Light scattering by resonant nanoparticles in a 2D lattice.

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Abstract. Photonic crystals are wide-spread optical materials that are actively applied for manipulating light in various cases. However, it is still a challenge to calculate optical properties of photonic crystals, which include small deep-subwavelength resonant inclusions, in a fast way with acceptable precision. Here, we present a method for calculation of scattering matrix of a 2D lattice of resonant nanoparticles embedded into a homogeneous layer far from any interfaces. The proposed approach combines both specialized techniques for a description of high-gradient nanoparticles’ near-field and theory, which accounts for the interactions between the nanoparticles. Our method makes it possible to increase the computational speed by several orders of magnitude in comparison with FEM and paves the way to a solution of several types of problems.

1. Introduction

Photonic crystal slabs and 2D photonic crystals are of great interest because of their unique optical properties, which appear in periodic structures and relative simplicity of fabrication. One of the most powerful methods for their description is Fourier modal method (FMM) [1-2], which is based on a decomposition of an electromagnetic field in terms of harmonics, which fulfill diffraction conditions. If the considered structure includes some tiny dielectric inclusions, then it is very likely that they might be just ignored because of negligible contribution in any observable quantity. Nevertheless, if these particles are plasmonic and have some resonances, then their influence becomes substantial and therefore very large number of harmonics are required to be taken into account. The requirement of FMM to calculate an inverse matrix, which size is proportional to the number of harmonics (N) leads to a cubic growth of algorithm complexity with N. Moreover, it is necessary to subdivide particles into many layers if they have a non-constant cross-section. These circumstances make FMM calculations for photonic crystals with small plasmonic nanoparticles almost impossible.

Near-field of small resonant particles can be efficiently calculated by such advanced methods as finite element method (FEM) or finite difference time domain (FDTD) method. However, straightforward utilization of these methods requires conducting calculations for a whole cell, which typically has relatively large dimensions. Thus, the problem again requires a huge amount of computational resources and time.

Problems of this type have been considered before. However, most studies are focused on some particular cases such as normal incidence of light and rectangular lattices [3-5]. The response of a single particle is often calculated analytically by Mie scattering theory [3] or conventional formulas for polarization of ellipsoids in electrostatic limit [4] or with dynamic corrections [5]. This strongly
limits capabilities of application of these approaches and makes it necessary to develop a more general one.

Here, we develop a theory and corresponding programming code, which calculates scattering matrix of a 2D lattice of resonant nanoparticles in a homogeneous layer (see figure 1). This approach allows us to calculate scattering matrix of arbitrary, not necessarily rectangular lattice for any angle of incidence of external light. The main feature of our theory, which makes it faster than conventional ones, is a combination of methods aimed at near and far-field calculations and utilization of their advantages. Moreover, we introduce both dipole and resonant approximation, which simplify the model and allow to conduct all the calculations knowing only eigenmodes of a particle.

![Figure 1. Schematic of a typical structure that might be calculated by the proposed theory. Plasmonic nanoparticles of a certain shape are embedded into a homogeneous layer far from interfaces.](image)

2. Self-consistent equation on induced polarization and its solution

FMM is a powerful tool for operating with periodic structures till electromagnetic fields vary in space slowly. Therefore, it is not a surprise that it fails to cope with a high-gradient field of resonances. In this way, it seems reasonable to subdivide a problem into two parts.

The first problem is a determination of background field that polarizes certain particle. It consists of external field and field reradiated by adjacent particles. Thus, we obtain the following formula

\[ \mathbf{E}_b(\mathbf{r}_i) = \mathbf{E}_{\text{ext}}(\mathbf{r}_i) + \sum_{j \neq i} \int \mathcal{G}(\mathbf{r}_i - \mathbf{r}_j) \mathbf{P}(\mathbf{r}_j) d^3\mathbf{r}_j, \]

where \( \mathbf{P} \) is the induced in particles excessive polarization field and \( \mathcal{G} \) is the dyadic Green function. Integration is conducted over the volume of particles and summation is conducting over all cells, except the considered one.

