Definition of an EM Continuum and Boundary Conditions for Electric Quadrupolar Continua

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***Abstract*—After defining a continuum using the rigorous spatial-dispersion equations for the macroscopic, fundamental Floquet modal fields of 3D periodic metamaterial arrays, boundary conditions are derived for electric quadrupolar continua.**

I. Introduction

Intuitively, it seems plausible that a three-dimensional (3D) periodic array of electrically isolated inclusions behaves as an electromagnetic continuum obeying Maxwellian macroscopic equations if the variation of the macroscopic fields is small over the distance separating the inclusions. In this paper, we use the equations of a recently developed representation for spatially dispersive periodic metamaterial arrays [1] to obtain sufficient conditions for the arrays to be treated as electromagnetic continua. We then derive the interface boundary conditions for continua with significant dipolar and electric quadrupolar polarization densities.

Maxwell's equations for the macroscopic fields of the fundamental Floquet mode of a periodic array excited by an applied plane-wave electric current density $\mathbf{J}_{\rm a}(\boldsymbol{\beta},\omega)e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$ can be written as [1]

$$i\boldsymbol{\beta}\times\mathbf{E}(\boldsymbol{\beta},\omega)-i\omega\mathbf{B}(\boldsymbol{\beta},\omega)=0 \tag{1a}$$

$$i\boldsymbol{\beta}\times\mathbf{H}(\boldsymbol{\beta},\omega)+i\omega\mathbf{D}(\boldsymbol{\beta},\omega)=\mathbf{J}_{\rm a}(\boldsymbol{\beta},\omega) \tag{1b}$$

with the constitutive relations

$$\mathbf{D}(\boldsymbol{\beta},\omega)\equiv\epsilon_0\mathbf{E}(\boldsymbol{\beta},\omega)+\mathbf{P}^e_\rho(\boldsymbol{\beta},\omega)+i\boldsymbol{\beta}\cdot\overline{\mathbf{Q}}^e(\boldsymbol{\beta},\omega)/2 \tag{2a}$$

$$\mathbf{H}(\boldsymbol{\beta},\omega)\equiv\mathbf{B}(\boldsymbol{\beta},\omega)/\mu_0-\mathbf{M}^e(\boldsymbol{\beta},\omega)-\mathbf{M}(\boldsymbol{\beta},\omega) \tag{2b}$$

where the macroscopic electric-dipole, magnetic-dipole, and electric-quadrupole polarization densities are given by integrations of the induced microscopic electric-current/polarization density over the volume of the unit cell of the array

$$\mathbf{P}^e_\rho(\boldsymbol{\beta},\omega)=\frac{1}{d^3}\int\limits_{\rm V_c}\rho^p_\omega(\mathbf{r})\mathbf{r}_c e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}d^3r \tag{3a}$$

$$\mathbf{M}^e(\boldsymbol{\beta},\omega)=\frac{1}{2d^3}\int\limits_{\rm V_c}\mathbf{r}_c\times\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}d^3r \tag{3b}$$

$$\overline{\mathbf{Q}}^e(\boldsymbol{\beta},\omega)=-\frac{1}{i\omega d^3}\int\limits_{\rm V_c}[\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})\mathbf{r}_c+\mathbf{r}_c\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})]e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}d^3r\,. \tag{3c}$$

and $\mathbf{r}_c$ is the position vector measured from a fixed point within the unit cell of integration. The macroscopic $(\boldsymbol{\beta},\omega)$ fields of the fundamental Floquet mode are determined by integrating the corresponding microscopic frequency-domain fields weighted by the factor $e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}$ over the volume of the unit cell; e.g., for the electric field

$$\mathbf{E}(\boldsymbol{\beta},\omega)=\frac{1}{d^3}\int\limits_{\rm V_c}\boldsymbol{\mathcal{E}}_\omega(\mathbf{r})e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}d^3r \tag{4}$$

where d is the sidelength (separation distance or lattice constant) of a cubic unit cell. The periodicity of the array requires that the fields and induced source densities satisfy Floquet modal expansions; e.g., the electric field can be expressed as

