On the correct form of optical force density

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We follow the procedure proposed by Ref.[1] to derive the correct form of optical force density for two-dimensional metamaterial systems. We use a mesoscopic lattice model as a numerically accurate reference, and compare its results with those obtained from an macroscopic effective media model using two different stress tensors. We show that only the Helmholtz stress tensor is able to give the just answer.

CONTENTS

I. INTRODUCTION

When studying metamaterial, it is almost always assumed that effective medium parameters provide sufficient information to determine the light-matter interaction. However, recent studies[2][3] have shown that when calculating infernal force density, one needs to carefully choose a specific stress tensor, or the effective medium would be misleading.

The debate between the correctness of the Minkowski or the Abraham tensor[4] has been on for nearly a century, and in recent years we are finally approaching its essence. Generally, when we go beyond the original Maxwell equations and obtained derived quantities by substituting one equation into another, one needs to be cautious of the risk of losing information about the system. In our case, we are able to show that the Maxwell tensor has discarded the system's electrostrictive properties, and calculations based on it results in a wrong distribution of force density.

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II. COMSOL MODEL SETUP

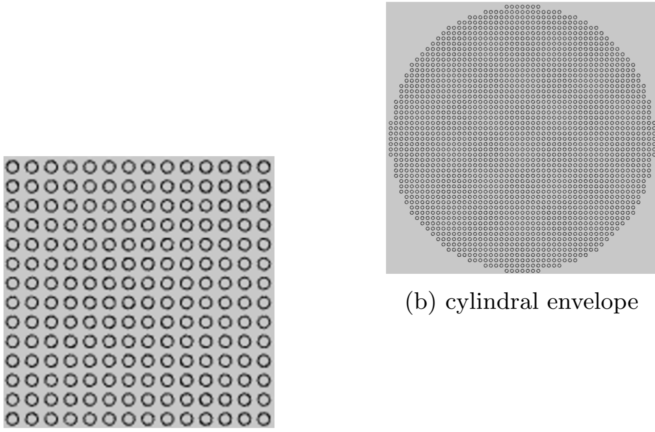
We are now trying to show the difference between force density in effective medium and its counterpart in the real lattice structure, which will lead to some illuminating results. The model under consideration is a kind of two-dimensional metamaterial consisting of an array of dielectric cylinders made from uniform electric permittivity and permeability ($\epsilon_r = 8, \mu_r = 1$).

The theory used in this work involves Multipole Scattering Theory (MST), Effective Medium Theory (EMT) and stress tensor derived from virtual force principle. Firstly, we use MST to derive the dispersion relation in the lattice structure which means the relation between bloch vector and the frequency of the incident electromagnetic wave. The block vector is, indeed , the effective vector that we will use to derive the effective permittivity. And then, we will use EMT to derive the effective permittivity, which turns out to be almost the same. Thirdly, we will use COMSOL[5] to calculate the exact field in the lattice structure as well as that of the effective medium. The incident waves include Ez polarization and Hz polarization(or TM and TE wave equivalently). Finally, we will use Maxwell tensor to calculate the force exerted on every single cylinder inclusion in real lattice structure and effective medium, and compare the result to force calculated using Helmholtz tensor using effective medium formalism.

The model now under consideration is a naïve two dimensional system made up of dielectric cylinders arranged in square lattice (See Fig. 1a) with the lattice constant $a = 10^{-8}$ m. The small circles represent dielectric cylinders, with uniform electric permittivity and permeability (($\epsilon_r = 8, \mu_r = 1$)). The overall shape of the cylinder array is a big circle, that is a big cylinder with infinite length (See Fig. 1b).

III. MULTIPLE SCATTERING THEORY

MST is a systematic method to derive the dispersion relation in the lattice structure. Its main idea is to take into consideration the wave scattered by every scatterer and thus figure out the eigenmode of the system by solving a secular equation determined by the boundary con-



(a) square lattice

(b) cylindral envelope

FIG. 1: Lattice structure

dition (which is the Mie coefficient in the system of dielectric cylinders). Graf's addition theorem also play an important role in collecting all the scattered wave as it enables us to write the complex amplitudes (b^q) of scattered waves from all the other cylinders ($Q \neq P$) as the complex amplitude of scattered wave (b^p) from cylinder P. Moreover, the coefficient derived using Graf's addition theorem lead to the lattice sum, which is another crucial quantity in the application of MST. We adopt the formalism and the notations of the a reference article[6].

