Calculation of Effective Material Parameters by Field Averaging Over Lattices with Non-Negligible Unit Cell Size

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Abstract

The Pendry *et al*. field averaging method for calculation of effective material parameters is reviewed and its limits explored. The method is then extended so that it can accurately calculate the effective material parameters of lattices where the unit cell size is appreciable but still quasistatic ($d \sim 0.1\lambda_0$). The new algorithm is verified by calculating the effective material properties of periodically placed particles suspended in free space, as the unit cell size becomes appreciable. Results of our proposed formulation are then compared with the Pendry *et al*. and conventional volumetric averaging algorithms.

1. Introduction

Artificial materials for electromagnetic and optical applications typically consist of lattices of dielectric or metal inclusions of various shapes and sizes [1]. Many inclusion geometries such as dielectric spheres, metal cylinders, swiss rolls, and split-ring resonators have been investigated for their unique electromagnetic behaviors. Successful use of these materials hinges on the accurate calculation of the effective permittivity ε_{eff} and permeability μ_{eff} of the material.

The effective parameters of lattices can be calculated using a plurality of methods that have been proposed over the years (see, e.g., [2-5]). In the quasistatic regime, when the size d of the unit cell of a lattice is small compared to the operating wavelength, $d << \lambda$, and the inclusion volume is small, it is possible to calculate the effective permittivity and permeability of the lattices based on the Maxwell Garnett formula [6]. However, beyond the quasistatic regime and for high inclusion volume geometries one has to use more sophisticated approaches.

One often used method to compute effective material parameters both in the lab and from computational data is to equate the scattering parameters of a plane wave incident on a finite thickness slab to the scattering parameters of an equivalent transmission line problem [7]. In the lab, free space measurement systems are used to measure such scattering parameters and computationally such problems can be solved trivially. However, contemporary work on artificial materials has focused on periodic materials that have lattice constants that are in the $0.05\lambda_0$ to $0.4\lambda_0$ range and are only a few layers thick in the direction of wave propagation. Calculation of effective material parameters from such geometries using transmission line equivalent problems is very difficult at best. As identified by others, periodic materials cannot be exactly modeled by a single section of homogeneous transmission line [8,9]. Near the edges of a finite thickness slab the truncation of the lattices cause the particles near the truncation to polarize differently than those in an infinite lattice. This edge effect results in both spatially varying and inherently anisotropic material parameters near the edge of the slab. To mitigate the effect this problem has on the calculated effective material problems one could create a finite thickness slab that is many cells thick in an attempt to average out the edge effect. However, this does not completely eliminate the error caused by the only approximate transmission line model and results in an unknown and unpredictable amount of inherent error in the calculated effective material parameters.

To avoid the inherent error of transmission line models, we instead chose to investigate methods of calculating effective materials using only the information contained within a single unit cell away from the lattice edges where the local electromagnetic behavior is nearly identical to that of the behavior of an infinite lattice. One particularly appealing method in the literature is proposed by Pendry *et al*. [5]. In the proposed method, effective material parameters of periodic materials are calculated using only the local E, D, H, and B fields averaged over unit cells. The average values of D and B fields are defined as surface integrals of the local field values while the averages of E and H fields are defined as line integrals of the local fields. These local fields can be obtained by numerically solving the corresponding boundary-value problem for Maxwell's equations with an appropriate solver.

Though this approach has been previously reported to give good results for lattices of some types, the proposers of the Pendry *et al.* method have identified two serious problems with the method [10,11]. First, it is only rigorously valid in the quasistatic limit and returns increasingly inaccurate material parameters as the size of the unit cell increases. Second, beyond the quasistatic limit it returns complex material parameters for lossless problems.

To eliminate these problems, we are proposing a modification to the Pendry *et al*. method. Our modification is based on using surface averages instead of line averages for the definition of the averaged electric and magnetic fields.

In this paper, we first briefly discuss the Pendry *et al.* method and its limitations. Next our modification to the Pendry *et al.* method is described and how it is applied. We then apply the Pendry *et al.* method, our proposed modified

method, and the conventional volume averaging method to three periodic materials consisting of (a) free space, (b) dielectric spheres, and (c) dielectric cubes. Lastly, we report the accuracy of the Pendry *et al.* method and our proposed modified method.