$$\boldsymbol{\mathcal{E}}_\omega(\mathbf{r})=e^{i\boldsymbol{\beta}\cdot\mathbf{r}}\sum_{(l,m,n)=-(\infty,\infty,\infty)}^{+(\infty,\infty,\infty)}\mathbf{E}_{lmn}(\boldsymbol{\beta},\omega)e^{i\mathbf{b}_{lmn}\cdot\mathbf{r}} \tag{5}$$

and similarly for the magnetic field and source densities. For simplicity, we shall assume a cubic array with lattice spacing d such that

$$\mathbf{b}_{lmn}=\frac{2\pi l}{d}\hat{\mathbf{x}}+\frac{2\pi m}{d}\hat{\mathbf{y}}+\frac{2\pi n}{d}\hat{\mathbf{z}} \tag{6}$$

where $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$ are the unit vectors in the (x,y,z) principal directions of the 3D cubic array. Since $\mathbf{b}_{000}=0$, the $(l,m,n)=(0,0,0)$ term in (5) with spatial propagation vector $\boldsymbol{\beta}$ is called the fundamental Floquet mode. Throughout we omit the subscripts 000 on the fundamental Floquet-mode fields and source densities. The applied plane-wave current spectrum $\mathbf{J}_{\rm a}(\boldsymbol{\beta},\omega)$ for all real $\boldsymbol{\beta}$ can be used to represent an arbitrary localized applied current density $\boldsymbol{\mathcal{J}}^{\rm a}_\omega(\mathbf{r})$ through the Fourier transform, and similarly for the other fields.

II. Definition of an electromagnetic continuum

An array of electrically isolated inclusions can be treated as an electromagnetic "continuum" if two conditions are satisfied:

1) $|\boldsymbol{\beta}d|$ is small enough (generally $|\boldsymbol{\beta}d|\ll 1$) that the ordinary averages (that is, averages without the $e^{-i\boldsymbol{\beta}\cdot\mathbf{r}}$ weighting factor) of the microscopic fields and sources over the unit cell approximately equal the fields and sources of the fundamental Floquet mode; e.g., for the electric field in (5)

$$\frac{1}{d^3}\int\limits_{\rm V_c}\boldsymbol{\mathcal{E}}_\omega(\mathbf{r})d^3r=\frac{1}{d^3}\int\limits_{\rm V_c}\Big[e^{i\boldsymbol{\beta}\cdot\mathbf{r}}\sum_{(l,m,n)=-(\infty,\infty,\infty)}^{+(\infty,\infty,\infty)}\mathbf{E}_{lmn}(\boldsymbol{\beta},\omega)e^{i\mathbf{b}_{lmn}\cdot\mathbf{r}}\Big]d^3r$$
$$\approx\ \mathbf{E}(\boldsymbol{\beta},\omega)e^{i\boldsymbol{\beta}\cdot\mathbf{r}_0} \tag{7}$$

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where $\mathbf{r}_0$ is the center of the unit cell, and similarly for the microscopic magnetic field, $\boldsymbol{\mathcal{B}}_\omega(\mathbf{r})$, and the microscopic sources, $\boldsymbol{\mathcal{P}}^e_{\rho\omega}(\mathbf{r}) = \rho^p_\omega(\mathbf{r})\mathbf{r}_c$, $\boldsymbol{\mathcal{M}}^e_\omega(\mathbf{r}) = \mathbf{r}_c \times \boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})/2$, $\boldsymbol{\mathcal{M}}_\omega(\mathbf{r})$, and $\overline{\boldsymbol{\mathcal{Q}}}^e_\omega(\mathbf{r}) = -[\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})\mathbf{r}_c + \mathbf{r}_c\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})]/(i\omega)$.

