Supplementary Material Beyond Mie Theory: Systematic Computation of Bulk Scattering Parameters based on Microphysical Wave Optics

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In this document we derive the far-field scattered field of clusters of particles from the Foldy-Lax equations. For completeness and selfcontainedness, we start by reviewing time-harmonic electromagnetics following the derivations described by Mishchenko et al. [2006] (§S1), and its formulation for a medium with multiple particles embedded using the Foldy-Lax equations [Foldy 1945; Lax 1951](§S2) and their far-field approximations (§S3.

From these, we later derive the scattering dyad encoding the response of a cluster of particles in the far field, which later can be used to compute the (radiative) optical properties of a scattering medium.

S1 ELECTROMAGNETIC SCATTERING

The propagation of a time-harmonic monochromatic electromagnetic field with frequency ω is defined by the Maxwell curl equations as

$$\begin{aligned} \nabla \times \mathbf{E}(\mathbf{r}) &= \mathrm{i}\omega\mu(\mathbf{r})\mathbf{H}(\mathbf{r}), \\ \nabla \times \mathbf{H}(\mathbf{r}) &= -\mathrm{i}\omega\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}), \end{aligned} \tag{S.1}$$

with $\nabla\times.$ the curl operator, $\mathbf{E}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r})$ the electric and magnetic field at $\mathbf{r}$ respectively, $\mu(\mathbf{r})$ and $\varepsilon(\mathbf{r})$ the magnetic permeability and electric permittivity at $\mathbf{r}$ respectively, and $\mathrm{i} = \sqrt{-1}$.

By assuming a non-magnetic medium (i.e. $\mu(\mathbf{r}) = \mu_0$, with μ_0 the magnetic permeability of a vacuum), and taking the curl on the first line in Equation (S.1) we get

$$\begin{aligned} \nabla^2\mathbf{E}(\mathbf{r}) &= \mathrm{i}\omega\mu(\mathbf{r})\nabla \times \mathbf{H}(\mathbf{r}) \\ &= -\mathrm{i}^2\omega^2\mu_0\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}), \end{aligned} \tag{S.2}$$

with $\nabla^2 = \nabla\times\nabla$, which by arithmetic reordering reduces to the *electric field wave equation*

$$\nabla^2 \times \mathbf{E}(\mathbf{r}) - k(\mathbf{r})^2\mathbf{E}(\mathbf{r}) = 0, \tag{S.3}$$

where $k(\mathbf{r}) = \omega\sqrt{\varepsilon(\mathbf{r})\mu_0}$ is the medium's wave number at $\mathbf{r}$. Note that the wave number k has a dependence on the frequency ω; in the following we omit such dependence for brevity.

Let us now assume an infinite homogeneous isotropic medium with permittivity ε_1, filled with scatterers with potentially inhomogeneous permittivity $\varepsilon_2(\mathbf{r})$. This separates the space in two different regions: The surrounding infinite region V_0, and the finite disjoint region occupied by the scatterers V, so that $V \bigcup V_0 = \mathbb{R}^3$. Under this configuration, we can express Equation (S.3) as two different wave equations

$$\nabla^2 \times \mathbf{E}(\mathbf{r}) - k_1^2\mathbf{E}(\mathbf{r}) = 0, \mathbf{r} \in V_0, \tag{S.4}$$

$$\nabla^2 \times \mathbf{E}(\mathbf{r}) - k_2(\mathbf{r})^2\mathbf{E}(\mathbf{r}) = 0, \mathbf{r} \in V, \tag{S.5}$$

with k_1 the constant wave number at the hosting medium, and $k_2(\mathbf{r})$ the potentially inhomogeneous wave number at the scatterers. Equations (S.4) and (S.5) can be expressed together in a single inhomogeneous differential equation as

$$\nabla^2 \times \mathbf{E}(\mathbf{r}) - k_1^2\mathbf{E}(\mathbf{r}) = U(\mathbf{r})\,\mathbf{E}(\mathbf{r}), \tag{S.6}$$

with $U(\mathbf{r}) = k_1^2[m^2(\mathbf{r}) - 1]$ the potential function at $\mathbf{r}$, and $m(\mathbf{r}) = k_2(\mathbf{r})/k_1$ the index of refraction at $\mathbf{r}$. It is trivial to verify that for $\mathbf{r} \in V_0$ in the hosting medium $m(\mathbf{r}) = 1$, then the potential function $U(\mathbf{r})$ vanishes, and Equation (S.6) reduces to Equation (S.4).

