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T-Matrix based Scattering Analysis of Photonic Materials with Periodicity in Different Dimensions

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Abstract. Optical devices and artificial photonic materials frequently make use of periodic arrangements of identical scatterers in 3D, 2D, and 1D, e.g. photonic crystals, meta-surfaces, or particle chains. To simplify their analysis, we present here a computational framework based on the T-matrix method that explicitly exploits spherical, cylindrical, and plane waves depending on the geometry and number of dimensions of the lattice. Due to the analytic properties of the chosen basis sets in combination with the use of Ewald's method for the lattice summation, we obtain an efficient framework to simulate such systems. The applicability will be illustrated at the conference by means of selected examples of contemporary interest.

Many designs for optical applications depend on periodic arrangements of individual scatterers. These designs can be a photonic crystal or metamaterial, where the underlying lattice is 3D, or a metasurface, which has a 2D lattice, or a particle chain with a 1D lattice.

Our approach to an efficient simulation method for such systems is the choice of a basis set for Maxwell's equations, that is adapted to the geometrical structure as close as possible. One prominent example for such a suiting basis set are the scattering properties of a sphere that are solved analytically in Mie theory using vector spherical waves (SWs). The approach from Mie theory can be generalized to the T-matrix method, such that calculations for arbitrary scatterers of finite size made from linear materials can be done [1]. If we build a 2D lattice from such scatterers, it is possible to calculate the mutual interaction of the particles with the T-matrix method. However, the effective response for a two-dimensional lattice is more conveniently described by vector plane waves (PWs) [2]. We find that there is a similar connection between a 1D lattice of scatterers described by SWs to an effective description by cylindrical waves (CWs) and a 1D lattice of CWs can be effectively described by PWs (see also fig. 1(a)-(c)). Thus, for each lattice dimension there is a basis set for an efficient description of its total response.

The efficiency of T-matrix based methods is partly due to the fact that the translation coefficients are analytically known [3]. This reduces the computation of the mutual interaction between multiple objects to simple linear algebra operations. For periodic arrangements, however, a notoriously slow converging lattice sum over the translation coefficients is necessary. This challenge can be met by using Ewald's method, where the sum is separated into a short-range and a long-range contribution which – individually – converge exponentially fast in real and reciprocal space, respectively [4]. With Ewald's method, adapted to the different lattice dimensions and the basis sets above, a wide range of optical system can be computed efficiently.

1 Plane, cylindrical, and spherical waves

All three basis sets can be derived by following a common procedure [5]. This solution is denoted by $\boldsymbol{M}_\nu(\boldsymbol{r})$ with the placeholder ν for the indices and it describes a transverse electric (TE) solution. A transverse magnetic (TM) solution is obtained by $\boldsymbol{N}_\nu(\boldsymbol{r}) = \frac{\nabla}{k} \times \boldsymbol{M}_\nu(\boldsymbol{r})$. The PWs are $\boldsymbol{M}_{\boldsymbol{k}}(\boldsymbol{r}) = \mathrm{i}\nabla \times (\hat{\boldsymbol{e}}_z \mathrm{e}^{\mathrm{i}\boldsymbol{kr}})/\sqrt{k_x^2 + k_y^2}$, the CWs are $\boldsymbol{M}^{(n)}_{k_z,m}(\boldsymbol{r}) = \mathrm{i}\nabla\times(\hat{\boldsymbol{e}}_z \mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}k_z z} Z^{(n)}_m(\sqrt{k^2 - k_z^2}\rho))/\sqrt{k^2 - k_z^2}$, and the SWs are $\boldsymbol{M}^{(n)}_{lm}(\boldsymbol{r}) = \mathrm{i}\nabla \times (\boldsymbol{r} Y_{lm}(\theta,\varphi) z^{(n)}_l(kr))$. For the PWs and the CWs the denominators assure a dimensionless basis function. We use $Z^{(n)}_l$ for the Bessel ($n = 1$) and Hankel ($n = 3$) functions of the first kind, $z^{(n)}_l$ for their spherical counterparts, and Y_{lm} for the spherical harmonics. All three solution sets include initially an infinite number of modes: PWs are defined by all wave vectors $\boldsymbol{k}$ that satisfy the dispersion relation, CWs are defined by $k_z \in \mathbb{R}$ and $m \in \mathbb{Z}$, and SWs are defined by $l \in \mathbb{N}$ and $m \in \mathbb{Z}$ with $|m| \leq l$. However, higher multipole or diffraction orders can be neglected by imposing a suitable threshold so that the solution space is restricted to a finite number of basis functions. The transition from the TE/TM basis to the helicity basis by defining $\sqrt{2}\mathbf{A}_{\pm,\nu}(\boldsymbol{r}) = \mathbf{N}_\nu(\boldsymbol{r}) \pm \mathbf{M}_\nu(\boldsymbol{r})$ facilitates the treatment of chiral materials and has also computational benefits over the TE/TM basis [2].

