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Application of Born series for modeling of Mie-resonant nanostructures

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Abstract. Born series formalism is a widely-used approach to solve a scattering problem in quantum mechanics and optics, including a problem of electromagnetic scattering on the ensembles of Mie-resonant nanoparticles. In the latter case, the Born series formalism can be used when the electromagnetic coupling between nanoparticles is weak. This can be violated near the multipole Mie-resonance of the nanoparticle. In this work, we analyze the applicability of the Born series approach for modeling the resonant optical response of Mie-nanoparticle ensembles and formulate quantitative criteria of Born series convergence and, subsequently, the applicability of this approach.

1. Introduction

The Born series formalism is a method to simulate scattering by a group of many nanoparticles in a perturbative manner [1, 2, 3, 4, 5, 6]. This method is based on constructing a convergent Born series and replacing it with a finite sum that successively approximate the interaction between particles where the accuracy depends on the number of terms included in the sum (i.e., on the Born approximation order). Born approximations of different orders have been used to simulate tip-substrate interaction [1, 2], calculate polarizability of a non-spherical particle [3, 4], and optimize metalens design [6]. All these problems require a simulation of the interaction in non-periodic structures of a large number of particles which is non-effective to perform, using full-wave simulation techniques; therefore, the Born series method, along with the coupled multipole model, [7, 8] was chosen. The applicability of the Born series method, as well as its convergence, are determined by the strength of electromagnetic coupling in the system. To the best of our knowledge, there is no exhaustive physical analysis of Born series applicability to simulate Mie-resonant nanostructures [9, 10] with quantitative criteria of the series convergence. In this work, we try to give such analysis and criteria and consider a nanosphere dimer having a simple analytical solution in the framework of the coupled dipole model.

2. Results and Discussion

We investigate the resonant scattering of a monochromatic electromagnetic plane wave $\mathbf{E}_0 e^{\mathrm{i}\mathbf{kr}-\mathrm{i}\omega t}$ on a dimer of identical nanospheres supporting dipole Mie-resonances at the optical range (as shown in Fig. 1(a)) [9, 10]. We use the electric dipole approximation of nanoparticle's optical

response admissible at the electric dipole resonance of nanoparticle. The self-consisted dipole moments of nanoparticles can be calculated using the coupled dipole model (CDM) [7]:

$$\begin{aligned} \mathbf{p}^1 &= \alpha(\omega)\mathbf{E}_0 + \alpha(\omega)k^2\varepsilon_0^{-1}\hat{\mathbf{G}}^{12}\mathbf{p}^2, \\ \mathbf{p}^2 &= \alpha(\omega)\mathbf{E}_0 + \alpha(\omega)k^2\varepsilon_0^{-1}\hat{\mathbf{G}}^{21}\mathbf{p}^1. \end{aligned} \tag{1}$$

where $\alpha(\omega)$ is the dipole polarizability, ε_0 is the vacuum permittivity, $k = 2\pi/\lambda$ is the free-space wavenumber, $\hat{\mathbf{G}}^{ij} \equiv \hat{\mathbf{G}}(\mathbf{r}_i, \mathbf{r}_j)$ is the dyadic dipole Green's function [7]. Here and further, we omit the time-dependence of fields and dipole moments. In accordance to Fig. 1(a), the incident wave propagates along the z-axis with a polarization along the x-axis $\mathbf{E}_0 = [E_0, 0, 0]^T$ (T-polarization) or y-axis $\mathbf{E}_0 = [0, E_0, 0]^T$ (L-polarization). The nanoparticles are placed at the positions $\mathbf{r}_1 = [0, +D/2, 0]$ and $\mathbf{r}_2 = [0, -D/2, 0]$, therefore dot product $\mathbf{k} \cdot \mathbf{r}_i = 0$ $(i = 1, 2)$ in Eq. (1).