Solving the inhomogeneous linear differential equation described in Equation (S.6) results in two terms: The contribution of the incident field $\mathbf{E}^{\mathrm{inc}}(\mathbf{r})$, which is the sole contribution in the case of a homogeneous medium, and the scattered field $\mathbf{E}^{\mathrm{sca}}(\mathbf{r})$ resulting of introducing inhomogeneities (i.e. scatterers) in the embedding medium, as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\mathrm{inc}}(\mathbf{r}) + \mathbf{E}^{\mathrm{sca}}(\mathbf{r}). \tag{S.7}$$

The fist part trivially satisfies Equation (S.4) for the incident field $\mathbf{E}^{\mathrm{inc}}(\mathbf{r})$. In order to compute the scattered field $\mathbf{E}^{\mathrm{sca}}(\mathbf{r})$, we enforce energy conservation by computing a solution that vanishes at large distances. We introduce the free-space dyadic Green function $\overleftrightarrow{G}(\mathbf{r}, \mathbf{r}')$ that satisfies the impulse response of the linear system in Equation (S.3), modeled as

$$\nabla^2 \times \overleftrightarrow{G}(\mathbf{r}, \mathbf{r}') - k_1^2\overleftrightarrow{G}(\mathbf{r}, \mathbf{r}') = \overleftrightarrow{I}\delta(\mathbf{r} - \mathbf{r}'), \tag{S.8}$$

where $\overleftrightarrow{I}$ is the identity dyad, and $\delta(\cdot)$ is the Dirac delta function. Note that the derivatives are with respect to $\mathbf{r}$. Multiplying both sides of the differential equation by $U(\mathbf{r})\,\mathbf{E}(\mathbf{r})$, and integrating both sides with respect to $\mathbf{r}'$ over the entire space $\mathbb{R}^3$, we get

$$\left(\nabla^2 \times \overleftrightarrow{I} - k_1^2\overleftrightarrow{I}\right)\overbrace{\int_{\mathbb{R}^3} U(\mathbf{r}')\,\overleftrightarrow{G}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'}^{\mathbf{E}^{\mathrm{sca}}(\mathbf{r})} = U(\mathbf{r})\,\mathbf{E}^{\mathrm{sca}}(\mathbf{r}), \tag{S.9}$$

with $.\cdot.$ the dyadic-vector dot-product. Since the potential function $U(\mathbf{r})$ vanishes everywhere outside V, we can express the scattered field $\mathbf{E}^{\mathrm{sca}}(\mathbf{r})$ as an integral on the space occupied by scatterers V

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only, as

$$\mathbf{E}^{\text{sca}}(\mathbf{r}) = \int_V U(\mathbf{r})\overleftrightarrow{G}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')\,\mathrm{d}\mathbf{r}' = k_1^2\int_V [m^2(\mathbf{r}')-1]\,\overleftrightarrow{G}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'. \tag{S.10}$$

Now, the only term missing for computing $\mathbf{E}^{\text{sca}}(\mathbf{r})$ is the Green function that solves Equation (S.8), which has a well-known solution as

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}') = \left(\overleftrightarrow{I} + k_1^{-2}\nabla\otimes\nabla\right)\frac{\exp(ik_1|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|}, \tag{S.11}$$

where $.\otimes.$ denotes the dyadic product of two vectors, and the derivative operator ∇ applies over $\mathbf{r}$.

Finally, by plugin Equation (S.10) into Equation (S.7) we get the *volume integral equation* [Mishchenko et al. 2006, Sec.3.1] that solves the Maxwell equations (S.1) as the sum of the incident field $\mathbf{E}^{\text{inc}}(\mathbf{r})$ and the scattered field $\mathbf{E}^{\text{sca}}(\mathbf{r})$ due to inhomogeneities in the medium in the form of scatterers:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \mathbf{E}^{\text{sca}}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \int_V \underbrace{k_1^2[m^2(\mathbf{r}')-1]}_{U(\mathbf{r}')}\overleftrightarrow{G}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'. \tag{S.12}$$

Intuitively, Equation (S.12) models the scattering field as the superposition of the spherical wavelets resulting from a change of permitivitty (i.e. with $m(\mathbf{r}')\neq 1$). This is a general equation that solves the Maxwell equations for non-magnetic media in arbitrary setups. Note also the recursive nature of Equation (S.12); we will deal with this recursivity in the following section, computing $\mathbf{E}^{\text{sca}}(\mathbf{r})$ as a function of the incident field $\mathbf{E}^{\text{inc}}(\mathbf{r})$.

