \sum_{p \neq q} \left(\bar{Z}^{N(qp)} + \bar{Z}^{D(qp)} \bar{Q}^{(p)} \right) \bar{\psi}(p). \quad (22)$$

Physically, the exciting field is the sum of the incident wave and scattered fields from all other scatterers $p \neq q$. Then

$$\bar{\psi}(q) = \left(\bar{Z}^{N(qq)} + \bar{Z}^{D(qq)} \bar{Q}^{(q)} \right)^{-1} \bar{\psi}^{\text{ex}}(q). \quad (23)$$

Substituting,

$$\bar{\psi}^{\text{ex}}(q) = \bar{\psi}^{\text{inc}}(q) + \sum_{p \neq q} \bar{C}^{E(qp)} \bar{\psi}^{\text{ex}}(p), \quad (24)$$

is the Foldy-Lax equation formulated by the MoM. The near-field T -matrix of scatterer p is expressed as

$$\begin{aligned} \bar{C}^{E(qp)} = - \left(\bar{Z}^{N(qp)} + \bar{Z}^{D(qp)} \bar{Q}^{(p)} \right) \\ \times \left(\bar{Z}^{N(pp)} + \bar{Z}^{D(pp)} \bar{Q}^{(p)} \right)^{-1}. \end{aligned} \quad (25)$$

This is the single-scatterer T -matrix because it depends only on the p th scatterer through $(\bar{Z}^{N(pp)} + \bar{Z}^{D(pp)} \bar{Q}^{(p)})^{-1}$. In scattering to q , $\bar{C}^{E(qp)}$ depends only on the position of q relative to p ; it does not depend on the scattering properties of scatterer q . In a more general framework, we note that

- (i) S does not have to be on the surface of the scatterer. This can be a convenient surface that encloses the scatterer. The surface S can tightly enclose the scatterer.
- (ii) The interior problem can be solved using CEM commercial software which provides $\bar{J}$ as a function of $\bar{\psi}$ on the enclosing surface S .
- (iii) The interior fields are not involved in the MST equations.

The formulation also permits more general constitutive models inside each scatterer. The derivation above requires the exterior/background medium, and therefore the Green's function used for inter-cell propagation, to retain the isotropic form assumed here. Within each enclosing surface, however, anisotropic or frequency-dispersive material response can be incorporated through the interior operator $\bar{Q}$ (or an equivalent numerically extracted surface operator) obtained with a solver that supports the desired constitutive model. For dispersive materials, this operator is recomputed or interpolated as a function of frequency, while the exterior ML-MST assembly is unchanged. An anisotropic background medium would instead require the corresponding anisotropic Green's function and translation/lattice operators.

3. MULTIPLE SCATTERING THEORY WITH VECTOR CYLINDRICAL WAVES

We describe the Foldy-Lax multiple scattering equations using VCW as a basis [6]. For a scatterer centered at $\bar{\rho}_p$, outgoing and regular VCW are defined by

$$\psi_n(\bar{\rho} - \bar{\rho}_p) = H_n^{(1)}(k|\bar{\rho} - \bar{\rho}_p|) e^{in\phi_{\bar{\rho}\bar{\rho}_p}}, \quad (26)$$

$$\text{Rg}\psi_n(\bar{\rho} - \bar{\rho}_p) = J_n(k|\bar{\rho} - \bar{\rho}_p|) e^{in\phi_{\bar{\rho}\bar{\rho}_p}}, \quad (27)$$

where $\phi_{\bar{\rho}\bar{\rho}_p}$ is the polar angle of $\bar{\rho} - \bar{\rho}_p$ with respect to the global x axis. For an isolated scatterer centered at $\bar{\rho}_p$ with a minimum enclosing circle of radius R_p ,

$$\psi^{E(p)}(\bar{\rho}) = \sum_n w_n^{(p)} \text{Rg}\psi_n(k(\bar{\rho} - \bar{\rho}_p)), \quad (28)$$

while the scattered field is expanded in outgoing waves valid for $|\bar{\rho} - \bar{\rho}_p| > R_p$,

$$\psi^{s(p)}(\bar{\rho}) = \sum_n a_n^{s(p)} \psi_n(k(\bar{\rho} - \bar{\rho}_p)). \quad (29)$$

The single-scatterer T -matrix is $a_n^{s(p)} = \sum_{n'} T_{nn'}^{(p)} w_{n'}^{(p)}$. The exciting field of scatterer q is the sum of the incident wave and the scattered waves from all other scatterers:

$$\psi^{E(q)}(\bar{\rho}) = \psi_{\text{inc}}(\bar{\rho}) + \sum_{p \neq q} \psi^{s(p)}(\bar{\rho}). \quad (30)$$

Let the incident wave be a plane wave in the $\bar{k}_i$ direction, $e^{i\bar{k}_i \cdot \bar{\rho}} = \sum_n \psi_n^{\text{inc}} \text{Rg} \psi_n(k\bar{\rho})$. For $\hat{k}_i = \cos \phi_i \hat{x} + \sin \phi_i \hat{y}$, $\psi_n^{\text{inc}} = i^n e^{-in\phi_i}$. Then

$$\begin{aligned} & \sum_n w_n^{(q)} \text{Rg} \psi_n(k(\bar{\rho} - \bar{\rho}_q)) \\ &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \sum_n \psi_n^{\text{inc}} \text{Rg} \psi_n(k(\bar{\rho} - \bar{\rho}_q)) \\ &+ \sum_{p \neq q} \sum_m a_m^{s(p)} \psi_m(k(\bar{\rho} - \bar{\rho}_p)) \\ &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \sum_n \psi_n^{\text{inc}} \text{Rg} \psi_n(k(\bar{\rho} - \bar{\rho}_q)) \\ &+ \sum_{p \neq q} \sum_m \sum_{n'} T_{mn'}^{(p)} w_{n'}^{(p)} \psi_m(k(\bar{\rho} - \bar{\rho}_p)). \end{aligned} \quad (31)$$

We next make use of the addition theorem, for $|\bar{\rho} - \bar{\rho}_q| \leq |\bar{\rho}_p - \bar{\rho}_q|$,

$$\begin{aligned} & H_m^{(1)}(k|\bar{\rho} - \bar{\rho}_p|) e^{im\phi_{\bar{\rho}\bar{p}}} \\ &= \sum_{n=-\infty}^{\infty} J_n(k|\bar{\rho} - \bar{\rho}_q|) e^{in\phi_{\bar{\rho}\bar{p}q}} \\ &\times H_{n-m}^{(1)}(k|\bar{\rho}_p - \bar{\rho}_q|) e^{-i(n-m)\phi_{\bar{p}\bar{p}q}}. \end{aligned} \quad (32)$$