Consider a SINGLE cylinder P first. The incident wave on P can be written as

$$E_z^{\text{in}}\left(\vec{r}_p\right) = \sum_m a_m^p J_m\left(k_0 r_p\right) e^{im\theta_p}$$

with J representing Bessel Function, $\overrightarrow{r_p} = (r, \theta_p)$ in polar coordinates representing a vector originating from scatter P and k_0 representing the wave vector in vacuum. While the scattered wave is

$$E_z^{\text{sca}}\left(\vec{r}_p\right) = \sum_m b_m^p H_m^{(1)}\left(k_0 r_p\right) e^{im\theta_p}$$

Then we consider the scattered waves from all the other cylinders except P, which are

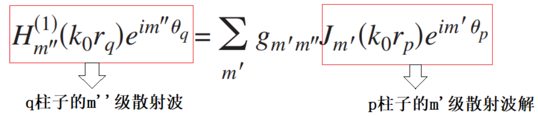
$$\vec{u}_p^{\text{in}}\left(\vec{r}_p\right) = \sum_{q\neq p}\sum_{m''} b^q_{m''} H^{(1)}_{m''}\left(k_0 r_q\right) e^{im''\theta_q}$$

Introduce the reciprocal vector

$$\overrightarrow{R_q} = \overrightarrow{r_p} - \overrightarrow{r_q}$$

And apply the Graff's addition theorem to write the outgoing scattered wave from cylinder Q of order m$''$ in terms of the sum of scattered wave from cylinder Q of order m$'$ multiplied by a coefficient $g_{m'm_0''}$
where

$$g_{m'm''} = H^{(1)}_{m'-m''}\left(k_0 R_q\right) e^{i\left(m''-m'\right)\Theta_q}$$



apply bloch's theorem and we will get

$$b^q{}_{m''} = b^q{}_{m''} e^{i\ \text{K}_{\text{eff}}\cdot R_q}$$

K_{eff} which shows up in the exponential term represents the periodic change of scattered amplitude induced by the space translational symmetry of the lattice field. The approach is actually an analogy of method used in dealing with electron's wave function in metallic material.

And this leads directly to the lattice sums

$$S_{m'-m''} = \sum_{q\neq p} g_{m'm''} e^{iK_{\text{eff}}\cdot R_q}$$

Then apply the boundary condition of cylinder P

$$b_m^p = \sum_{m'} t_{mm'} a_{m'}^p$$

Consider the incident wave, scattered waves from $Q \neq P$ together, and we will get

$$b_m^p = \sum_{m'} t_{mm'}\left(a_{m'}^p + \sum_{q\neq p}\sum_{m''} g_{m'm''} b^q_{m''}\right)$$

where

$$t_{mm'} = D_m \delta_{mm'}$$

and the Mie coefficient D_m

$$D_m = \frac{\mu_0 k_s J_m\left(k_0 r_s\right)\left(\left.\frac{\partial J_m(\phi)}{\partial\phi}\right|_{\phi=k_s r_s}\right) - k_0\mu_s J_m\left(k_s r_s\right)\left(\left.\frac{\partial J_m(\phi)}{\partial\phi}\right|_{\phi=k_0 r_s}\right)}{k_0\mu_s J_m\left(k_s r_s\right)\left(\left.\frac{\partial H_m^{(1)}(\phi)}{\partial\phi}\right|_{\phi=k_0 r_s}\right) - \mu_0 k_s H_m^{(1)}\left(k_0 r_s\right)\left(\left.\frac{\partial J_m(\phi)}{\partial\phi}\right|_{\phi=k_s r_s}\right)}$$

Drop the incident term $a_{m'}^p$, since we are now trying to find the eigenmode, then we will get the secular equation

$$\det\left|\sum_{m'} t_{mm'}\sum_{q\neq p} g_{m'm''} e^{i\bar{K}\cdot\vec{R}_q} - \delta_{mm''}\right| = 0$$