S2 FOLDY-LAX EQUATIONS

Let us consider a medium filled with N finite discrete particles with volume V_i and index of refraction $m_i(\mathbf{r})$. We can now define the potential function $U_i(\mathbf{r})$ for each particle i as

$$U_i(\mathbf{r}) = \begin{cases} 0, & \mathbf{r}\notin V_i \\ k_1^2[m_i^2(\mathbf{r})-1] & \mathbf{r}\in V_i, \end{cases} \tag{S.13}$$

with the total potential function U in Equation (S.12) defined as $U(\mathbf{r}) = \sum_{i=1}^N U_i(\mathbf{r})$. By combining Equations (S.12) and (S.13), we can express the field at any position $\mathbf{r}\in\mathbb{R}^3$ following the so-called *Foldy-Lax equation* [Foldy 1945; Lax 1951] as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \sum_{i=1}^N \int_{V_i}\overleftrightarrow{G}(\mathbf{r},\mathbf{r}')\cdot\int_{V_i}\overleftrightarrow{T_i}(\mathbf{r}',\mathbf{r}'')\cdot\mathbf{E}_i(\mathbf{r}'')\,\mathrm{d}\mathbf{r}''\,\mathrm{d}\mathbf{r}' = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \sum_{i=1}^N \mathbf{E}_i^{\text{sca}}(\mathbf{r}), \tag{S.14}$$

with $\mathbf{E}_i(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \sum_{j(\neq i)=1}^N \mathbf{E}_{ij}^{\text{exc}}(\mathbf{r})$, where the partial exciting field $\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r})$ from particles j to i and $\mathbf{E}_i^{\text{sca}}(\mathbf{r})$ the scattered field from particle i. Note that we overload the dot-product operator accounting for the dyad-dyad case. The dyad transition operator $\overleftrightarrow{T_i}(\mathbf{r},\mathbf{r}')$ for particle i defined as [Tsang et al. 1985]

$$\overleftrightarrow{T_i}(\mathbf{r},\mathbf{r}') = U_i(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\overleftrightarrow{I} + U_i(\mathbf{r})\int_{V_i}\overleftrightarrow{G}(\mathbf{r},\mathbf{r}'')\cdot\overleftrightarrow{T_i}(\mathbf{r}'',\mathbf{r}')\,\mathrm{d}\mathbf{r}'', \tag{S.15}$$

with $\delta(x)$ the Dirac delta, $\overleftrightarrow{I}$ the identity dyad. The partial exciting field $\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r})$ is defined as

$$\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r}) = \int_{V_j}\overleftrightarrow{G}(\mathbf{r},\mathbf{r}')\cdot\int_{V_j}\overleftrightarrow{T_j}(\mathbf{r}',\mathbf{r}'')\cdot\mathbf{E}_j(\mathbf{r}'')\,\mathrm{d}\mathbf{r}''\,\mathrm{d}\mathbf{r}', \tag{S.16}$$

with $\mathbf{r}\in V_i$. Note that the exciting field $\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r})$ has essentially the same form as the scattered field $\mathbf{E}_j^{\text{sca}}(\mathbf{r})$ from particle j. As shown by Mishchenko [2002], the Foldy-Lax equations (S.14) solve exactly the volume integral equation (S.12) for multiple arbitrary particles in the medium without any assumptions on their composition or packing rate, beyond the assumption of a homogeneous hosting medium.

S3 FAR-FIELD FOLDY-LAX EQUATIONS

Equation (S.16) define the exact exciting field resulting from scattering by particle j on particle i. However, if the distance between particles $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$, with $\mathbf{R}_i$ the origin of particle i, is large, so that $k_1R_{ij}\gg 1$, we can approximate the propagation distance between points $\mathbf{r}\in V_i$ and $\mathbf{r}'\in V_j$ as $|\mathbf{r}-\mathbf{r}'|\approx R_{ij} + (\hat{\mathbf{R}}_{ij}\cdot\Delta\mathbf{r}) - (\hat{\mathbf{R}}_{ij}\cdot\Delta\mathbf{r}')$, with $\hat{\mathbf{R}}_{ij} = \frac{\mathbf{R}_i-\mathbf{R}_j}{R_{ij}}$, $\Delta\mathbf{r} = \mathbf{r}-\mathbf{R}_i$ and $\Delta\mathbf{r}' = \mathbf{r}'-\mathbf{R}_j$. With this approximation, and after some algebraic operations, we can now approximate the dyadic Green's function as