2. Pendry *et al.* and modified averaging methods

According to Pendry *et al.*, the effective permittivity and permeability tensors of a lattice of inclusions can be calculated as [10,11]

$$(\varepsilon_{\text{eff}})_{ij} \equiv \frac{\langle D_i \rangle_S}{\langle E_j \rangle_L}, \qquad (\mu_{\text{eff}})_{ij} \equiv \frac{\langle B_i \rangle_S}{\langle H_j \rangle_L} \tag{1}$$

where F_i is the i th component of the respective field ($F = E, D, H, B$) and the averages $\langle F_i \rangle_S$, $\langle F_i \rangle_L$ are defined as surface and line integrals

$$\langle F_i \rangle_S \equiv \frac{1}{S} \iint_S F_i dS, \tag{2}$$

$$\langle F_i \rangle_L \equiv \frac{1}{L} \int_L F_i dL \tag{3}$$

with specific integration surface S and integration path L. The latter is designated along one of the edges of the unit cell and the surface S is designated as one of the cell's faces as illustrated in Fig. 1.

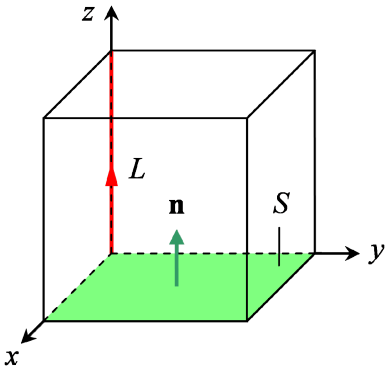

Figure 1: The integration surface S and integration path L used in Eqs. (2)-(3) to calculate the average values of z-components of the fields. For x- and y-components, both the line L and the surface normal **n** must be in the respective directions.

Eqs. (1)-(3) play a central role in the Pendry *et al.* averaging method. They define how to calculate the effective permittivity and permeability tensors ε_{eff} and μ_{eff} if the local distributions of all the fields E, D, H, and B are known. The distributions of E and H fields can be obtained by numerically solving the respective boundary value problem with a full wave solver. The distributions of D and B fields can then be calculated from those of E and H fields by using the constitutive relations

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}, \qquad \mathbf{B} = \mu_0 \mu_r \mathbf{H},$$

with $\varepsilon_0 = 8.85 \times 10^{-12}$ F/m and $\mu_0 = 4\pi \times 10^{-7}$ H/m being the permittivity and permeability of free space and ε_r and μ_r are the local *relative* permittivity and permeability within the unit cell.

Note the following advantages of the Pendry *et al.* method:

i) it only utilizes local field information and thus simulations can be created that have little or negligible edge effect problems;
ii) the field quantities used in the method can be easily calculated using an appropriate commercial software.

However, the Pendry *et al.* method also has the following limitation: it is only correct, strictly speaking, in the quasistatic case. For lattices with an appreciable unit cell size, it provides a poor description of their effective parameters [10,11].

As an illustration, we calculated, based on Eqs. (1)-(3), the effective parameters of a lattice of empty cells with non-negligible unit cell size when compared to the wavelength of the incident wave. The local field data sets used in Eqs. (2)-(3) were obtained from *CST Microwave Studio Suite* by simulating the propagation of a plane wave incident normally onto a slab of free space. The slab was split into simple cubic cells (SCCs) of cell size d. The total thickness of the slab was 9 unit cells and the necessary field calculations were performed on the unit cell at the center of the slab. The time domain solver was used to calculate the numerical results and was set to terminate after the energy of the system had run down to -80 dB. Automatic meshing of the geometry was set to 50 lines per wavelength (convergence of this and the geometries discussed later in this paper were verified but are not shown here). Once calculated, post processing templates within the software were used to calculate the necessary line and surface averages. Ratios of the averaged quantities were finally used to calculate the effective material parameters. The calculation results for both the real and imaginary parts of the relative values $\varepsilon_{\text{eff},r} \equiv \varepsilon_{\text{eff}} / \varepsilon_0$ and $\mu_{\text{eff},r} \equiv \mu_{\text{eff}} / \mu_0$ of ε_{eff} and μ_{eff} as functions of the unit cell size are presented in Fig. 2 (red dashed curves).