2 T-matrix for CWs and SWs in lattices

While usually defined for SWs, we present the T-matrix method here in a more general way that also applies to

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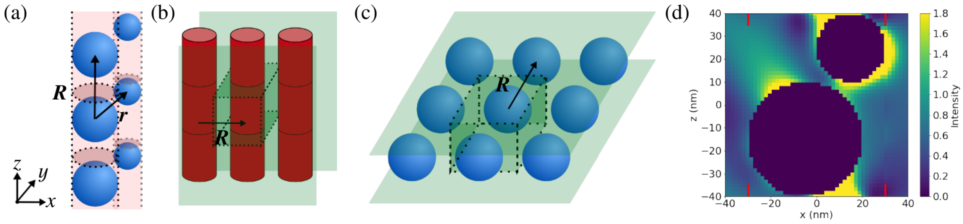

Figure 1. Panels (a) to (c) show the different possible layouts for transitions between SWs, CWs, and PWs which are color-coded in blue, green, and red. In each sketch one unit cell is highlighted. In panel (a) the unit cell contains two scatters. Panel (d) shows the simulated intensities for the arrangement in panel (a) under a PW illumination with along $(\sin\frac{\pi}{3}, 0, \cos\frac{\pi}{3})$ of negative helicity. The electric fields between the red marks are calculated directly with Ewald's method, outside it is much faster to use the efficient CW description. The lack of a discontinuity between these domains shows the accurate match of both approaches.

CWs. These two basis sets allow the electric field to be separated into an incident part $\boldsymbol{E}_{\text{inc}}(\boldsymbol{r}) = \sum_{\lambda,\nu} a_{\lambda,\nu}\boldsymbol{A}^{(1)}_{\lambda,\nu}(\boldsymbol{r})$ and a scattered part $\boldsymbol{E}_{\text{sca}}(\boldsymbol{r}) = \sum_{\lambda,\nu} p_{\lambda,\nu}\boldsymbol{A}^{(3)}_{\lambda,\nu}(\boldsymbol{r})$.

Thus, we can now write down the linear relationship between the incident and scattered mode coefficients, that each are placed in a vector, as $\boldsymbol{p} = \mathbf{T}\boldsymbol{a}$ with the T-matrix $\mathbf{T}$. A particular strength of the T-matrix method are the analytically known translation coefficients $C^{(3)}_{\nu',\nu}(\boldsymbol{r})$. We write the multi-scattering equation within a lattice as

$$\boldsymbol{p}_{i\alpha} = \mathbf{T}_i\left(\boldsymbol{a}_{i\alpha} + \sum_{j=1}^{N}\sum_{\beta}{}' \mathbf{C}^{(3)}(\boldsymbol{r}_{ij} + \boldsymbol{R}_{\alpha\beta})\boldsymbol{p}_{j\beta}\right) \quad (1)$$

where Latin indices i, j refer to N different particles within one unit cell and Greek indices α, β to different positions on the lattice. We now make the assumption that there is a constant phase difference along different positions on the lattice defined by $\boldsymbol{k}_\parallel$. Then, we can find the relation $\boldsymbol{a}_{i\alpha} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel\boldsymbol{R}}\boldsymbol{a}_{i0}$ for the incident and, analogously, for the scattered field. After rearranging eq. (1) slightly, we obtain