$$\overleftrightarrow{G}(\mathbf{r},\mathbf{r}') \approx (\overleftrightarrow{I} - \hat{\mathbf{R}}_{ij}\otimes\hat{\mathbf{R}}_{ij})\frac{\exp(ik_1R_{ij})}{4\pi R_{ij}}g(\hat{\mathbf{R}}_{ij},\Delta\mathbf{r})g(-\hat{\mathbf{R}}_{ij},\Delta\mathbf{r}'), \tag{S.17}$$

with $g(\hat{\mathbf{n}},\mathbf{r}) = \exp(ik_1\hat{\mathbf{n}}\cdot\mathbf{r})$. With this approximation, we can now express $\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r})$ for a point $\mathbf{r}\in V_i$ using its *far-field* approximation, as

$$\mathbf{E}_{ij}^{\text{exc}}(\mathbf{r}) = \frac{\exp(ik_1\,R_{ij})}{R_{ij}}g(\hat{\mathbf{R}}_{ij},\Delta\mathbf{r})\,\mathbf{E}_{1ij}^{\text{exc}}(\hat{\mathbf{R}}_{ij}), \tag{S.18}$$

with $\mathbf{r}\in V_i$ a point in particle i, and $\mathbf{E}_{1ij}^{\text{exc}}$ the far-field exciting field from particle j to particle i defined as

$$\mathbf{E}_{1ij}^{\text{exc}}(\hat{\mathbf{R}}_{ij}) = \frac{(\overleftrightarrow{I} - \hat{\mathbf{R}}_{ij}\otimes\hat{\mathbf{R}}_{ij})}{4\pi}\cdot\int_{V_j} g(-\hat{\mathbf{R}}_{ij},\Delta\mathbf{r}')\int_{V_j}\overleftrightarrow{T_j}(\mathbf{r}',\mathbf{r}'')\cdot\mathbf{E}_j(\mathbf{r}'')\,\mathrm{d}\mathbf{r}''\,\mathrm{d}\mathbf{r}'. \tag{S.19}$$

The dyad $(\overleftrightarrow{I} - \hat{\mathbf{R}}_{ij}\otimes\hat{\mathbf{R}}_{ij})$ to ensure a transverse planar field, which allows to solely characterize $\mathbf{E}_{1ij}^{\text{exc}}(\hat{\mathbf{R}}_{ij})$ by the propagation direction $\hat{\mathbf{R}}_{ij}$. In order to Equation (S.19) to be valid, the distance R_{ij} needs to hold the far-field criteria, which relates the R_{ij} with the radius of the particle a_j following the inequality [Mishchenko et al. 2006]

$$k_1R_{ij}\gg\max\left(1,\frac{k_1^2a_j^2}{2}\right). \tag{S.20}$$

The two forms of computing the exciting field from particle j to i (Equations (S.16) and (S.19)) suggest that we can consider two subsets of particles j depending on their distance with respect to the point of interest $\mathbf{r}$: One set of N_{near} particles in the near field and another set of N_{far} particles in the far field. With that, we can now the exciting field in particle i as

$$\mathbf{E}_i(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \sum_{j(\neq i)=1}^{N_{\text{near}}} \mathbf{E}^{\text{exc}}_{ij}(\mathbf{r}) + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}^{\text{exc}}_{ik}(\mathbf{r}). \tag{S.21}$$

In the following, we will use this as motivation for defining the exciting field on a particle from a group of particles in the far field.

S4 FAR-FIELD FOLDY-LAX EQUATIONS FOR CLUSTERS OF PARTICLES

Here we derive the far-field Foldy-Lax equations for groups of particles where the a cluster of these particles are in their respective near-field region, while the other elements in the system are in the far field. For simplicity in our derivations, we consider a single far-field incident field, as well as single particle k in the far field region of the cluster of particles. More formally, let us now consider a cluster C of N_C particles, where all particles $j \in C$ are in their respective near-field region, and that the particles of the cluster are bounded on a sphere centered at $\mathbf{R}_C$ with radius a_C.