Substituting the addition theorem into the scattered-field terms gives

$$\begin{aligned} & \sum_n w_n^{(q)} \text{Rg} \psi_n(k(\bar{\rho} - \bar{\rho}_q)) \\ &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \sum_n \psi_n^{\text{inc}} \text{Rg} \psi_n(k(\bar{\rho} - \bar{\rho}_q)) \\ &+ \sum_{p \neq q} \sum_m \sum_{n'} \sum_n T_{mn'}^{(p)} w_{n'}^{(p)} J_n(k|\bar{\rho} - \bar{\rho}_q|) e^{in\phi_{\bar{\rho}\bar{p}q}} \\ &\times H_{n-m}^{(1)}(k|\bar{\rho}_p - \bar{\rho}_q|) e^{-i(n-m)\phi_{\bar{p}\bar{p}q}}. \end{aligned} \quad (33)$$

Balancing the coefficients gives

$$\begin{aligned} w_n^{(q)} &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \psi_n^{\text{inc}} \\ &+ \sum_{p \neq q} \sum_m \sum_{n'} H_{n-m}^{(1)}(k|\bar{\rho}_p - \bar{\rho}_q|) \\ &\times e^{-i(n-m)\phi_{\bar{p}\bar{p}q}} T_{mn'}^{(p)} w_{n'}^{(p)}. \end{aligned} \quad (34)$$

Let $[\bar{\sigma}^{(qp)}]_{nm} = H_{n-m}^{(1)}(k|\bar{\rho}_p - \bar{\rho}_q|) e^{-i(n-m)\phi_{\bar{p}\bar{p}q}}$. Then, in matrix form,

$$\bar{w}^{(q)} = e^{i\bar{k}_i \cdot \bar{\rho}_q} \bar{\psi}^{\text{inc}} + \sum_{p \neq q} \bar{\sigma}^{(qp)} \bar{T}^{(p)} \bar{w}^{(p)}, \quad (35)$$

for $q = 1, \dots, N$. This is the MST equation in VCW with the translational addition theorem.

4. MULTILEVEL MULTIPLE SCATTERING THEORY

Let q_N be the set of nearest neighbors of q . We separate the scattered waves into $p \in q_N$ and $p \notin q_N$. For the MST-VCW,

$$\begin{aligned} \bar{w}^{(q)} &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \bar{\psi}^{\text{inc}} + \sum_{p \in q_N} \bar{\sigma}^{(qp)} \bar{T}^{(p)} \bar{w}^{(p)} \\ &+ \sum_{p \notin q_N} \bar{\sigma}^{(qp)} \bar{T}^{(p)} \bar{w}^{(p)}. \end{aligned} \quad (36)$$

For the MST-MoM,

$$\begin{aligned} \bar{\psi}^{E(q)} &= \bar{\psi}^{\text{inc}(q)} + \sum_{p \in q_N} \bar{C}^{E(qp)} \bar{\psi}^{E(p)} \\ &+ \sum_{p \notin q_N} \bar{C}^{E(qp)} \bar{\psi}^{E(p)}. \end{aligned} \quad (37)$$

First, we note that the dimension of $\bar{w}$ is $2N_{\text{max}} + 1$. The dimension of $\bar{\psi}^E$ is N_ψ , which is the number of MoM points on the tightest enclosing surface of the scatterer. The two should be consistent; therefore, N_{max} must be such that the VCW exciting field can reproduce the variation of $\bar{\psi}^{\text{ex}}$. Generally, $2N_{\text{max}} + 1 \leq N_\psi$. Let $\bar{T}_{\psi^{(q)}w^{(q)}}$ be the transformation from $\bar{w}^{(q)}$ to $\bar{\psi}^{E(q)}$,

$$\bar{\psi}^{E(q)} = \bar{T}_{\psi^{(q)}w^{(q)}} \bar{w}^{(q)}, \quad (38)$$

of dimension $N_\psi \times (2N_{\text{max}} + 1)$. The matrix $\bar{T}_{\psi^{(q)}w^{(q)}}$ is constructed column by column; its n th column is the surface field $\bar{\psi}^{E(q)}$ at the N_ψ points on S_q produced by the n th regular VCW basis function. For a scatterer with boundary S_q centered at the origin, the VCW basis function of $\bar{w}^{(q)}$ is $J_{m-N_{\text{max}}-1}(k\rho) \exp(i(m-N_{\text{max}}-1)\phi)$, $m = 1, \dots, 2N_{\text{max}}+1$. Decomposing S_q into intervals σ_n with center (ρ_n, ϕ_n) ,

$$\begin{aligned} \left(\bar{T}_{\psi^{(q)}w^{(q)}} \right)_{nm} &= J_{m-N_{\text{max}}-1}(k\rho_n) e^{i(m-N_{\text{max}}-1)\phi_n}, \\ n &= 1, \dots, N_\psi, \quad m = 1, \dots, 2N_{\text{max}} + 1. \end{aligned} \quad (39)$$

The inverse transformation $\bar{T}_{w(q)\psi(q)}$ is

$$\bar{w}^{(q)} = \bar{T}_{w(q)\psi(q)} \bar{\psi}^{E(q)}, \quad (40)$$

where we use the Moore–Penrose pseudo-inverse of $\bar{T}_{\psi(q)w(q)}$. The two-level MST is obtained by replacing the $p \notin q_N$ term of MST-MoM with that of MST-VCW, transforming to VCW, and back to MoM:

$$\begin{aligned} \bar{\psi}^{E(q)} &= \bar{\psi}^{\text{inc}(q)} + \sum_{p \in q_N} \bar{C}^{E(qp)} \bar{\psi}^{E(p)} \\ &+ \bar{T}_{\psi(q)w(q)} \sum_{p \notin q_N} \bar{\sigma}^{(qp)} \bar{T}^{(p)} \bar{T}_{w(p)\psi(p)} \bar{\psi}^{E(p)}. \end{aligned} \quad (41)$$

Because $\bar{w}$ must be compatible with $\bar{\psi}^{\text{ex}}$, we use the $p \in q_N$ MST-MoM term to replace the $p \in q_N$ term of MST-VCW. Similar transformations give

$$\begin{aligned} \bar{w}^{(q)} &= e^{i\bar{k}_i \cdot \bar{\rho}_q} \bar{\psi}^{\text{inc}} \\ &+ \bar{T}_{w(q)\psi(q)} \sum_{p \in q_N} \bar{C}^{E(qp)} \bar{T}_{\psi(p)w(p)} \bar{w}^{(p)} \\ &+ \sum_{p \notin q_N} \bar{\sigma}^{(qp)} \bar{T}^{(p)} \bar{w}^{(p)}. \end{aligned} \quad (42)$$

In the two-level scheme, multipole truncation plays two distinct roles, and a different order is assigned to each. The near level, which carries the rapidly varying near fields of overlapping cells through $\bar{C}^{E(qp)}$ and the basis transformations $\bar{T}_{\psi w}$ and $\bar{T}_{w\psi}$, is retained to a high order N_{max} so that the regular VCW expansion can reproduce the strong field variation on the enclosing surface of close scatterers. The single-scatterer T -matrix $\bar{T}$ is truncated at a lower order $N_{\text{max},s} \leq N_{\text{max}}$. For scatterers that are small compared with the wavelength, the high-order regular-wave amplitudes $J_n(kR)$ become very small; therefore, the high-order rows and columns of $\bar{T}$ are formed from the inversion of nearly singular blocks and are dominated by numerical noise. Retaining $\bar{T}$ at the lower order $N_{\text{max},s}$ keeps it numerically stable. The two orders are combined by computing $\bar{T}$ at $N_{\text{max},s}$ and applying it within the order- N_{max} space; the bookkeeping is provided in Appendix B. In practice, both orders are increased until the band solution converges.