As seen from Fig. 2(a), the calculated values of the real parts $\varepsilon'_{\text{eff},r} \equiv \text{Re}\,\varepsilon_{\text{eff},r}$ and $\mu'_{\text{eff},r} \equiv \text{Re}\,\mu_{\text{eff},r}$ progressively diverge away from the value $\varepsilon'_r = \mu'_r = 1$ of free space as the unit cell size increases from $d/\lambda_0 = 0$ to approx. 0.7 and then converges in an oscillating manner to a final value of $\varepsilon'_{\text{eff},r} = \mu'_{\text{eff},r} = 0$. A similar oscillating behavior is observed for the imaginary parts $\varepsilon''_{\text{eff},r} \equiv \text{Im}\,\varepsilon_{\text{eff},r}$ and $\mu''_{\text{eff},r} \equiv \text{Im}\,\mu_{\text{eff},r}$, as seen in Fig. 2(b). Conversely, and purely coincidentally because of the loss free geometry, the final value of calculated $\varepsilon''_{\text{eff},r}$ and $\mu''_{\text{eff},r}$ coincides with the true value $\varepsilon''_r = \mu''_r = 0$ for vacuum.

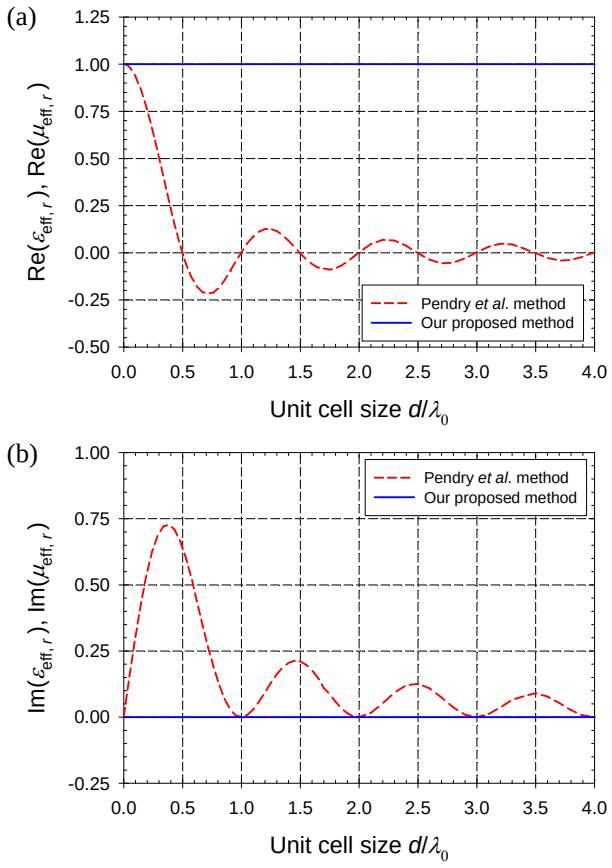

Figure 2: Computed (a) real and (b) imaginary parts of the relative effective permittivity and permeability of free space considered as a lattice of empty cells.

Dependence of the error in the real part of the computed permittivity value $\Delta \equiv (\varepsilon_0 - \varepsilon'_{\text{eff}})/\varepsilon_0$ on the unit cell size d is presented in Fig. 3. As seen from the plot, even at $d/\lambda_0 = 0.2$, where one might expect the Pendry *et al.* method to give quite satisfactory results, the calculated value of $\varepsilon'_{\text{eff}}$ of free space contains an error approximately 25%.

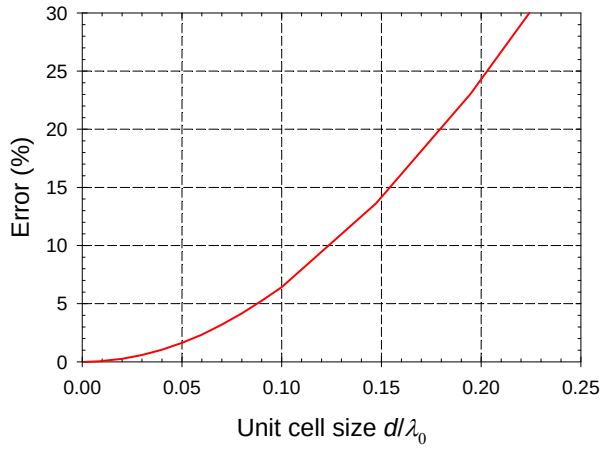

Figure 3: The error in the effective permittivity of free space computed by Pendry *et al.* method.

