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Multiple-Scattering T-Matrix Simulations for Nanophotonics: Symmetries and Periodic Lattices

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Abstract. The multiple scattering method T-matrix (MSTMM) can be used to solve the electromagnetic response of systems consisting of many compact scatterers, retaining a good level of accuracy while using relatively few degrees of freedom, largely surpassing other methods in the number of scatterers it can deal with. Here we extend the method to infinite periodic structures using Ewald-type lattice summation, and we exploit the possible symmetries of the structure to further improve its efficiency, so that systems containing tens of thousands of particles can be studied with relative ease. We release a modern implementation of the method, including the theoretical improvements presented here, under GNU General Public Licence.

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1 Introduction

The problem of electromagnetic response of a system consisting of many relatively small, compact scatterers in various geometries, and its numerical solution, is relevant to several branches of nanophotonics. In practice, the scatterers often form some ordered structure, such as metallic or dielectric nanoparticle arrays [12,29,61,70] that offer many degrees of tunability, with applications including structural color, ultra-thin lenses [28], strong coupling between light and quantum emitters [48,57,58], weak and strong coupling lasing and Bose-Einstein condensation [16,18,19,49,59,60,67,69], magneto-optical effects [27], or sensing [32]. The number of scatterers tends to be rather large; unfortunately, the most common general approaches used in computational electrodynamics are often unsuitable for simulating systems with larger number of scatterers due to their computational

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complexity: differential methods such as the finite difference time domain (FDTD, [56]) method or the finite element method (FEM, [46]) include the field degrees of freedom (DoF) of the background medium (which can have very large volumes), whereas integral approaches such as the boundary element method (BEM, a.k.a the method of moments, MOM [21, 40, 51]) need much less DoF but require working with dense matrices containing couplings between each pair of DoF. Therefore, a common (frequency-domain) approach to get an approximate solution of the scattering problem for many small particles has been the coupled dipole approximation (CD) [68] where a drastic reduction of the number of DoF is achieved by approximating individual scatterers to electric dipoles (characterised by a polarisability tensor) coupled to each other through Green's functions.

CD is easy to implement and demands relatively little computational resources but suffers from at least two fundamental drawbacks. The obvious one is that the dipole approximation is too rough for particles with diameter larger than a small fraction of the wavelength, which results to quantitative errors. The other one, more subtle, manifests itself in photonic crystal-like structures used in nanophotonics: there are modes in which the particles' electric dipole moments completely vanish due to symmetry, and regardless of how small the particles are, the excitations have quadrupolar or higher-degree multipolar character. These modes, belonging to a category that is sometimes called *optical bound states in the continuum (BIC)* [22], typically appear at the band edges where interesting phenomena such as lasing or Bose-Einstein condensation have been observed [16, 18, 19, 45, 67] – and CD by definition fails to capture such modes.

The natural way to overcome both limitations of CD mentioned above is to take higher multipoles into account. Instead of a polarisability tensor, the scattering properties of an individual particle are then described with more general *transition matrix* (commonly known as *T*-matrix), and different particles' multipole excitations are coupled together via translation operators, a generalisation of the Green's functions used in CDA. This is the idea behind the *multiple-scattering T-matrix method* (MSTMM), a.k.a. *superposition T-matrix method* [34], and it has been implemented many times in the context of electromagnetics [52], but usually only as specific codes for limited subsets of problems, such as scattering by clusters of spheres, circular cylinders, or Chebyshev particles [9, 35, 36, 66]; there also exists a code for modeling photonic slabs including 2D-periodic infinite arrays of spheres [54, 55]. From the rather rare examples in this field of publicly available codes with clear public licence and without proprietary dependences we point out FaSTMM [37, 38], which has been perhaps the most general MSTMM software with respect to the system geometry for particle ensembles with homogeneous background, and SMUTHI [7, 8] for dealing with finite ensembles of particles in a layered medium.

However, the potential of MSTMM reaches far beyond its past implementations. Here we present several enhancements to the method, which are especially useful in metamaterial and nanophotonics simulations. We extend the method on infinite periodic lattices (in all three possible dimensionalities) using Ewald-type summation techniques. This enables, among other things, to use MSTMM for fast solving of the lattice modes of such