5. APPLICATION TO BAND THEORY AND THE MULTILEVEL KKR EQUATION

For band theory, let $\bar{R}_{\alpha\beta} = \alpha\bar{a}_1 + \beta\bar{a}_2$, where $\bar{a}_1, \bar{a}_2$ are the lattice vectors, and use the combined index $(\alpha, \beta) \rightarrow p$. There is no incident wave; let $q = (0, 0)$ and $\bar{w}^{(q)} = \bar{w}$. For the Bloch vector $\bar{k}_i$, the Bloch condition is $\bar{w}^{(p)} = e^{i\bar{k}_i \cdot \bar{R}_p} \bar{w}$. All scatterers are identical, $\bar{T}^{(p)} = \bar{T}$, $\bar{T}_{\psi(p)w(p)} = \bar{T}_{\psi w}$, and $\bar{T}_{w(p)\psi(p)} = \bar{T}_{w\psi}$. The ML-MST equation becomes

$$\begin{aligned} \bar{w} &= \bar{T}_{w\psi} \sum_{p \in 0_N} \bar{C}^{E(0p)} e^{i\bar{k}_i \cdot \bar{R}_p} \bar{T}_{\psi w} \bar{w} \\ &+ \sum_{p \notin 0_N} \bar{\sigma}^{(0p)} e^{i\bar{k}_i \cdot \bar{R}_p} \bar{T} \bar{w}. \end{aligned} \quad (43)$$

We next sum the $p \notin 0_N$ terms using the broadband Green's function (BBGF):

$$\left[\sum_{p \notin 0_N} \bar{\sigma}^{(0p)} e^{i\bar{k}_i \cdot \bar{R}_p} \bar{T} \bar{w} \right]_n = \sum_m D_{n-m}^M(k, \bar{k}_i) (\bar{T} \bar{w})_m, \quad (44)$$

where the D coefficients, with the nearest neighbors subtracted, are

$$D_{n-m}^M(k, \bar{k}_i) = \sum_{p \notin 0_N} H_{n-m}^{(1)}(k|\bar{R}_p|) e^{-i(n-m)\phi_{\bar{R}_p}} e^{i\bar{k}_i \cdot \bar{R}_p}. \quad (45)$$

In matrix notation, $\sum_{p \notin 0_N} \bar{\sigma}^{(0p)} e^{i\bar{k}_i \cdot \bar{R}_p} \bar{T} \bar{w} = \bar{D}^M \bar{T} \bar{w}$.

We apply the BBGF to compute the $p \notin 0_N$ sum. The lattice Green's function is

$$\begin{aligned} g_p(k, \bar{\rho}, \bar{k}_i) &= \sum_p \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \\ &= \frac{i}{4} H_0^{(1)}(k\rho) + \sum_{p \in 0_N} \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \\ &+ \sum_{p \notin 0_N} \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p}. \end{aligned} \quad (46)$$

Using the addition theorem for $\rho \leq |\bar{R}_p|$,

$$H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) = \sum_{n=-\infty}^{\infty} J_n(k\rho) e^{in\phi} H_n^{(1)}(k|\bar{R}_p|) e^{-in\phi_{\bar{R}_p}}, \quad (47)$$

we obtain

$$\begin{aligned} &\sum_{p \notin 0_N} \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \\ &= \frac{i}{4} \sum_{\ell} J_{\ell}(k\rho) e^{i\ell\phi} D_{\ell}^M(k, \bar{k}_i) \\ &= g_p(k, \bar{\rho}, \bar{k}_i) - \frac{i}{4} H_0^{(1)}(k\rho) \\ &- \sum_{p \in 0_N} \frac{i}{4} H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p}. \end{aligned} \quad (48)$$

Let $\rho = R$. Integrating with $\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi}$,

$$\begin{aligned} D_{\ell}^M(k, \bar{k}_i) &= \frac{4}{iJ_{\ell}(kR)} \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} g_p(k, \bar{\rho}, \bar{k}_i) \right. \\ &- \frac{i}{4} \delta_{\ell 0} H_0^{(1)}(kR) \\ &- \sum_{p \in 0_N} \frac{i}{4} \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} \\ &\times H_0^{(1)}(k|\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \left. \right], \end{aligned} \quad (49)$$

where $\bar{\rho} = R \cos \phi \hat{x} + R \sin \phi \hat{y}$ and the contour radius $R_c \equiv R$ is chosen smaller than the smallest center-to-center distance to a non-neighbor cell. A detailed expansion of D_ℓ^M is provided in Appendix A. The multilevel KKR equation based on the multilevel MST is expressed as

$$\bar{w} = \sum_{p \in 0_N} \bar{T}_{w\psi} \bar{C}^{(0p)} \bar{T}_{\psi w} e^{i\bar{k}_i \cdot \bar{R}_p} \bar{w} + \bar{D}^M \bar{T} \bar{w}. \quad (50)$$

The eigenvalue problem becomes

$$\bar{\Lambda} \bar{w} = 0, \quad (51)$$

where

$$\bar{\Lambda} = \bar{I} - \bar{D}^M \bar{T} - \sum_{p \in 0_N} \bar{T}_{w\psi} \bar{C}^{E(0p)} \bar{T}_{\psi w} e^{i\bar{k}_i \cdot \bar{R}_p}. \quad (52)$$

Equation (51) is the central result of this formulation and exhibits a multilevel structure. The second term in $\bar{\Lambda}$ accounts for all non-neighbor cell interactions through the truncated BBGF lattice sum $\bar{D}^M$, which excludes near neighbors. They are handled by the third term, which represents the explicitly computed near-field T -matrix interactions mapped into the VCW basis.

The near-neighbor block $\bar{T}_{w\psi} \bar{C}^{E(0p)} \bar{T}_{\psi w}$ also has a useful connection to the hopping description used in tight-binding (TB) models. In a TB model, nearest-neighbor coupling is represented by one or a few hopping parameters after the field is projected onto a selected set of localized cell modes. In the present full-wave formulation, no phenomenological hopping parameter is introduced; instead, the near-neighbor block maps the complete retained vector of VCW amplitudes of one cell into the exciting-field amplitudes of another. It is therefore a matrix-valued, frequency-dependent full-wave representation of nearest-neighbor coupling. If this operator were further projected onto a reduced localized-mode basis, its matrix elements would play a role analogous to TB hopping amplitudes; in a single-mode-per-cell reduction, the corresponding coupling could reduce to a scalar hopping coefficient.