All we need to do now is to compute the lattice sum until it converges and solve the secular equation and the outcome will the dispersion relationship

$$K_{\text{eff}} \sim \omega$$

which is exactly what we want to describe the effective medium

$$\epsilon_{\text{eff}} = \left(\frac{K_{\text{eff}}}{k_0}\right)^2$$

IV. EFFECTIVE MEDIUM THEORY

The E_z polarization there is a well know result that according to the Maxwell Garnett Relation, we can derive that $\epsilon_{\text{eff}} = \epsilon_0 + p\epsilon_0\chi_e$, which means $\epsilon_{\text{eff}} = \epsilon_0 + p(\epsilon_s - 1)$ in the lattice field. Here p represent the filling rate, which is $p = 0.283$ in the current case. Thus we get $\epsilon_{\text{eff}} = 2.97$, which exactly matches with the result derived from MST. While for H_z polarization EMT gives $\epsilon_{\text{eff}} = 1.57$.

V. MAXWELL TENSOR AND HELMHOLTZ TENSOR

Maxwell tensor is a well-known result in classical electrodynamics, since now we are considering the time average of the force, we can safely drop the term of intrinsic electromagnetic momentum in the volume under consideration (which averages out at zero). Thus the electromagnetic force exerted on a single cylinder could be written as

$$\vec{f}(i,j) = \oint_{\mathrm{C}} \overleftrightarrow{T} \cdot d\vec{l}$$

where T stand for

$$\begin{aligned} T_{\text{Maxwell },ik} =& \frac{1}{2}\operatorname{Re}\left[\varepsilon_0 E_i E_k^* - \frac{1}{2}\varepsilon_0 E^2 \delta_{ik} \right. \\ & \left. + \mu_0 H_i H_k^* - \frac{1}{2}\mu_0 H^2 \delta_{ik}\right] \end{aligned}$$

$$\begin{aligned} T_{\text{Helmholt },ik} =& \frac{1}{2}\operatorname{Re}\left[\varepsilon_0\varepsilon_{\mathrm{r}} E_i E_k^* - \frac{1}{2}\varepsilon_0\left(\varepsilon_{\mathrm{r}}\delta_{ik} + \frac{\partial\varepsilon_{\mathrm{r}}}{\partial u_{ik}}\right)E^2 \right. \\ & \left. + \mu_0 H_i H_k^* - \frac{1}{2}\mu_0 H^2 \delta_{ik}\right] \end{aligned}$$

Furthermore, the procedure of line intergral actually represent the opreation of average over the volume of every single cylinder, and thus comes the “force density”.

VI. SIMULATION RESULTS

We utilizes a comercial software package COMSOL to build the lattice model and the effective medium model and calculate the field distributions throughout the lattice using the wave optics module. Based on which, we calculate the values of the non-trivial components of the Maxwell and the Helmholtz tensors.

The two figures, Fig. 2 and Fig. 3, both consist of 6 subfigures. The first row is retrieved from the square lattice model, where both tensors give the same results as there’s only vacuum between cylindrals. This is considered to be the accurate numerical force density of the lattice, and is used as a reference to be compared with the rest of the subfigures. The model we use is composed of approximately 2000 cylinders, and with each pixel of the subfigure, we perform a numerical integration around a cuboid column that contains the cylinder. The so called “force density” here is actually the total force acting on a cylinder, as it’s relatively a small piece in the effective medium. The second and third column is obtained with similar manner. The integration is done at the exact same coordinates with the first column, only replacing the model from a square lattice model to the effective medium one.

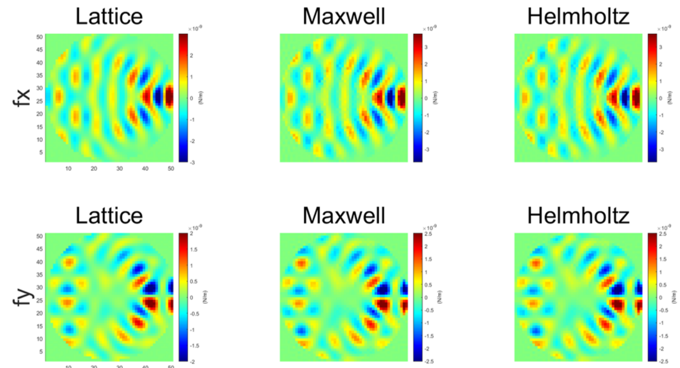


FIG. 2: E_z polarization. Both tensors give the same results.