In Eq. (1), the dipole moment of the nanoparticle determines by the external field (the first term) and the dipole field generated by another particle (the second term). Due to the structure symmetry, both dipole moments have only one non-zero component along the incident field:

$$p_l^i = \frac{\alpha(\omega)E_0}{1 - \alpha(\omega)k^2\varepsilon_0^{-1}G_{ll}^{12}}, \quad i = 1, 2. \tag{2}$$

where $l = x$ for T-polarization, and $l = y$ for L-polarization. The corresponding elements of Green's function:

$$G_{xx}^{12} = \frac{e^{\mathrm{i}kD}}{4\pi D}\left[1 + \frac{\mathrm{i}}{kD} - \frac{1}{k^2D^2}\right], \quad G_{yy}^{12} = \frac{e^{\mathrm{i}kD}}{4\pi D}\left[-\frac{2\mathrm{i}}{kD} - \frac{4}{k^2D^2}\right]. \tag{3}$$

Dipole moments calculating by Eq. (2) rigorously takes into account the electromagnetic coupling between two dipoles. We can also approximate the coupling expanding moments (2) in the Born series. In this case, the Born series is an expansion of the denominator of (2) in geometric series:

$$p_l^i = \alpha(\omega)E_0\sum_{n=0}^{\infty}\left(\alpha(\omega)k^2\varepsilon_0^{-1}G_{ll}^{12}\right)^n, \quad i = 1, 2. \tag{4}$$

The solution of Eq. (1) in the Born approximation of m-th order is given by transition from an infinite series to a finite sum in Eq. (4), i.e., $\sum\limits_{n=0}^{\infty} \to \sum\limits_{n=0}^{m}$.

We can use the Born series approach if the Born series converges. The convergence criteria of geometric series such as Eq. (4) is well-known:

$$|\alpha(\omega) \cdot k^2\varepsilon_0^{-1}G_{ll}^{12}| < 1. \tag{5}$$

Electric-dipole polarizability of a homogeneous nanosphere can be expressed through the Mie-coefficient $a_1(nkR)$ [7, 11], depending on the particle refractive index n and radius R, and incident wavelength:

$$\alpha(\omega) = \mathrm{i}\frac{6\pi\varepsilon_0}{k^3}a_1, \tag{6}$$

then the convergence criteria (5) can be formulated as follows:

$$6\pi \cdot |a_1| \cdot |k^{-1}G_{ll}^{12}| < 1. \tag{7}$$

Non-absorptive particles ($\varepsilon'' = 0$). In this case, the resonance condition provides [12]:

$$a_1 = 1, \tag{8}$$

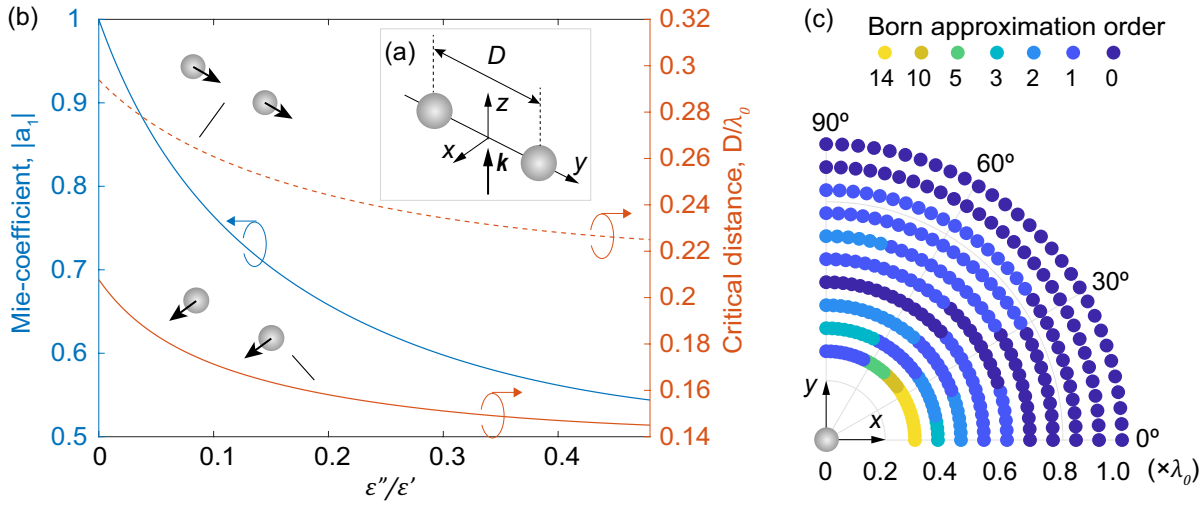

Figure 1. Analysis of the applicability of the Born series approach. (a) Schematic view of identical nanosphere dimer embedded in a vacuum with the marked wavevector of the external incident wave. Dipole moments with the orientation along the y-axis or x-axis are excited by y-polarized (L-polarized) or x-polarized (T-polarized) external wave, respectively. (b) The absolute value of Mie-coefficient (blue line) and critical center-center distance between particles (red lines) as functions of particle material ε'' (where $\varepsilon' = 12.5$). Red solid and red dashed lines correspond to T- and L-polarization of dipole moments, respectively. The Born series converges at the dipole Mie-resonance $\lambda = \lambda_0$ (where $\lambda_0 = 555$ nm) if the distance between particles D is higher than the critical one. (c) The Born approximation order as a function of the second particle position while the first particle is placed at the coordinates' origin. The position of the circle point indicates the second particle position, and its color corresponds to the order of Born approximation that allows calculating the extinction cross section in this approximation with an error (10) of less than 10%. The distance between particles is measured in resonant wavelength $\lambda_0 = 1140$ nm. The minimal inter-particle distance is $D = 0.3\lambda_0$, radius of particles $R = 100$ nm, permittivity of particle material $\varepsilon' = 64$, $\varepsilon'' = 0$. The normally incident plane wave is x-polarized.

corresponding to the resonance wavelength λ_0. By substitution of resonance condition (8) and expressions (3) in inequality (7), we obtain at-resonance convergence criteria of the Born series:

$$6\pi \cdot |k_0^{-1} G_{ll}^{12}| < 1, \tag{9}$$

explicitly independent on the particle refractive index and size (but the resonant wavelength depends). From (9), we find the *critical* distances for L- and T-polarization: $D^{\mathrm{L}} = 0.3\lambda_0$ and $D^{\mathrm{T}} = 0.21\lambda_0$, respectively. A word *critical* highlights that the Born series diverges when the center-center distance between particles is less than critical.

Absorptive particles ($\varepsilon'' \neq 0$). For the particles with absorption (Ohmic) losses, a condition (8) is not valid. The criteria of Born series convergence (7) depends on the absolute value of the Mie-coefficient $|a_1|$. As shown in Fig. 1(b), at-resonance value $|a_1|$ decreases as imaginary part of permittivity increases. Solving the inequality (7) for varying ε'', we find the critical distances and also show their in Fig. 1(b). It is seen that, for both T- and L-polarizations, the critical distances decrease as the absorption losses increase.

Knowing the critical distances between particles, we investigate the accuracy of calculating resonant optical response via the Born series approach. We put the first particle in the origin of the Cartesian coordinate system and vary the position of the second particle. The distance

between two particles is higher than $D = 0.3\lambda_0$. The error of the m-order Born approximation is defined as the relative error of the extinction cross section (ECS):

$$\Delta = \frac{|\sigma^{(m)} - \sigma^{(\mathrm{CDM})}|}{\sigma^{(\mathrm{CDM})}} \times 100\%, \tag{10}$$

where $\sigma = k_0\varepsilon_0^{-1}|E_0|^{-2}\mathrm{Im}\left[\sum_{i=1}^{2}\mathbf{E}_0^*(\mathbf{r}_i)\cdot\mathbf{p}^i\right]$ is the ECS of resonant dimer in the dipole approximation [7], $\sigma^{(\mathrm{CDM})}$ and $\sigma^{(m)}$ is ECS calculated using the rigorous dipole moments (2) and dipole moments in the m-th Born approximation (4), respectively. We set a limit of 10% on the error value Δ and find the Born approximation order when a condition $\Delta \leq 10\%$ is satisfied. The results are presented in Fig. 1(c) for the dimer of non-absorptive nanoparticles. We see in Fig. 1(c) that particles separated higher than λ_0 can be considered as non-interacting because their collective response is accurately described in the zero-order Born approximation. This because a strong near-field coupling between particles becomes weak for inter-particle distances $D \gtrsim \lambda_0$.

3. Conclusion

We analyzed when and how the Born series approach can be used to accurately simulate a resonant optical response of nanoparticle structures. Studying a dimer of the nanospheres under the electric dipole approximation, we derive convergence criteria of the Born series, independent of the particle size and refractive index for non-absorptive particles.

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