The single-scatterer T -matrix $\bar{T}$ that multiplies $\bar{D}^M$ in the non-neighbor term is evaluated at the reduced order $N_{\max,s}$, while the near-neighbor term $\bar{T}_{w\psi} \bar{C}^{(0p)} \bar{T}_{\psi w}$ is retained at the higher order $N_{\max}$, so the dimension of $\bar{\Lambda}$ is set by $N_{\max}$. The order bookkeeping is detailed in Appendix B.

6. NUMERICAL RESULTS AND DISCUSSION

In the numerical results, the multilevel KKR-MST formulation was applied to the band calculation of a two-dimensional hexagonal periodic structure consisting of equilateral triangular dielectric scatterers. The geometry is illustrated in Fig. 3. Each scatterer had a relative permittivity $\epsilon_r = 20$, and the background medium had a relative permittivity $\epsilon_{rb} = 2.5$. The triangle side length was fixed at $L = 9$ mm, and the center-to-center distance between neighboring cells, R , was varied to scan from the well-separated regime to the regime, in which the minimum enclosing circles of neighboring cells overlapped. Four values were considered: $R = 10.5, 9, 8.5$, and 8 mm.

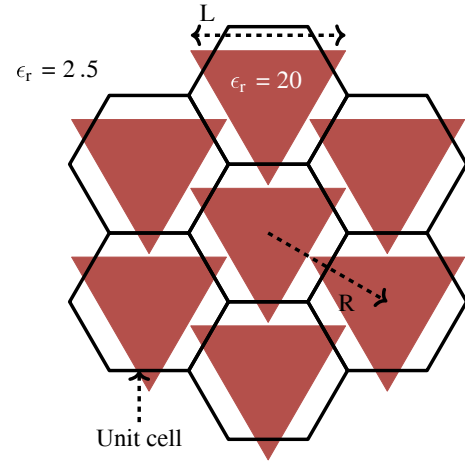


FIGURE 3. Layout of the 2D hexagonal grid of triangular dielectric scatterers. L is the triangle side length, and R is the center-to-center distance between neighboring cells.

The minimum enclosing circle of an equilateral triangle with side L has radius $L/\sqrt{3}$, which gives an enclosing radius of approximately 5.196 mm. The enclosing circles of two neighboring cells just touch when $R \approx 10.39$ mm. Thus, $R = 10.5$ mm lies in the well-separated regime, in which the standard KKR equation with only T -matrices is valid, and the near-neighbor set in (52) becomes empty. The remaining three cases, $R = 9, 8.5$, and 8 mm, all have overlapping enclosing circles among the six nearest neighbors, and the multilevel formulation in Section 4 is required. For these cases, the near-neighbor set is taken to consist of six nearest neighbors, and the corresponding pair near-field T -matrices $\bar{C}^{E(qp)}$ are computed once per frequency sample.

Both polarizations are considered. For TM_z , the nonzero electric-field component is E_z and the boundary-condition factor in (16) is $\rho = \mu_p/\mu_1 = 1$. For TE_z , the nonzero magnetic-field component is H_z and $\rho = \epsilon_p/\epsilon_1 = 8$. The single-scatterer T -matrix and the pair near-field T -matrices were computed independently for the two polarizations.

The hexagonal Bravais lattice is generated by the primitive vectors $\bar{a}_1 = R\hat{y}$ and $\bar{a}_2 = R(\sqrt{3}\hat{x}/2 - \hat{y}/2)$, with reciprocal vectors $\bar{b}_1 = (2\pi/R)(\hat{x}/\sqrt{3} + \hat{y})$ and $\bar{b}_2 = (2\pi/R)(2\hat{x}/\sqrt{3})$. The band diagram was computed along the standard high-symmetry path $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$ in the first Brillouin zone, with $\Gamma = (0, 0)$, $K = (\bar{b}_1 + \bar{b}_2)/3$, and $M = \bar{b}_1/2$.

6.1. Numerical Parameters

The boundary S_p of each scatterer is discretized with $N = 60$

pulse-basis patches in the MoM evaluation of $\bar{\bar{Z}}^N$, $\bar{\bar{Z}}^D$, $\bar{\bar{Z}}^{N,\text{int}}$, and $\bar{\bar{Z}}^{D,\text{int}}$. The same boundary discretization is used to construct the basis-transformation matrices $\bar{T}_{\psi w}$ and $\bar{T}_{w\psi}$ in (38). For a fair comparison, the COMSOL mesh inside the scatterer uses an average triangle edge length equal to the patch length adopted in this study.

For the COMSOL validation, a custom finite-element mesh was used with a maximum element size of $L/5 = 1.8$ mm and a minimum element size of $L/15 = 0.6$ mm, the latter applied

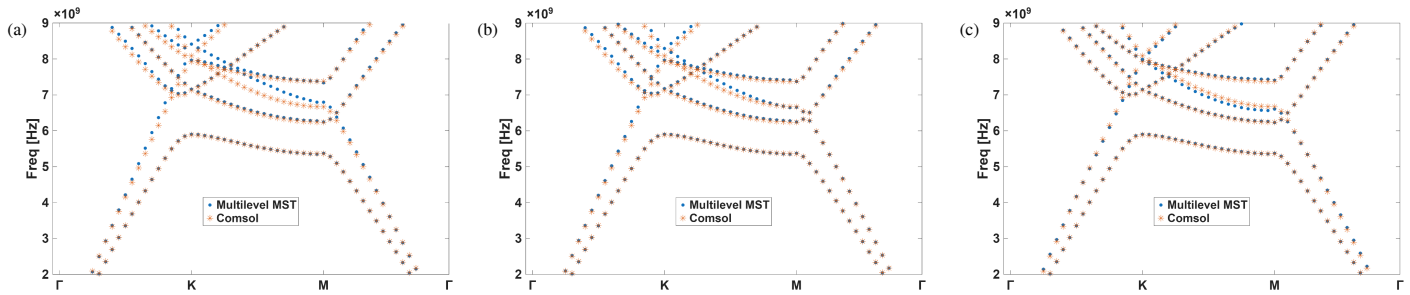


FIGURE 4. Truncation-order convergence for the strongly overlapping case $R = 8$ mm. The adopted pair $(N_{\max}, N_{\max,s}) = (5, 4)$ gives the best agreement with COMSOL without extra or missing bands. (a) $N_{\max} = 4$, $N_{\max,s} = 3$. (b) $N_{\max} = 5$, $N_{\max,s} = 3$. (c) $N_{\max} = 5$, $N_{\max,s} = 4$.

especially inside the dielectric triangle. At 9 GHz, these sizes correspond to approximately $\lambda_b/11.5$ in the background and $\lambda_{\text{int}}/12.5$ inside the scatterer, respectively. For the $R = 8$ mm case, the mesh contained 986 domain elements and 141 boundary elements, resulting in 7035 degrees of freedom. Robust analysis setting and quadratic field representation were used. Eigenfrequencies were computed with the ARPACK solver using a search centered at 5 GHz.

