Application of Born series for modeling of Mie-resonant nanostructures

N Ustimenko¹, D Kornovan¹, K V Baryshnikova¹, A B Evlyukhin²,¹, and M Petrov¹

¹School of Physics and Engineering, ITMO University, St. Petersburg 197101, Russia
²Leibniz Universität Hannover, Hannover 30167, Germany
E-mail: nikita.ustimenko@metalab.ifmo.ru

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 $E_0e^{i(kr-\omega t)}$ 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]:

\[
\mathbf{p}^1 = \alpha(\omega)\mathbf{E}_0 + \alpha(\omega)k^2\varepsilon_0^{-1}\mathbf{G}_{12}^0 \mathbf{p}^2,
\]

\[
\mathbf{p}^2 = \alpha(\omega)\mathbf{E}_0 + \alpha(\omega)k^2\varepsilon_0^{-1}\mathbf{G}_{21}^0 \mathbf{p}^1.
\]  

(1)

where \(\alpha(\omega)\) is the dipole polarizability, \(\varepsilon_0\) is the vacuum permittivity, \(k = 2\pi/\lambda\) is the free-space wavenumber, \(\mathbf{G}^{ij} = \mathbf{G}(\mathbf{r}_i, \mathbf{r}_j)\) 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:

\[
p_i^j = \frac{\alpha(\omega)E_0}{1 - \alpha(\omega)k^2\varepsilon_0^{-1}G_{ll}^{12}}, \quad i, j = 1, 2.
\]  

(2)

where \(l = x\) for T-polarization, and \(l = y\) for L-polarization. The corresponding elements of Green’s function:

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

(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:

\[
p_i^j = \alpha(\omega)E_0 \sum_{n=0}^{\infty} (\alpha(\omega)k^2\varepsilon_0^{-1}G_{ll}^{12})^n, \quad i, j = 1, 2.
\]  

(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., \(\sum_{n=0}^{\infty} \to \sum_{n=0}^{m}\).

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:

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

(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:

\[
\alpha(\omega) = \frac{6\pi \varepsilon_0}{k^3}a_1,
\]  

(6)

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

\[
6\pi \cdot |a_1| \cdot |k^{-1}G_{ll}^{12}| < 1.
\]  

(7)

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

\[
a_1 = 1,
\]  

(8)
corresponding to the resonance wavelength $\lambda_0$. By substitution of resonance condition (8) and expressions (3) in inequality (7), we obtain at-resonance convergence criteria of the Born series:

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

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: $D^L = 0.3\lambda_0$ and $D^T = 0.21\lambda_0$, 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 $\varepsilon''$, 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):

\[
\Delta = \frac{|\sigma^{(m)} - \sigma^{(CDM)}|}{\sigma^{(CDM)}} \times 100\%,
\]

where \( \sigma = k_0\varepsilon_0^{-1}|E_0|^2 \text{Im} \left[ \sum_{i=1}^{2} \mathbf{E}_0^i(\mathbf{r}_i) \cdot \mathbf{p}^i \right] \) is the ECS of resonant dimer in the dipole approximation \([7]\), \( \sigma^{(CDM)} \) 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 \( \Delta \) 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 \( \lambda_0 \) 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.

4. Acknowledgments

The work was supported by the Russian Science Foundation (project No. 21-79-10190).

References

[1] Labani B, Courjon D, Labeke D V and Girard C 1990 J. Opt. Soc. Am. B 7 936
[2] Keller O, Xiao M and Bozhevolnyi S 1993 Surf. Sci. 280 217–230
[3] Fan Z H, Wang D X, Chen R S and Yung E K N 2006 Microw. Opt. Techn. Lett. 48 1741–1746
[4] Singham S B and Bohren C F 1988 J. Opt. Soc. Am. A 5 1867–1872
[5] Bereza A S, Nemykin A V, Perminov S V, Frumin L L and Shapiro D A 2017 Phys. Rev. A 95 063839
[6] Ustimenko N A, Baryshnikova K V, Melnikov R V, Kornov D F, Ulyantsev V I, Chichkov B N and Evlyukhin A B 2021 Multipole optimization of light focusing by silicon nanosphere structures (Preprint arXiv:2103.01482)
[7] Evlyukhin A B, Reinhartd C, Seidel A, Luk’yanchuk B S and Chichkov B N 2010 Phys. Rev. B 82 045404
[8] Babicheva V E and Evlyukhin A B 2019 Phys. Rev. B 99 195444
[9] Evlyukhin A B, Novikov S M, Zywietz U, Eriksen R L, Reinhartd C, Bozhevolnyi S I and Chichkov B N 2012 Nano Lett. 12 3749–3755
[10] Kuznetsov A I, Miroshnichenko A E, Brongersma M L, Kivshar Y S and Luk’yanchuk B 2016 Science 354 aag2472
[11] Bohren C F and Huffman D R 1983 Absorption and Scattering of Light by Small Particles, (Wiley, New York)
[12] Tribelsky M I and Luk’yanchuk B S 2006 Phys. Rev. Lett. 97 263902