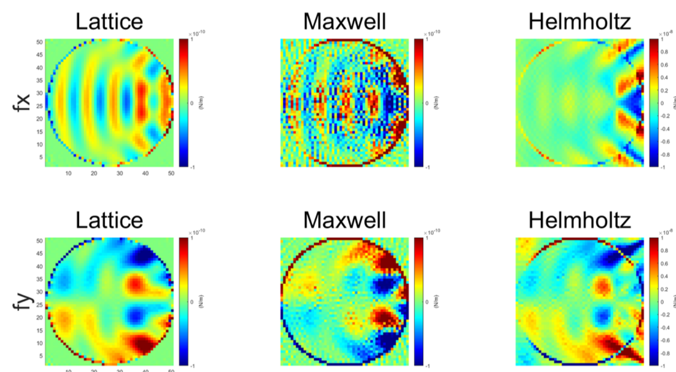


FIG. 3: H_z polarization. The results obtained from the Maxwell tensor deviates from the correct ones, whereas the Helmholtz tensor is still able to provide appropriate force density distributions.

It’s worth noticing that COMSOL doesn’t feature conducting arrays of integrations, so this tedious process is actually done by hand-written python numerical integration.

Additionally, we conducted a comparison between the fine shape (or phase) of the electromagnetic field of the two models by plotting the following term:

$$\frac{\operatorname{Norm}[E_{\text{lattice }}]}{\operatorname{Max}[\operatorname{Norm}[E_{\text{lattice }}]]} - \frac{\operatorname{Norm}[E_{\text{effective }}]}{\operatorname{Max}[\operatorname{Norm}[E_{\text{lattice }}]]}$$

The term describes the proportion of the E field at a certain point to the maximum value of E in the lattice, and reflects the local responses that is neglected by K_{eff} .

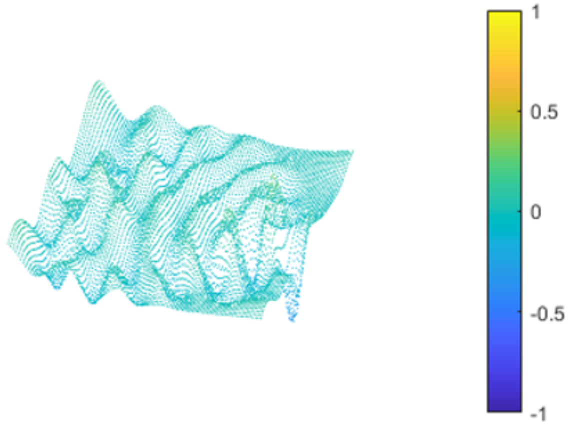


FIG. 4: Comparison of E field proportion between the two models. It shows that the effective medium model fails to grasp the local responses that exist in the lattice model.

VII. SUMMARY AND OUTLOOK

In this work, we mainly followed a passage shown in the reference. Our main focus is on the difference between the lattice field and its counterpart in the effective medium. Using force density as a property to examine it, we have shown that in the long-wave limit, the EMT does well describe the behavior of TM wave, while it fails when it comes to the TE wave. An important reason is that we set μ_r=1, which means that there will be no dipole term or higher term of response in the lattice field. When it comes to the TE wave, the situation is totally different ($\epsilon_r \neq 1$) due to the higher order response.

When comparing the difference between the periodicity of lattice structure and effective medium, we can see that they are almost the same in the large scare while there are bumps in a rather small scale. In fact, a simple understanding of this effect is that the effective medium gives the effective phase change required by the traveling of wave and thus produce a field highly similar to that of the real lattice structure. The information of the local effect of lattice field, however, is lost in the formalism of EMT, which is also why we failed to describe the force density correctly using the field given by the effective medium. And this matches with our previous explanation of EMT's failure in the context of the TE wave. We shall also point out that our lattice structure is a try to relate the macroscopic property with the microscopic property. Thus we use cylinders of uniform permittivity and permeability inclusion as an alternative to calculating the real field of molecules and atoms.

AUTHOR CONTRIBUTIONS

T.S.-H. conducted the numerical simulation, programming, and data post-processing. J.C.-L. conducted the theoretical analysis, and calculated the lattice band structure via Mathematica. T.S.-H. and J.C.-L. wrote the paper and the PPT together. L.-Z. supervised the project.

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