The VCW cylindrical-wave truncation index $N_{\max}$ is selected on a case-by-case basis. When the scatterers are not close, a smaller $N_{\max}$ value is sufficient. As the scatterers move closer together, close-neighbor near-field interactions become stronger, and the MoM exciting fields exhibit more spatial variation; consequently, a larger $N_{\max}$ is required to represent the fields consistently on the enclosing surface. For the $R = 10.5$ mm case, $N_{\max} = 4$ is sufficient, because the cells are well separated and no near-field T -matrix is needed. For the overlapping cases, the multipole truncation takes two distinct values, as introduced in Section 4. The near level, comprising the pair near-field T -matrices and the basis transformations $\bar{T}_{\psi w}$ and $\bar{T}_{w\psi}$, is retained at the higher order $N_{\max} = 5$ to capture the strong close-neighbor interactions. The single-scatterer T -matrix is truncated at the lower, numerically stable order $N_{\max,s} = 4$. The eigenproblem dimension is set by $N_{\max} = 5$.

The single-scatterer size is $L = 9$ mm, and the frequency range extends to 9 GHz. The scatterer is not large compared with the wavelength. Thus, the single-scatterer T -matrix and the near-field T -matrix are smooth functions of frequency. They are evaluated at 20 frequency samples and interpolated during the band search.

For the BBGF evaluation of the lattice sum coefficients $\tilde{D}_l$ via (A3), the spatial-truncation parameter is $N_{\text{spa}} = 13$, and the spectral-truncation parameter is $N_{\text{spe}} = 2$. The contour radius R_c in (A3) is chosen smaller than the smallest center-to-center distance to a non-neighbor cell. BBGF lattice sum is evaluated directly at every $(k, \bar{k}_i)$ pair because the BBGF setup makes this evaluation algebraically inexpensive.

The number of Bloch vectors sampled along the path was $N_\beta = 150$ for the reference case $R = 10.5$ mm and $N_\beta = 60$ for the overlapping cases $R = 9, 8.5$, and 8 mm. For each Bloch vector along the path, the band eigenfrequencies are extracted as local minima of the smallest singular value of $\bar{\Lambda}(k, \bar{k}_i)$ as a function of k , retaining minima below a tolerance of 0.1.

A truncation-order convergence test was also performed for the most strongly overlapping case, $R = 8$ mm. Three combinations of the near-level order $N_{\max}$ and the single-scatterer order $N_{\max,s}$ were compared with COMSOL, as shown in Fig. 4. With $(N_{\max}, N_{\max,s}) = (5, 4)$, which is used for the reported overlapping cases, the maximum frequency difference from the corresponding COMSOL bands was approximately 120 MHz, with no extra or missing bands. Reducing $N_{\max,s}$ to 3 while retaining $N_{\max} = 5$ increased the maximum difference to approximately 210 MHz and produced additional duplicate bands. Reducing both orders to $(4, 3)$ produced substantial deviations in several branches. We therefore adopt $(N_{\max}, N_{\max,s}) = (5, 4)$ as an adequate truncation for the overlapping cases considered here.

6.2. Reference Case: $R = 10.5$ mm

For $R = 10.5$ mm, the enclosing circles of the neighboring cells do not overlap, and the standard KKR equation applies without near-field T -matrices. The near-neighbor sum in (52) is empty, and the multilevel formulation reduces to the conventional BBGF-KKR-MST. This case serves as a verification of both the BBGF lattice-sum implementation and the VCW T -matrix construction in a regime where the standard method is known to be accurate.

Figure 5 presents the band diagram along the $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$ path, obtained using the proposed method, compared with the COMSOL solution using the same triangle discretization. Both polarizations were overlaid on the same plot. Excellent agreement was observed across the entire path. Fig. 6 presents the same band diagram with the TM_z and TE_z modes plotted separately. A band gap was observed in the TM mode between the first and second bands, located between approximately 5 GHz and 6.3 GHz at the K and M points, respectively. The TE mode does not exhibit a gap in this frequency range, and its bands fill the spectral region of the TM gap; therefore, the gap is polarization-selective rather than complete.

6.3. Overlapping Enclosing-Circle Cases: $R = 9, 8.5, 8$ mm

For $R = 9, 8.5$, and 8 mm, the enclosing circles of the six nearest-neighbor cells overlap with that of the reference cell, and the convergence condition of the translation addition theorem (32) fails for those neighbors. Therefore, the standard KKR equation is inapplicable, and the multilevel formulation (50) is

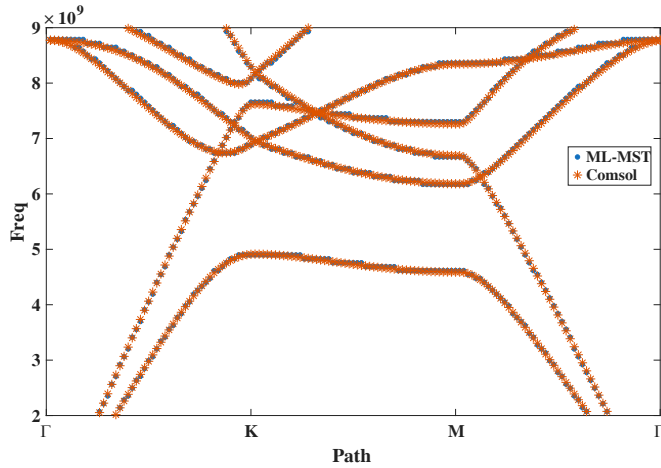


FIGURE 5. Band diagram for $R = 10.5$ mm along $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$. Overlay of the multilevel KKR-MST method (markers) and COMSOL (asterisks) with both TM_z and TE_z polarizations.

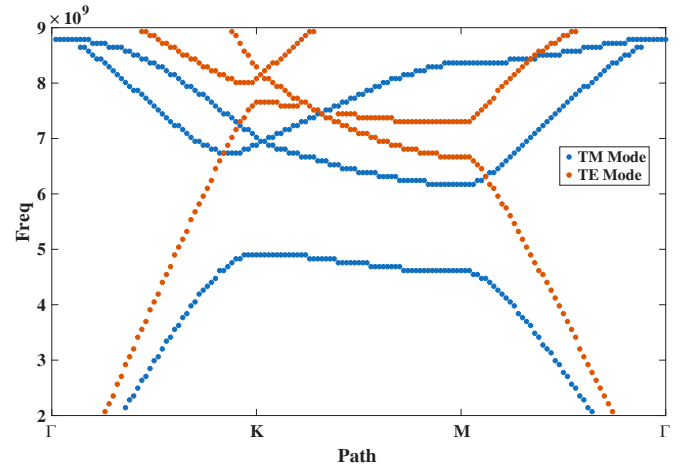


FIGURE 6. Band diagram for $R = 10.5$ mm with the TM_z and TE_z modes plotted separately. A band gap is visible in the TM mode between the first and second bands.