The discrepancy between the calculated and true values of ε_{eff}, μ_{eff} of free space has been explained [10,11] as caused by the spatial variation of the electric and magnetic fields of the incident wave over large enough unit cells. Due to this variation, the effective parameters of free space calculated from Eqs. (1)-(3) become [10]

$$\varepsilon_{\text{eff}} = \varepsilon_0 \frac{\exp(ikd)-1}{ikd}, \qquad \mu_{\text{eff}} = \mu_0 \frac{\exp(ikd)-1}{ikd}, \tag{4}$$

with their real parts [11]

$$\varepsilon'_{\text{eff}} = \varepsilon_0 \frac{\sin(kd)}{kd}, \qquad \mu'_{\text{eff}} = \mu_0 \frac{\sin(kd)}{kd}, \tag{5}$$

and imaginary parts

$$\varepsilon''_{\text{eff}} = \varepsilon_0 \frac{1-\cos(kd)}{kd}, \qquad \mu''_{\text{eff}} = \mu_0 \frac{1-\cos(kd)}{kd}, \tag{6}$$

where k is the wave number of the incident wave propagating along one of the lattice's axis. The oscillating behavior of both the real and imaginary parts of ε_{eff} and μ_{eff} as functions of the unit cell size d, which is predicted by analytical expressions (5)-(6), is exactly what is observed in our numerical results shown in Fig. 2.

It should be mentioned that the calculation of ε_{eff} and μ_{eff} of a lattice of empty cells was performed, within the Pendry *et al.* averaging method, for the first time in [10] and then repeated in [11]. However, the expressions (6) for the imaginary parts $\varepsilon''_{\text{eff}}$, μ''_{eff} are not given explicitly in either of these works.

Formally, the difference between $(\varepsilon_{\text{eff}}, \mu_{\text{eff}})$ and (ε_0, μ_0) is due to the oscillating factors appearing in Eqs. (4)-(6). To match the values of $(\varepsilon_{\text{eff}}, \mu_{\text{eff}})$ calculated by the Pendry *et al.* method to the values (ε_0, μ_0) of free space, it has been proposed [10,11] to simply remove the respective phase factors $[\exp(ikd)-1]/(ikd)$ or $\sin(kd)/(kd)$ from Eqs. (4)-(5). However, such "handmade correction" is valid for only the case of empty cells considered here. For the general case of non-empty cells with arbitrary inclusions it is still not clear what is the "phase factor" that has to be eliminated from the calculation results to obtain correct values of ε_{eff}, μ_{eff}.

Since at large enough d/λ values the line integral definition (3) for the average E and H fields cannot take into account the phase variation of the fields over the unit cells in the direction of wave propagation, we propose to modify the Pendry *et al.* method in order to automatically account for the variation. Namely, we propose the use of surface averages for E and H fields instead of the line averages (3). Accordingly, Eqs. (1) are replaced by

$$(\varepsilon_{\text{eff}})_{ij} \equiv \frac{\langle D_i \rangle_S}{\langle E_j \rangle_{S'}}, \tag{7}$$

$$(\mu_{\text{eff}})_{ij} \equiv \frac{\langle B_i \rangle_S}{\langle H_j \rangle_{S'}}, \tag{8}$$

where the surface averages $\langle E_j \rangle_{S'}$, $\langle H_j \rangle_{S'}$ are calculated similarly to Eq. (2) but now over the surface S' selected as explained in Fig. 4. Note that our modified definitions for the averages of E and H in Eqs. (7)-(8) do not compute the average value normal to the plane as used in the definitions for the average electric or magnetic flux densities. Rather, it calculates the average tangential value in the i th direction over the plane S'.

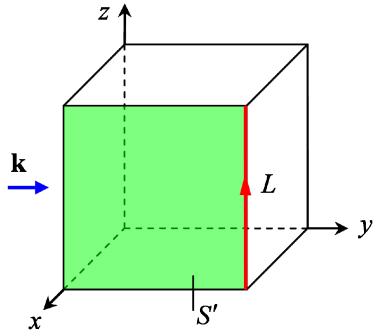

Figure 4: The integration surface S' used in Eqs. (7)-(8) to calculate the average values of z -components of E and H fields. For the other two components, surface S' is defined by the respective axis and the wave vector **k** of the incident wave.