Since both the incident field $\mathbf{E}^{\text{inc}}(\mathbf{r})$ and the exciting field $\mathbf{E}^{\text{exc}}_{Ck}$ from particle k are in the far-field region, we can assume that both fields are planar waves defined as

$$\mathbf{E}^{\text{inc}}(\mathbf{r}) = \mathbf{E}^{\text{inc}}_0 \exp(ik_1 \hat{\mathbf{n}} \cdot \Delta\mathbf{r}) = \mathbf{E}^{\text{inc}}_0\, g(\hat{\mathbf{n}}, \Delta\mathbf{r}), \tag{S.22}$$

$$\mathbf{E}^{\text{exc}}_{Ck}(\mathbf{r}) = \mathbf{E}^{\text{exc}}_{0Ck} \exp(ik_1 \hat{\mathbf{R}}_{Ck} \cdot \Delta\mathbf{r}) = \mathbf{E}^{\text{exc}}_{0Ck}\, g(\hat{\mathbf{R}}_{Ck}, \Delta\mathbf{r}) \tag{S.23}$$

with $\mathbf{E}^{\text{inc}}_0$ and $\mathbf{E}^{\text{exc}}_{0Ck} = \frac{\exp(ik_1 R_{Ck})}{R_{Ck}} \mathbf{E}^{\text{exc}}_{1Ck}(\hat{\mathbf{R}}_{Ck})$ (S.19) the amplitude of the planar incident field and the exciting field from particle k respectively, $\hat{\mathbf{n}}$ and $\hat{\mathbf{R}}_{Ck}$ the propagation direction of the each field, and $\Delta\mathbf{r} = \mathbf{r} - \mathbf{R}_C$.

Now, let us slightly abuse the dot product notation defining $(\varphi_1 \bullet \varphi_2) = \int \varphi_1(x) \cdot \varphi_2(x)\,\mathrm{d}x$, and remove the spatial dependency on each term. By the planar incident field assumption, and plugging Equation (S.21) into the definition of the scattered field from particle $i \in C$ (S.14), we get

$$\begin{aligned}\mathbf{E}^{\text{sca}}_i(\mathbf{r}) &= \overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \mathbf{E}_i \\ &= \overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}^{\text{exc}}_{Ck} + \sum_{j(\neq i)=1}^{N_{\text{near}}} \mathbf{E}^{\text{exc}}_{ij}\right].\end{aligned} \tag{S.24}$$

By recursively expanding $\mathbf{E}^{\text{exc}}_{ij}$, Equation (S.24) becomes

$$\begin{aligned}\mathbf{E}^{\text{sca}}_i(\mathbf{r}) = \overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \Bigg[&\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}^{\text{exc}}_{Ck} \\ &+ \sum_{j(\neq i)=1}^{N_{\text{near}}} \overleftrightarrow{G} \bullet \overleftrightarrow{T_j} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}^{\text{exc}}_{Ck} + \sum_{l(\neq j)=1}^{N_{\text{near}}} [\ldots]_l\right]\Bigg],\end{aligned} \tag{S.25}$$

where the "$[\ldots]_l$" term represents the recursivity as

$$[\ldots]_l = \overleftrightarrow{G} \bullet \overleftrightarrow{T_l} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}^{\text{exc}}_{Ck} + \sum_{m(\neq l)=1}^{N_{\text{near}}} [\ldots]_m\right]. \tag{S.26}$$

By reordering Equation (S.25) we get

$$\begin{aligned}\mathbf{E}^{\text{sca}}_i(\mathbf{r}) &= \overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{j(\neq i)=1}^{N_{\text{near}}} \overleftrightarrow{G} \bullet \overleftrightarrow{T_j} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{l(\neq j)=1}^{N_{\text{near}}} [\ldots]_l^{\mathbf{E}^{\text{inc}}}\right]\right] \\ &+ \sum_{k=1}^{N_{\text{far}}} \left[\overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[\mathbf{E}^{\text{exc}}_{Ck} + \sum_{j(\neq i)=1}^{N_{\text{near}}} \overleftrightarrow{G} \bullet \overleftrightarrow{T_j} \bullet \left[\mathbf{E}^{\text{exc}}_{Ck} + \sum_{l(\neq j)=1}^{N_{\text{near}}} [\ldots]_l^{\mathbf{E}^{\text{exc}}_{Ck}}\right]\right]\right],\end{aligned} \tag{S.27}$$

where "$[\ldots]_l^{\varphi}$" is similar to Equation (S.26), with form

$$[\ldots]_l^{\varphi} = \overleftrightarrow{T_l} \bullet \overleftrightarrow{G} \bullet \left[\varphi + \sum_{m(\neq l)=1}^{N_{\text{near}}} [\ldots]_m^{\varphi}\right]. \tag{S.28}$$