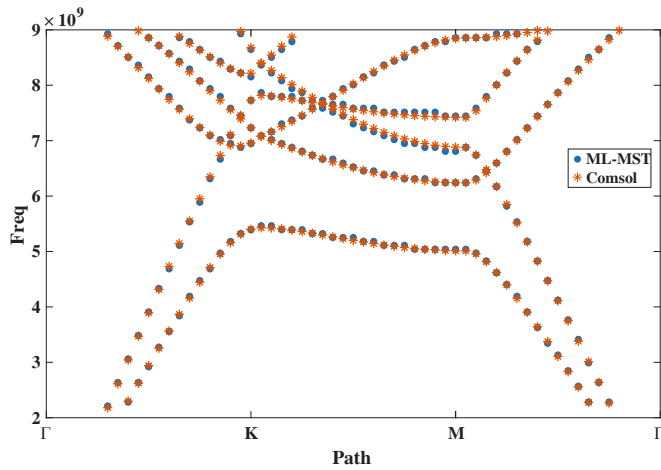


FIGURE 7. Band diagram for $R = 9$ mm along $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$. Overlay of the multilevel KKR-MST method (markers) and COMSOL (asterisks) with both TM_z and TE_z polarizations.

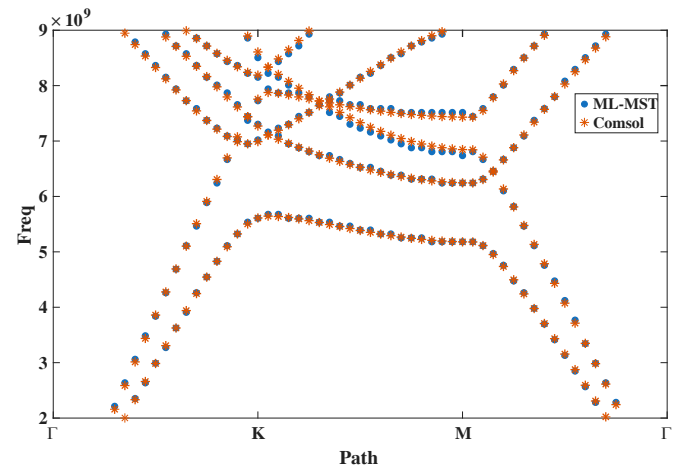


FIGURE 8. Band diagram for $R = 8.5$ mm along $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$. Overlay of the multilevel KKR-MST method (markers) and COMSOL (asterisks) with both TM_z and TE_z polarizations.

used. The six nearest-neighbor interactions are handled by the explicitly computed pair near-field T -matrices $\bar{C}^{E(qp)}$ derived in (52), whereas all other lattice cells continue to be handled by the truncated BBGF sum $\bar{D}^M$.

Figs. 7, 8, and 9 show computed band diagrams for $R = 9$, 8.5, and 8 mm, each compared with the corresponding COMSOL solution with both polarizations overlaid. Fig. 10 presents the band diagram for $R = 8$ mm with the TM_z and TE_z modes plotted separately. The agreement with COMSOL remains excellent across the path for all three values of R , confirming that the multilevel splitting between near-field T -matrices and the truncated BBGF sum reproduces the band structure correctly, even in the regime where the conventional KKR method breaks down.

To directly assess the effect of the near-neighbor treatment, Fig. 11 compares the $R = 8$ mm ML-MST result with conventional MST calculations using $N_{\max} = 5$ and $N_{\max} = 4$, in both cases without the pair near-field coupling matrices, as well as

with COMSOL. The conventional MST solutions follow COMSOL along some portions of the bands but depart from the reference along several branches and can follow different band paths. These deviations occur in the regime where the close-neighbor interaction is strongest, and the translation-addition representation is outside its convergence region. In contrast, the ML-MST solution remains in agreement with COMSOL because the six overlapping-neighbor interactions are supplied by the MoM near-field coupling matrices.

The TM mode retains a band gap between the first and second bands across all three overlapping cases, similar to that in the reference case. As R decreases, the gap shrinks. The TE mode did not exhibit a gap in this range for any of the three cases.

6.4. Computational Efficiency

Table 1 summarizes CPU times for the three overlapping cases, along with the corresponding COMSOL run times on the same

TABLE 1. CPU time comparison between the multilevel KKR-MST method and COMSOL for one full band diagram along $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$, for the overlapping (neighbor) cases. T-mat: assembly of the single-scatterer VCW T -matrix and the six pair near-field T -matrices, including frequency interpolation. KKR: assembly and eigen-extraction of $\bar{\bar{A}}$ at all sampled $(k, \bar{k}_i)$.

R (mm)	Regime	T-mat (s)	KKR (s)	Total (s)	COMSOL (s)
9.0	Multilevel KKR-MST	0.19	0.08	0.27	87
8.5	Multilevel KKR-MST	0.19	0.08	0.27	84
8.0	Multilevel KKR-MST	0.19	0.08	0.27	83

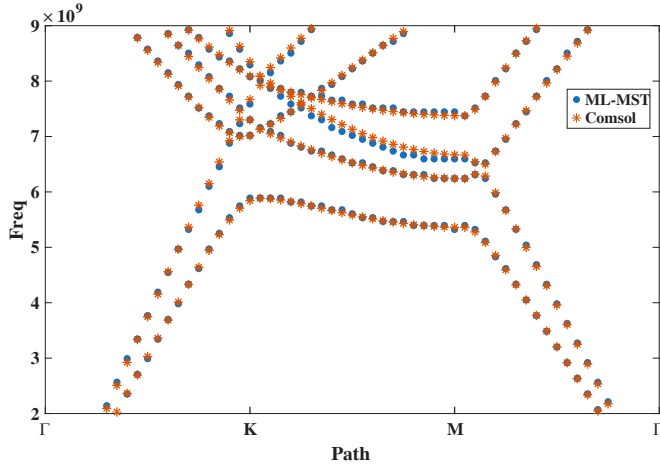


FIGURE 9. Band diagram for $R = 8$ mm along $\Gamma \rightarrow K \rightarrow M \rightarrow \Gamma$. Overlay of the multilevel KKR-MST method (markers) and COMSOL (asterisk), with both TM_z and TE_z polarizations.