$$\left(\mathbb{1}\delta_{ij} + \mathbf{T}_i\sum_{j=1}^{N}\sum_{\beta}{}' \mathbf{C}^{(3)}(\boldsymbol{r}_{ij} + \boldsymbol{R}_{0\beta})\mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel\boldsymbol{R}_{0\beta}}\right)\boldsymbol{p}_{j0} = \mathbf{T}_i\boldsymbol{a}_{i0} \quad (2)$$

which is the regular multiple scattering equation for T-matrices with the exception of the lattice series $\sum_\beta C_{\nu',\nu}(\boldsymbol{r}_{ij} + \boldsymbol{R}_{0\beta})\mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel\boldsymbol{R}_{0\beta}}$. For both the CWs and the SWs these series can be solved for 1D, 2D, and 3D lattices by means of Ewald's method.

3 Transitions between basis sets

Besides the coupling between different cells of the lattice, where the Ewald summation is a key ingredient for an efficient computation, we need the expansion of the incident wave of a particular type into other types, e.g. expanding a CW into PWs. These properties can be summarized by $\boldsymbol{A}_{\pm,\boldsymbol{k}}(\boldsymbol{r}) = \sum_{m=-\infty}^{\infty} \mathrm{i}^m \mathrm{e}^{-\mathrm{i}m\varphi_k}\boldsymbol{A}^{(1)}_{\pm,k_z m}(\boldsymbol{r})$ and $\boldsymbol{A}^{(1)}_{\pm,k_z m}(\boldsymbol{r}) = \sum_{l=|m|}^{\infty} \mathrm{i}^{l-m} 4\pi\gamma_{lm} f_{\lambda,lm}(\theta_{\boldsymbol{k}})\boldsymbol{A}^{(1)}_{\pm,lm}(\boldsymbol{r})$ using $\gamma_{lm} = \sqrt{\frac{(2l+1)}{4\pi l(l+1)}\frac{(l-m)!}{(l+m)!}}$ and the function $f_{\pm,lm}(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}P_l^m(\cos\theta) \pm \frac{m}{\sin\theta}P_l^m(\cos\theta)$ with the Legendre Polynomial P_l^m. The transition from PWs to SWs can be obtained by combining both equations. As a last main ingredient we need the expansion of the scattered field in different basis sets which is more involved because it includes a lattice summation and is necessary, e.g. for the effective description of a chain of (SW-)T-matrices with a CW-T-matrix (fig. 1(a, d)). We make use of the integral representation of the scattered fields in combination with Poisson's formula to arrive at

$$\sum_\beta \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel\boldsymbol{R}_\beta}\boldsymbol{A}^{(3)}_{\lambda,lm}(\boldsymbol{r} - \boldsymbol{R}_\beta) = \frac{\pi\gamma_{lm}}{ak\mathrm{i}^{l-m}}\sum_\beta f_{\lambda,lm}(\theta_{\boldsymbol{k}+\boldsymbol{G}_\beta})\boldsymbol{A}^{(3)}_{\lambda,k_\parallel+G_\beta m}(\boldsymbol{r}) \quad (3)$$

$$\sum_\beta \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel\boldsymbol{R}_\beta}\boldsymbol{A}_{\lambda,k_z m}(\boldsymbol{r} - \boldsymbol{R}_\beta) = \frac{2}{ak\mathrm{i}^m}\sum_\beta \frac{\mathrm{e}^{\mathrm{i}m\varphi_{\boldsymbol{k}+\boldsymbol{G}_\beta}}\boldsymbol{A}_{\boldsymbol{k}+\boldsymbol{G}_\beta}(\boldsymbol{r})}{\sqrt{k^2 - k_z^2 - (\boldsymbol{k}_\parallel + \boldsymbol{G})^2}} \quad (4)$$

where $\boldsymbol{G}_\beta$ are reciprocal lattice vectors and a the lattice pitch. The transitions from SWs to PWs are possible by a combination of the results.

4 Conclusion

With the T-matrix method for lattices and Ewald's method from section 2 and the transitions between different basis sets from section 3 we can efficiently calculate the interaction of objects in a lattice and also have a description of the total response in the most suitable basis set. We implemented the sketched procedure in a program whose open source publication is in preparation.

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