Our approach can be proven rigorously [12] in the static approximation based on conventional volumetric averaging [13]

$$(\varepsilon_{\text{eff}})_{ij} \equiv \frac{\langle D_i \rangle_V}{\langle E_j \rangle_V},$$

$$(\mu_{\text{eff}})_{ij} \equiv \frac{\langle B_i \rangle_V}{\langle H_j \rangle_V},$$

$$\langle F_i \rangle_V \equiv \frac{1}{V}\iiint_V F_i dV,$$

(V is the entire volume of the unit cell under investigation) and first principles—the general properties of the static electric and magnetic fields as described by Maxwell's integral equations

$$\oint_C \mathbf{E}\cdot d\mathbf{l} = 0,$$

$$\oint_C \mathbf{H}\cdot d\mathbf{l} = \mathbf{J},$$

$$\oiint_S \mathbf{D}\cdot d\mathbf{S} = Q_{\text{free}},$$

$$\oiint_S \mathbf{B}\cdot d\mathbf{S} = 0,$$

($\mathbf{J}$ and Q_{free} being the current density and total free charge enclosed by the contour C and surface S, respectively) as well as periodicity of all the fields in an infinite lattice. Moreover, in the static limit our proposed method turns to be identical to the Pendry *et al.* method due to [12]

$$\langle E_i \rangle_L = \langle E_i \rangle_{S'},$$

$$\langle H_i \rangle_L = \langle H_i \rangle_{S'}.$$

However, as the unit cell size increases, our approach provides more accurate results for lattices of larger unit cell size in the region of d/λ_0 values where the Pendry *et al.* method fails.

To illustrate the advantages of our modified method, we first calculated, based on Eqs. (7)-(8), the effective parameters of free space. The results are presented in Fig. 2 by the blue solid curves. As seen from Fig. 2, our approach returns correct results for ε_{eff} and μ_{eff} of free space regardless of the unit cell size. Such perfect agreement between these calculated and theoretical results is a unique case and will not generalize to any other unit cell geometry. Generally, our proposed method will give only approximate values of the effective parameters, but far more accurate than the Pendry *et al.* method.

Lastly, the very concept of the effective parameters is questionably applicable to lattices with unit cells that are of the order of the wavelength of incident waves. Therefore, as the unit cell size becomes too large it should be expected that our averaging method will also fail.

3. Numerical results and discussion

To further investigate the validity of our proposed method, we have applied it to simple cubic lattices of dielectric spheres and cubes. For comparison, we have also implemented the Pendry *et al.* method as well as the rigorous volume averaging method. While volume averaging as defined above may appear to be an appealing method, it becomes very difficult to implement once highly conducting materials are added to the unit cell design due to the polarization of the conducting object. However, since we are only dealing with dielectric materials here it provides highly accurate data to compare with our proposed method.

3.1. Dielectric spheres

A simple cubic lattice of dielectric spheres with a volume fill factor of 0.3 and relative permittivity of 8 was modeled and its effective permittivity was computed. The real and imaginary components of the effective permittivity are shown in Fig. 5. As seen from the data, our proposed method returns nearly identical effective permittivity parameters as the volume averaging method up to a unit cell size of 0.3 free space wavelengths. In contrast, the Pendry *et al.* method immediately diverges away. To quantify the divergence of both our proposed method and the Pendry *et al.* method away from the volume averaging method, we have computed the difference between the computations and normalized the resulting difference to that of the volume averaging method, $\Delta \equiv \left|(\varepsilon_{\text{eff},V} - \varepsilon_{\text{eff}})/\varepsilon_{\text{eff},V}\right|$. This divergence is shown in Fig. 6 and is plotted in percent. As seen from the plot, the Pendry *et al.* method incurs significant error (up to approx. 210% at $d/\lambda_0 = 0.3$) while our proposed method incurs little error.