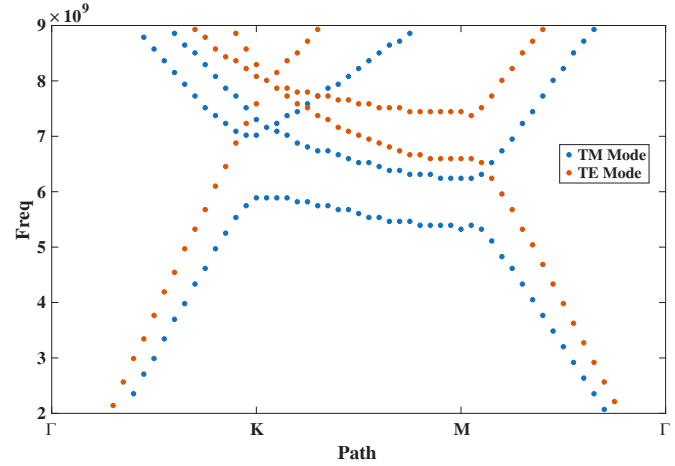


FIGURE 10. Band diagram for $R = 8$ mm with the TM_z and TE_z modes plotted separately.

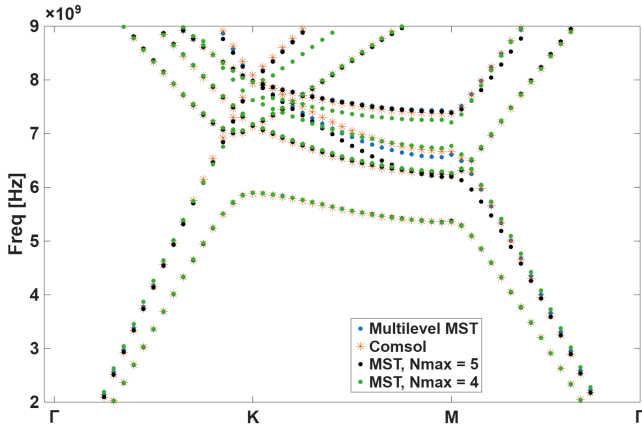


FIGURE 11. Direct comparison for $R = 8$ mm among the adopted ML-MST solution, COMSOL, and conventional MST using $N_{\max} = 5$ and $N_{\max} = 4$ without pair near-field coupling matrices.

machine. All calculations were performed on a single PC, and the reported values were the average of 10 independent executions. The multilevel KKR-MST run time decomposes into two parts: the construction of the single-scatterer VCW T -matrix and the six pair near-field T -matrices, which together require approximately 0.19 s per band diagram, and the assembly and eigen-extraction of $\bar{\bar{A}}$ at the 100 sampled frequencies along the path, which requires approximately 0.08 s. The total CPU time per band diagram was approximately 0.27 s. The COMSOL solution, which used a mesh resolution to be comparable to the MoM boundary discretization, required approximately 83 s

on the same hardware. Thus, the proposed method is approximately two orders of magnitude ($300\times$) faster than COMSOL for this problem.

The method efficiency is rooted in the same three properties identified in Section 4. First, the single-scatterer VCW T -matrix is independent of $\bar{k}_i$ and smooth in k , so it is tabulated at a small number of frequencies and interpolated. Second, the pair near-field T -matrices are also independent of $\bar{k}_i$ and smooth in k , and the same interpolation strategy applies; this is what makes the overlapping-circle cases nearly as inexpensive as the well-separated case. Third, the BBGF lattice sum is broadband by construction: after a one-time setup, $\bar{D}_l(k, \bar{k}_i)$ is obtained algebraically from $F_l(\bar{k}_i, k)$, given in Appendix A; therefore, adding more frequencies incurs negligible cost. The eigen-extraction at each $(k, \bar{k}_i)$ acts on a small 11×11 matrix in the overlapping cases (and a 9×9 matrix in the reference case). Within this 11×11 system, the single-scatterer T -matrix enters at the reduced order $N_{\max, s} = 4$, as a 9×9 block, while the near-field contributions are carried at order $N_{\max} = 5$.

The dimension of $\bar{\bar{A}}$ is two orders of magnitude smaller than the matrices that arise in plane-wave or finite-element band calculations for the same problem, where typical matrix sizes are in the thousands. This dimensional reduction, made possible by the cylindrical-wave representation in the scatterer's extinction region, is the underlying reason for the speedup. The near-field T -matrix machinery extends this dimensional reduction to the dense-packing regime, where the standard cylindrical-wave method alone would fail.

7. CONCLUSIONS

Standard KKR formulations for periodic structures rely on the translation addition theorem, whose convergence fails when the minimum enclosing circles of neighboring cells overlap. This study resolves this by partitioning the lattice into two groups according to whether each cell's enclosing circle overlaps with that of the reference cell, with each group handled in its own representation of the exciting field. Non-overlapping cells remain in the VCW basis, where the lattice sum is evaluated using the broadband Green's function. Overlapping cells are treated using pairs of near-field T -matrices constructed from the surface integral equations of multiple scattering by the method of moments. Projecting these pair operators onto the VCW basis allows both contributions to be combined in a single eigenvalue equation, whose size is set by the VCW truncation alone. The two contributions are carried at different multipole orders: the overlapping (near) level is retained to a higher order to capture the strong close-neighbor interactions, while the non-overlapping level uses a reduced order that keeps the single-scatterer T -matrix numerically stable; thus, the truncation order decreases from the near level to the non-near level.

Numerical tests on a hexagonal lattice of equilateral dielectric triangles were performed at four center-to-center distances, spanning the well-separated case through the strongly overlapping case. The resulting band diagrams reproduce the COMSOL solutions at the high-symmetry points of the first Brillouin zone for both TM and TE polarizations. The runtime on the same hardware was shorter than that of COMSOL by approximately two orders of magnitude. Changes in scatterer shape, material anisotropy, or frequency dispersion require only recomputation of the corresponding interior and pair near-field operators (as functions of frequency for dispersive media); the exterior ML-MST machinery remains unchanged so long as the background Green's function retains the form assumed here.

In this paper, we developed a multi-level, multiple scattering theory. The ML-MST formulation allows neighboring scatterers to be close to each other and also covers cases in which the enclosing circles overlap. The MST-MoM equations were derived and synthesized with the MST-VCW equations so that MST-MoM near-field T -matrices are used for close-neighbor interactions. The ML-KKR results are in good agreement with COMSOL and are computationally much more efficient.

In this paper, we used two expansions for the exciting field: VCW and MoM. Transformations are derived between the exciting-field expansions of VCW and MoM. We also call the method the MMMST method (Multi-expansion, Multi-level, Multiple Scattering theory). We are currently extending the MMMST theory to the three-dimensional scattering of vector electromagnetic waves. The MMMST theory will also be adapted for microwave remote sensing and metasurfaces.