The second problem is a determination of polarization operator \( \hat{\alpha} \) that shows what polarization is induced in a solitary particle under the influence of background field \( \mathbf{P}(\mathbf{r}) = \hat{\alpha} [\mathbf{E}_b(\mathbf{r})] \). It can be easily shown that this polarization field might be expressed in terms of full electric field \( \mathbf{E} = \mathbf{E}_b + \mathbf{E}_s \), which includes both background and scattered parts. Indeed, \( \mathbf{P}(\mathbf{r}) = (\varepsilon - \varepsilon_b) \mathbf{E}(\mathbf{r})/(4\pi) \), where \( \varepsilon \) and \( \varepsilon_b \) are permittivities of a particle and background medium respectively. Thus, this problem reduces to an issue of determination of full electric field, which may be solved in an efficient way. For simple geometries, it can be done analytically, whereas non-trivial cases can be resolved by FEM or any other appropriate numerical method. However, since we consider resonant nanoparticles, according to the theory of quasinormal modes (see figure 2) scattered field can be expressed as a superposition of eigenmodes \( \mathbf{E}_s = \sum_i A_i \hat{\mathbf{E}}_i \) [6-7]. That is why all the Lorentz-like frequency dependences of a single particle polarization can be described by resonances’ fields \( \hat{\mathbf{E}}_i \) that can be found, for instance, by FEM and corresponding amplitudes \( A_i \) that are given by theory [6].
Thus, gathering these two observations we obtain self-consistent equation on induced polarization, which is a modified form of volume-integral equation method [8].

\[ \mathbf{P}(\mathbf{r}_i) = \tilde{\alpha} \left[ \mathbf{E}_{\text{ext}}(\mathbf{r}_i) + \sum_{j \neq i} \int \mathbf{G}(\mathbf{r}_i - \mathbf{r}_j) \mathbf{P}(\mathbf{r}_j) d^3\mathbf{r}_j \right] \]  

(1)

The equation (1) fully describes the structure. If it included sum over all cells, then it might have been easily reduced to a system of linear equations by application of Fourier method. In order to do that we have implemented a special filter that is equal to zero at the zero point and smoothly raises up to the unity on a distance of a lattice period. Therefore, application of this filter helps to make the equation homogeneous, but absolutely identical to the initial one. Moreover, we have managed to compose such a filter, that it is still possible to make a Fourier transform of a filtered Green function analytically, which is very important for efficient calculations.

After reducing to the system of linear equations it might be additionally simplified for small particles, which corresponds to dipole approximation. Indeed, small particles reradiate the most part of energy through dipole emission [9], which means that we need to account for only 3 degrees of freedom. Finally, we obtain the following system of equations on a total background electric field:

\[ \mathbf{E}_b = \mathbf{E}_{\text{ext}}(0) + \frac{2\pi^2 k_0^2}{S} \tilde{\alpha}_d \mathbf{D} \]  

(2)

where $S$ is the area of a cell, $k_0$ is a wavenumber in the vacuum, $\tilde{\alpha}_d$ is the polarizability tensor of an isolated particle (which can be expressed in resonant form), $\mathbf{D} = \mathbf{G}\mathbf{D}$ is a complex matrix which is fully determined by Green function, geometrical properties of a lattice and wave vectors of external incident waves. Finally, $\mathbf{E}_b$ is a total background field, which is a sum of an external one and a field induced by other particles. Also, it can be considered as $\mathbf{E}_b = \tilde{\alpha}_d^{-1}\mathbf{D}$, where $\mathbf{D}$ is a full dipole moment of a particle in the central cell. Thus, by solving this equation numerically, which is not a challenging task, we obtain the value of induced dipole moment. After that, we can easily calculate reemitted field which together with transmitted one forms the scattered field of a lattice.

In order to illustrate the operation of the developed script, we consider a square lattice of gold nanospheres of 20 nm radius in a medium with $\varepsilon_b = 10$. Period of the lattice is equal to 300 nm and gold is described by Drude model with the following parameters: $\omega_p = 1.34 \cdot 10^{16}$ s$^{-1}$, $\gamma = 1.09 \cdot 10^{14}$ s$^{-1}$, $\varepsilon_\infty = 8.5$. The projection of an incident wave’s wave vector on a lattice plane is directed along one of the lattice axis. From the figure 3, it is seen that coupling between nanoparticles leads to a significant bending of plasmonic resonance band.
3. Conclusion

In this work, we have constructed a theory, which makes it possible to calculate both polarization of resonant nanoparticles in a 2D lattice and their scattering matrix. In dipole approximation, this theory requires knowing of polarizability tensor, which might be calculated analytically, numerically using FEM or in any different way. Also, we propose to calculate this tensor in resonant approximation, which strongly accelerates all the calculations. The typical calculation time of scattering matrix turns out to be of an order of several milliseconds whereas full FEM calculations take at least several dozens of seconds, which is four orders of magnitude longer. Such speed paves the way to large-scale computations for purposes of design of optoelectronic devices and other photonic crystals based structures. Also, our method can be easily expanded on more useful and practical problems of a lattice placed on an interface between two layers and a lattice with a basis of several nanoparticles, which will be done in further studies.

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