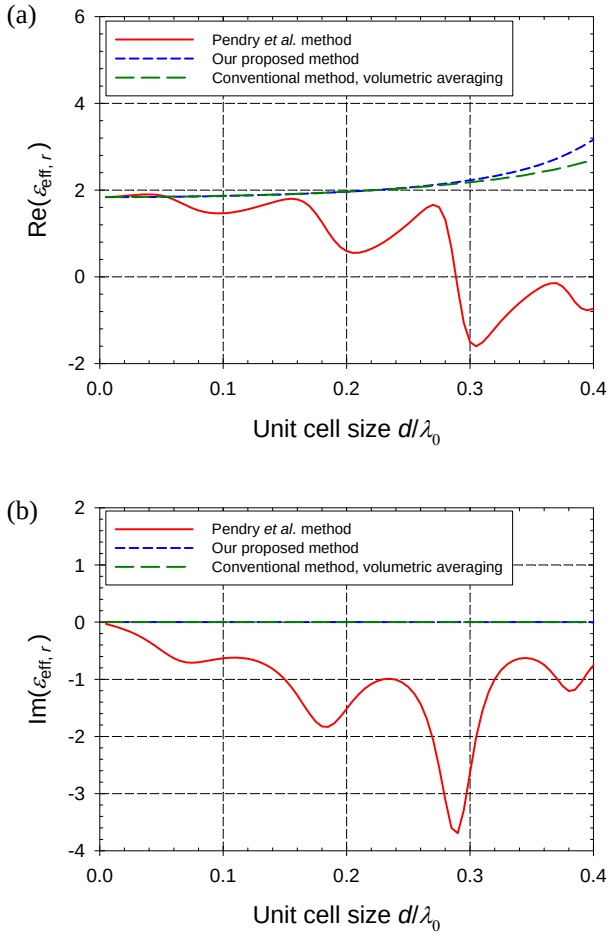

Figure 5: Computed (a) real and (b) imaginary parts of the relative effective permittivity of periodic material consisting of dielectric spheres of $\varepsilon_r = 8$ at a fill factor of 0.3 vs. normalized unit cell size of the material.

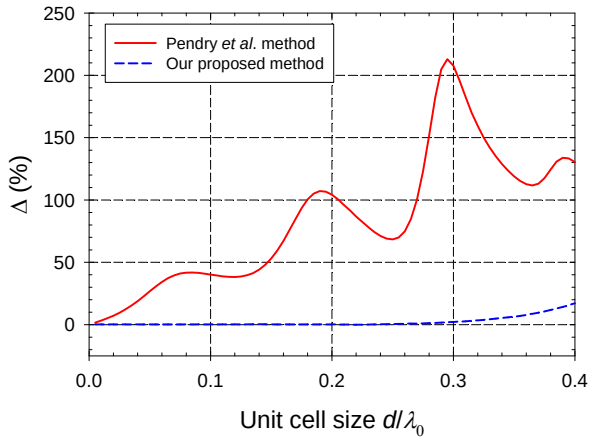

Figure 6: Difference between Pendry *et al.* method or our proposed method from the volume averaging method.

Note that the values of ε_{eff}, μ_{eff} computed by using the Pendry *et al.* method are complex even in cases of lossless inclusions such as those presented here. This is due first to the peculiarities of the Pendry *et al.* method itself and second the complex representation of the local electromagnetic fields provided by *CST Microwave Studio Suite* [which uses an $\exp(j\omega t)$ time convention] or any other electrodynamic solver. Within the Pendry *et al.* method, one might avoid the appearance of nonzero imaginary parts of the effective parameters of lossless lattices by using a real-valued representation of all the fields. However, such an approach cannot be exploited in *numerical* calculations if complex values of the local fields provided by eigensolvers by default are used to calculate the average fields.

To avoid the appearance of nonzero imaginary parts of numerically calculated effective parameters of lossless lattices, Smith and Pendry proposed [11] to calculate the field averages at two phases of the incident wave 90º apart. This correction to the initial Pendry *et al.* method allows one to obtain plausible results on $\varepsilon''_{\text{eff}}$, μ''_{eff}. Comparatively, our modified method yields correct values $\varepsilon''_{\text{eff}} = 0$, $\mu''_{\text{eff}} = 0$ from complex local fields *automatically*, see Fig. 5(b), without invoking any additional correction procedures.