Finally, by exploiting Equations (S.22) and (S.23), and contracting the recursion, we transform Equation (S.27) into

$$\begin{aligned}\mathbf{E}^{\text{sca}}_i(\mathbf{r}) = &\overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[g(\hat{\mathbf{n}}) + \sum_{j(\neq i)=1}^{N_{\text{near}}} [\ldots]_j^{g(\hat{\mathbf{n}})}\right] \cdot \mathbf{E}^{\text{inc}}_0 \\ &+ \sum_{k=1}^{N_{\text{far}}} \left[\overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[g(\hat{\mathbf{R}}_{Ck}) + \sum_{j(\neq i)=1}^{N_{\text{near}}} [\ldots]_j^{g(\hat{\mathbf{R}}_{Ck})}\right] \cdot \mathbf{E}^{\text{exc}}_{0Ck}\right].\end{aligned} \tag{S.29}$$

Note that each element in the sum in the equation above is the result of the amplitude of the far-field incident or exciting fields, and a series that encode all the near-field scattering in the cluster C. We can thus define the scattering dyad $\overleftrightarrow{A}^{\text{near}}_i(\hat{\mathbf{n}}^{\text{inc}}, \mathbf{r})$ relating a field incoming at particle i from direction $\hat{\mathbf{n}}^{\text{inc}}$ with the field at point $\mathbf{r}$ as

$$\boxed{\overleftrightarrow{A}^{\text{near}}_i(\hat{\mathbf{n}}^{\text{inc}}, \mathbf{r}) = \overleftrightarrow{G} \bullet \overleftrightarrow{T_i} \bullet \left[g(\hat{\mathbf{n}}^{\text{inc}}) + \sum_{j(\neq i)=1}^{N_{\text{near}}} [\ldots]_j^{g(\hat{\mathbf{n}}^{\text{inc}})}\right].} \tag{S.30}$$

Trivially, following our assumption of constant $\mathbf{E}^{\text{inc}}_0$ and $\mathbf{E}^{\text{exc}}_{0Ck}$ for the whole cluster C, we can compute the cluster's scattering dyad as:

$$\overleftrightarrow{A}^{\text{near}}_C(\hat{\mathbf{n}}^{\text{inc}}, \mathbf{r}) = \sum_{i=1}^{N_C} \overleftrightarrow{A}^{\text{near}}_i(\hat{\mathbf{n}}^{\text{inc}}, \mathbf{r}). \tag{S.31}$$

The scattering dyad $\overleftrightarrow{A}^{\text{near}}_C(\hat{\mathbf{n}}^{\text{inc}}, \mathbf{r})$ solves the scattering field for a unit-amplitude incoming planar field in a scene consisting of the particles forming cluster C, and can be computed using any method from computational electromagnetics.

Far-field approximation. Equation (S.30) represents the general form of the scattering dyad for particle i, which results into a five-dimensional function. Assuming that $\mathbf{r}$ is in the far-field region of a particle $i \in C$, and by using the far-field approximation of the Green's function (S.18), Equation (S.24) becomes

$$\mathbf{E}^{\text{sca}}_i(\mathbf{r}) \approx (\overleftrightarrow{I} - \hat{\mathbf{R}}_i \otimes \hat{\mathbf{R}}_i) \frac{\exp(ik_1 R_i)}{4\pi R_i} \cdot g(-\hat{\mathbf{R}}_i) \bullet \overleftrightarrow{T_i} \cdot \mathbf{E}_i, \tag{S.32}$$

with $R_i = |\mathbf{r} - \mathbf{R}_i|$ and $\hat{\mathbf{R}}_i = \frac{\mathbf{r}-\mathbf{R}_i}{R_i}$. Note that the term $g(\hat{\mathbf{R}}_i, \Delta\mathbf{r})$ inEquation (S.18) vanishes for a single particle, since $|\Delta\mathbf{r}| = 0$ and therefore $g(\hat{\mathbf{R}}_i, \Delta\mathbf{r}) = 1$.

Now, using the definition of the scattered field $\mathbf{E}_i$ in Equation (S.21), and expanding $\mathbf{E}^{\text{exc}}$ following Equation (S.24), and expanding $\mathbf{E}_{ij}^{\text{exc}}$ following Equation (S.25) we get

$$\mathbf{E}_i^{\text{sca}}(\mathbf{r}) = (\overleftrightarrow{I} - \hat{\mathbf{R}}_i \otimes \hat{\mathbf{R}}_i)\frac{\exp(\mathrm{i}k_1 R_i)}{4\pi R_i} \cdot g(-\hat{\mathbf{R}}_i) \bullet \overleftrightarrow{T_i} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}_{Ck}^{\text{exc}} + \sum_{j(\neq i)=1}^{N_{\text{near}}} \overleftrightarrow{G} \bullet \overleftrightarrow{T_j} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \mathbf{E}_{Ck}^{\text{exc}} + \sum_{l(\neq j)=1}^{N_{\text{near}}} [\ldots]_l\right]\right], \quad \text{(S.33)}$$