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APPENDIX A. $D_\ell^M(k, \bar{k}_i)$ WITH NEIGHBOR SUBTRACTION

We follow the definitions in [33]. Define

$$F_l(k, \bar{k}_i) = \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi g_P(k, \bar{k}_i, \bar{\rho}) e^{-i\ell\phi} \right]_{\rho=R}. \quad (\text{A1})$$

Because F_l is a coefficient, it is evaluated by fixing $\rho = R$, with $\bar{\rho} = R \cos \phi \hat{x} + R \sin \phi \hat{y}$, and integrating over ϕ . Then

$$D_l(k, \bar{k}_i) = \frac{1}{J_l(kR)} [F_l(k, \bar{k}_i) + \frac{1}{4} \delta_{l0} N_0(kR)], \quad (\text{A2})$$

$$\tilde{D}_l(k, \bar{k}_i) = \frac{4}{i} D_l(k, \bar{k}_i) - \delta_{l0}. \quad (\text{A3})$$

The explicit expressions for F_l to the sixth order in the BBGF are given in Eqs. (28)–(38) of [33].

In the main text,

$$\begin{aligned} D_\ell^M(k, \bar{k}_i) = \frac{4}{iJ_\ell(kR)} \left\{ \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} g_p(k_0, \bar{\rho}, \bar{k}_i) \right]_{\rho=R} \right. \\ \left. - \frac{i}{4} \delta_{l0} H_0^{(1)}(k_0 R) \right. \\ \left. - \sum_{p \in 0_N} \frac{i}{4} \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} \right. \right. \\ \left. \left. \times H_0^{(1)}(k_0 |\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \right]_{\rho=R} \right\}. \end{aligned} \quad (\text{A4})$$

Using (A1)–(A3),

$$\begin{aligned} D_\ell^M(k, \bar{k}_i) = \frac{4}{iJ_\ell(kR)} \left\{ D_l J_l(kR) - \frac{i}{4} \delta_{l0} J_0(kR) \right. \\ \left. - \sum_{p \in 0_N} \frac{i}{4} \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} \right. \right. \\ \left. \left. \times H_0^{(1)}(k_0 |\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \right]_{\rho=R} \right\}. \end{aligned} \quad (\text{A5})$$

For $|\bar{\rho}| = R \leq |\bar{R}_p|$,

$$H_0^{(1)}(k |\bar{\rho} - \bar{R}_p|) = \sum_n J_n(k\rho) e^{in\phi} H_n^{(1)}(k |\bar{R}_p|) e^{-in\phi_{\bar{R}_p}}. \quad (\text{A6})$$

Then

$$\begin{aligned} \left[\frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\ell\phi} H_0^{(1)}(k_0 |\bar{\rho} - \bar{R}_p|) e^{i\bar{k}_i \cdot \bar{R}_p} \right]_{\rho=R} \\ = J_\ell(kR) H_\ell^{(1)}(k |\bar{R}_p|) e^{-i\ell\phi_{\bar{R}_p}}. \end{aligned} \quad (\text{A7})$$

Substituting,

$$D_\ell^M(k, \bar{k}_i) = \tilde{D}_l - \sum_{p \in 0_N} e^{i\bar{k}_i \cdot \bar{R}_p} H_\ell^{(1)}(k|\bar{R}_p|) e^{-i\ell\phi_{\bar{R}_p}}. \quad (\text{A8})$$

For the hexagonal structure in this study, the six neighbors are $\bar{R}_p = \pm\bar{a}_1, \pm\bar{a}_2, \pm\bar{a}_3$, with $\bar{a}_3 = \bar{a}_1 + \bar{a}_2$. By the symmetry between opposite neighbors,

$$\begin{aligned} & \sum_{p \in 0_N} e^{i\bar{k}_i \cdot \bar{R}_p} H_\ell^{(1)}(k|\bar{R}_p|) e^{-i\ell\phi_{\bar{R}_p}} \\ &= H_\ell^{(1)}(k|\bar{a}_1|) e^{-i\ell\phi_{\bar{a}_1}} \left[e^{i\bar{k}_i \cdot \bar{a}_1} + (-1)^\ell e^{-i\bar{k}_i \cdot \bar{a}_1} \right] \\ &+ H_\ell^{(1)}(k|\bar{a}_2|) e^{-i\ell\phi_{\bar{a}_2}} \left[e^{i\bar{k}_i \cdot \bar{a}_2} + (-1)^\ell e^{-i\bar{k}_i \cdot \bar{a}_2} \right] \\ &+ H_\ell^{(1)}(k|\bar{a}_3|) e^{-i\ell\phi_{\bar{a}_3}} \left[e^{i\bar{k}_i \cdot \bar{a}_3} + (-1)^\ell e^{-i\bar{k}_i \cdot \bar{a}_3} \right]. \end{aligned} \quad (\text{A9})$$

Only the Hankel functions depend on k ; the remaining terms do not. For the hexagonal lattice, $|\bar{a}_1| = |\bar{a}_2| = |\bar{a}_3|$.

APPENDIX B. ORDER CONSIDERATIONS FOR $\bar{\bar{A}}$, $N_{\max, s}$, AND $N_{\max}$

In the main text,

$$\bar{\bar{A}} \bar{w} = 0, \quad (\text{B1})$$

$$\bar{\bar{A}} = \bar{\bar{I}} - \bar{\bar{D}}^M \bar{\bar{T}} - \sum_{p \in 0_N} \bar{\bar{T}}_{\psi\psi} \bar{\bar{C}}^{(0p)} \bar{\bar{T}}_{\psi w} e^{i\bar{k}_i \cdot \bar{R}_p}. \quad (\text{B2})$$

The product $\bar{\bar{D}}^M \bar{\bar{T}} \bar{w}$ arises from the contributions of the non-neighbor scatterers. For these terms, a small $N_{\max}$ is sufficient, because $\bar{\bar{T}}$ is small for large $N_{\max}$. Therefore, we adopt an order $N_{\max, s}$ that is held constant for all cases, consistent with the size

of the scatterer and the magnitude of the entries of $\bar{\bar{T}}$,

$$N_{\max, s} \leq N_{\max}. \quad (\text{B3})$$

For example, $N_{\max, s} = 4$, whereas $N_{\max}$ varies with R .

The exciting-field coefficient $\bar{w}$ has dimension $2N_{\max} + 1$, whereas in

$$[\bar{\bar{D}}^M \bar{\bar{T}}]_{mn'} = \sum_n [D^M]_{m-n} [\bar{\bar{T}}]_{nn'}, \quad (\text{B4})$$

we set

$$[\bar{\bar{T}}]_{nn'} = 0, \quad |n| > N_{\max, s} \text{ or } |n'| > N_{\max, s}. \quad (\text{B5})$$

The coefficients $[D^M]_{m-n}$ need to be computed only for

$$-N_{\max, s} \leq m - n \leq N_{\max, s}, \quad (\text{B6})$$

$$[D^M]_{m-n} = 0, \quad |m - n| > N_{\max, s}. \quad (\text{B7})$$

In the numerical results, with the fixed scatterer size used in this paper,

$$N_{\max, s} = 4 \quad (\text{B8})$$

for all cases, whereas $N_{\max}$ increases as R decreases, as indicated in the Results section.

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