3.2. Dielectric cubes

A simple cubic lattice of dielectric cubes with a volume fill factor of 0.4 and relative permittivity of 8 was modeled and its effective permittivity was computed. The real and imaginary components of the effective permittivity are shown in Fig. 7.

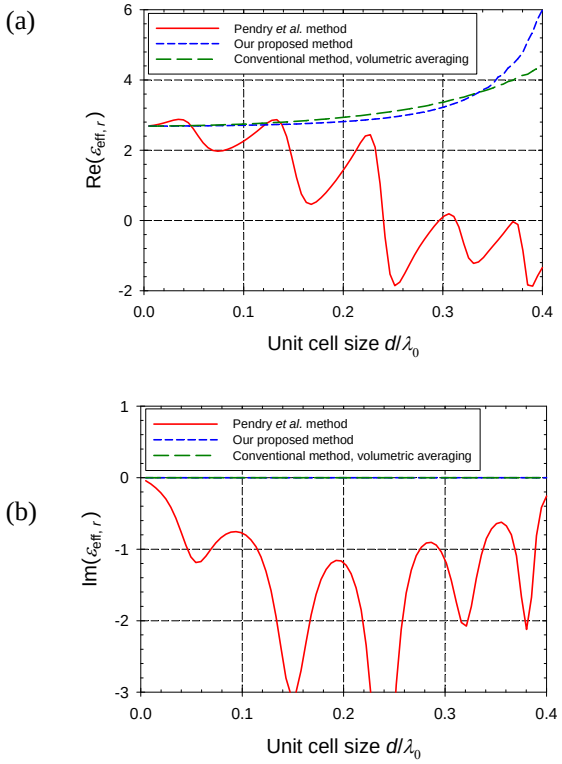

Figure 7: Computed (a) real and (b) imaginary parts of the relative effective permittivity of periodic material consisting of dielectric cubes of $\varepsilon_r = 8$ at a fill factor of 0.4 vs. normalized unit cell size.

As seen from the data, our proposed method returns effective permittivity parameters that are very close to those returned by the volume averaging method. In contrast, the Pendry *et al.* method immediately diverges away. The divergence of both our proposed method and the Pendry *et al.* method away from the volume averaging method is shown in Fig. 8 and is plotted in percent. As seen from the plot, until a unit cell size of 0.35 wavelengths our proposed method incurs approximately 5% error or less. Comparatively, the Pendry *et al.* method incurs more than 5% error after a unit cell size of just $0.013\,\lambda_0$.

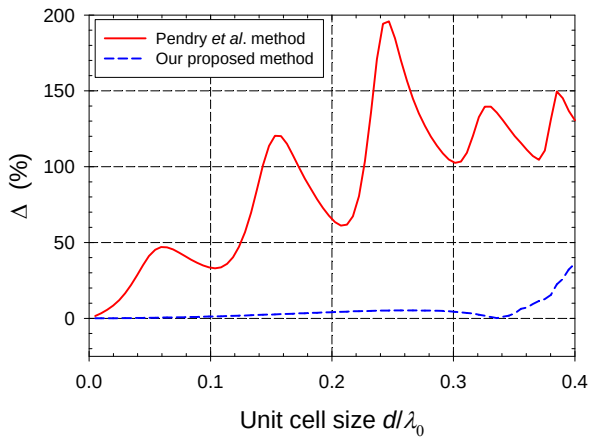

Figure 8: Difference between Pendry *et al.* method or our proposed method from the volume averaging method.

4. Conclusions

Our proposed modification to the averaging method of Pendry *et al.* allows one to calculate the effective material parameters of lattices of particles to a much higher degree of accuracy for the case of appreciable unit cell size. For small unit cell sizes, $d << \lambda_0$, our proposed method returns identical results to that of the Pendry *et al.* method as well as the conventional volume averaging method. For the intermediate region $0.02 < d/\lambda_0 < 0.3$, our method provides more favorable results than the Pendry *et al.* method. Our quantification of the error of the calculated effective material parameters of cube and sphere media show that the Pendry *et al.* method incurs 5% or more error for $d/\lambda_0 > 0.02$. Comparatively, our proposed method incurs more than 5% error for a much larger value $d/\lambda_0 > 0.35$.

Acknowledgements

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