with "$[\ldots]_l$" representing the recursivity (S.26). Following Equations (S.27) and (S.29) we reorder the equation to separate the contribution of the incident $\mathbf{E}^{\text{inc}}$ and exciting fields $\mathbf{E}_{Ck}^{\text{exc}}$ respectively, and exploit the far field assumption to put $\mathbf{E}^{\text{inc}}$ and $\mathbf{E}_{Ck}^{\text{exc}}$ in their planar field form [Equations (S.22) and (S.23)], as

$$\mathbf{E}_i^{\text{sca}}(\mathbf{r}) \approx \frac{e^{\mathrm{i}k_1 R_i}}{R_i}\left(\overleftrightarrow{A_i}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_0^{\text{inc}} + \sum_{k=1}^{N_{\text{far}}} \overleftrightarrow{A_i}(\hat{\mathbf{R}}_{Ck}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_{0Ck}^{\text{exc}}\right), \quad \text{(S.34)}$$

with $\overleftrightarrow{A_i}(\hat{\mathbf{n}}^{\text{inc}}, \hat{\mathbf{n}}^{\text{sca}})$ the far-field scattering dyad relating incident and scattered directions $\hat{\mathbf{n}}^{\text{inc}}$ and $\hat{\mathbf{n}}^{\text{sca}}$ as

$$\boxed{\overleftrightarrow{A_i}(\hat{\mathbf{n}}^{\text{inc}}, \hat{\mathbf{n}}^{\text{sca}}) = (\overleftrightarrow{I} - \hat{\mathbf{R}}_i \otimes \hat{\mathbf{R}}_i) \cdot \frac{g(-\hat{\mathbf{n}}^{\text{sca}})}{4\pi} \bullet \overleftrightarrow{T_i} \bullet \left[g(\hat{\mathbf{n}}^{\text{inc}}) + \sum_{j(\neq i)=1}^{N_{\text{near}}} [\ldots]_j^{g(\hat{\mathbf{n}}^{\text{inc}})}\right].} \quad \text{(S.35)}$$

Finally, since $\hat{\mathbf{R}}_i \approx \hat{\mathbf{R}}_C$ for all particles $i \in C$ we can approximate the far-field scattered field of cluster C as

$$\begin{aligned}
\mathbf{E}_C^{\text{sca}}(\mathbf{r}) &= \sum_{i=1}^{N_C} \mathbf{E}_i^{\text{sca}}(\mathbf{r}) \\
&= \sum_{i=1}^{N_C} \frac{e^{\mathrm{i}k_1 R_i}}{R_i}\left(\overleftrightarrow{A_i}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_0 + \sum_{k=1}^{N_{\text{far}}} \overleftrightarrow{A_i}(\hat{\mathbf{R}}_{Ck}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_{0Ck}^{\text{exc}}\right), \\
&\approx \frac{e^{\mathrm{i}k_1 R_C}}{R_C}\left(\sum_{i=1}^{N_C} \overleftrightarrow{A_i}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_0 + \sum_{k=1}^{N_{\text{far}}} \sum_{i=1}^{N_C} \overleftrightarrow{A_i}(\hat{\mathbf{R}}_{Ck}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_{0Ck}^{\text{exc}}\right) \\
&= \frac{e^{\mathrm{i}k_1 R_C}}{R_C}\left(\overleftrightarrow{A_C}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_0 + \sum_{k=1}^{N_{\text{far}}} \overleftrightarrow{A_C}(\hat{\mathbf{R}}_{Ck}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_{0Ck}^{\text{exc}}\right),
\end{aligned} \quad \text{(S.36)}$$

with $\overleftrightarrow{A_C}(\hat{\mathbf{n}}^{\text{inc}}, \hat{\mathbf{n}}^{\text{sca}}) = \sum_{i=1}^{N_C} \overleftrightarrow{A_i}(\hat{\mathbf{n}}^{\text{inc}}, \hat{\mathbf{n}}^{\text{sca}})$ the far-field scattering dyad of cluster C.

Computing the far-field exciting field. Let us know compute the far-field exciting field $\mathbf{E}_{kC}^{\text{exc}}$ from a cluster C to a particle k placed in the far-field region of C. By plugging Equation (S.21) into Equation (S.19), and under the assumption of far-field incident fields (Equations (S.22) and (S.23)) we get the exciting field from a particle $i \in C$ over particle j as:

$$\mathbf{E}_{ki}^{\text{exc}}(\mathbf{r}) \approx (\overleftrightarrow{I} - \hat{\mathbf{R}}_{ki} \otimes \hat{\mathbf{R}}_{ki}) \cdot \frac{e^{\mathrm{i}k_1(R_{ki} + \hat{\mathbf{R}}_{ki} \cdot \Delta\mathbf{r})}}{4\pi R_{ki}} g(\hat{\mathbf{R}}_{ki}) \bullet \overleftrightarrow{T_j} \bullet \left[\mathbf{E}^{\text{inc}} + \sum_{k'=1}^{N_{\text{far}}} \mathbf{E}_{ik'}^{\text{exc}} + \sum_{j(\neq i)=1}^{N_{\text{near}}} \mathbf{E}_{ij}^{\text{exc}}\right]. \quad \text{(S.37)}$$

This equation has the same form as Equation (S.34), and thus we can express it using the far-field scattering dyad defined in Equation (S.35) as

$$\mathbf{E}_{ki}^{\text{exc}}(\mathbf{r}) = \frac{e^{\mathrm{i}k_1(R_{ki} + \hat{\mathbf{R}}_{ki} \cdot \Delta\mathbf{r})}}{R_{ki}}\left(\overleftrightarrow{A_i}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_0^{\text{inc}} + \sum_{k'=1}^{N_{\text{far}}} \overleftrightarrow{A_i}(\hat{\mathbf{R}}_{Ck'}, \hat{\mathbf{R}}_i) \cdot \mathbf{E}_{0Ck'}^{\text{exc}}\right), \quad \text{(S.38)}$$

which by summing the exciting field of all particles $i \in C$ and following the far-field approximation ($\hat{\mathbf{R}}_{ki} \approx \hat{\mathbf{R}}_{kC}, \forall i \in C$ we get

$$\mathbf{E}_{kC}^{\text{exc}}(\mathbf{r}) \approx \frac{e^{\mathrm{i}k_1(R_{kC} + \hat{\mathbf{R}}_{kC} \cdot \Delta\mathbf{r})}}{R_{kC}}\left(\overleftrightarrow{A_C}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_0^{\text{inc}} + \sum_{k'=1}^{N_{\text{far}}} \overleftrightarrow{A_C}(\hat{\mathbf{R}}_{Ck'}, \hat{\mathbf{R}}_C) \cdot \mathbf{E}_{0Ck'}^{\text{exc}}\right). \quad \text{(S.39)}$$

Finally, if particle k is itself contained in the near-field of a cluster of particles C_1, then it is trivial to compute the exciting field from cluster C to C_1 as

$$\mathbf{E}_{C_1 C}^{\text{exc}}(\mathbf{r}) = \sum_{k=1}^{N_{C_1}} \mathbf{E}_{kC}^{\text{exc}}(\mathbf{r}). \quad \text{(S.40)}$$

Thus, by grouping the individual particles into N^{cls} near-field clusters, and assuming that all clusters and observation point $\mathbf{r}$ lay in their respective far field, we can approximate the Foldy-Lax equation (S.14) as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \sum_{C_j=1}^{N^{\text{cls}}} \mathbf{E}_{C_j}^{\text{sca}}(\mathbf{r}), \quad \text{(S.41)}$$

with $\mathbf{E}_{C_j}^{\text{sca}}(\mathbf{r})$ defined by pluging Equation (S.40) into Equation (S.36) as

$$\mathbf{E}_{C_j}^{\text{sca}}(\mathbf{r}) = \frac{e^{\mathrm{i}k_1 R_{C_j}}}{R_{C_j}}\left(\overleftrightarrow{A}_{C_j}(\hat{\mathbf{n}}, \hat{\mathbf{R}}_{C_j}) \cdot \mathbf{E}_0^{\text{inc}} \quad \text{(S.42)}\right.$$

$$\left. + \sum_{C_k(\neq C_j)=1}^{N^{\text{cls}}} \overleftrightarrow{A}_{C_j}(\hat{\mathbf{R}}_{C_j C_k}, \hat{\mathbf{R}}_{C_j}) \cdot \mathbf{E}_{0C_j C_k}^{\text{exc}}\right), \quad \text{(S.43)}$$

with $\mathbf{E}_{0C_jC_k}^{\text{exc}}$ the amplitude of the far-field exciting field from cluster C_k to cluster C_j.

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