2) $|k_0 d| = |\omega d/c|$ is small enough (generally $|k_0 d| \ll 1$) that the wave numbers $\boldsymbol{\beta}_{\rm eig}(\omega)$ of the "propagating" source-free eigenmodes of the array (that would be excited by discontinuities or terminations of the array) satisfy the requirement of condition 1) of small enough $|\boldsymbol{\beta}_{\rm eig} d|$ that the fundamental Floquet modes dominate. This second continuum condition implies that the quasi-static fields of the electrically separated inclusions dominate over the length of several or more unit cells. On lossy arrays, the $\boldsymbol{\beta}_{\rm eig}$ of the propagating eigenmodes can be complex with small imaginary parts for small values of $|k_0 d|$. In addition, even for small values of $|k_0 d|$, there may be "evanescent" complex eigenmodes on lossy and lossless arrays with $|{\rm Im}(\boldsymbol{\beta}_{\rm eig} d)| > 1$. However, these evanescent waves are irrelevant for defining a continuum because they decay to a negligible value in "transition layers" a small fraction of a wavelength from discontinuities or terminations of an array.

If the above conditions 1) and 2) are met, ordinary averages over electrically small (quasi-static) macroscopic volumes ΔV within the array, but outside any transition layers of discontinuities or terminations of the array, and containing many inclusions will produce physically meaningful averages at each value of $\boldsymbol{\beta}$ and ω satisfying the small $|\boldsymbol{\beta} d|$ and small $|k_0 d|$ criteria of conditions 1) and 2). Specifically, we can write

$$\mathbf{E}_{\rm ave}(\mathbf{r}, t) \approx \mathbf{E}(\boldsymbol{\beta}, \omega) e^{i(\boldsymbol{\beta}\cdot\mathbf{r} - \omega t)} \tag{8}$$

and similarly for the other macroscopic fields and source densities. That is, the ordinary macroscopic-volume averages at each $\boldsymbol{\beta}$ and ω within the small spatial and temporal bandwidths defining the continuum are given approximately by the fundamental Floquet mode. The constitutive parameters of a continuum, in particular the permittivity and permeability dyadics, can be spatially dispersive (as well as temporally dispersive).

With the help of the polarizations defined in (3), we will show that the continuum can be characterized by ordinary multipole moments with ordinary electric-dipole, magnetic-dipole, and electric-quadrupole moments dominating at sufficiently small values of $|\boldsymbol{\beta} d|$. Consider the integrations in (3) over the unit cell in which the coordinate-system origin of the position vector $\mathbf{r}$ is located, and then let $\mathbf{r}_c = \mathbf{r}$. With $|\boldsymbol{\beta} d|$ sufficiently < 1, the approximation $e^{-i\boldsymbol{\beta}\cdot\mathbf{r}} \approx 1 - i\boldsymbol{\beta}\cdot\mathbf{r}$ holds for this unit cell and, thus, to first order in $|\boldsymbol{\beta} d|$ (3) yields

$$\mathbf{P}^e_\rho(\boldsymbol{\beta}, \omega) = \mathbf{P}^e_0(\boldsymbol{\beta}, \omega) - i\boldsymbol{\beta}\cdot\overline{\mathbf{Q}}^e_0(\boldsymbol{\beta}, \omega) + O(|\boldsymbol{\beta} d|^2) \tag{9a}$$

$$\mathbf{M}^e(\boldsymbol{\beta}, \omega) + \mathbf{M}(\boldsymbol{\beta}, \omega) = \mathbf{M}^e_0(\boldsymbol{\beta}, \omega) + \mathbf{M}_0(\boldsymbol{\beta}, \omega) + O(|\boldsymbol{\beta} d|) \tag{9b}$$

where the ordinary (continuum) electric and magnetic dipole-moment densities, and the ordinary electric quadrupole-moment density in the unit cell containing the origin of the position vector $\mathbf{r}$ are given by

$$\mathbf{P}^e_0(\boldsymbol{\beta}, \omega) = \frac{1}{d^3}\int_{\rm V_c} \rho^p_\omega(\mathbf{r})\mathbf{r} d^3r = \frac{1}{d^3}\int_{\rm V_c} [\rho_\omega(\mathbf{r})\mathbf{r} + \boldsymbol{\mathcal{P}}_\omega(\mathbf{r})]\, d^3r \tag{10a}$$

$$\mathbf{M}^e_0(\boldsymbol{\beta}, \omega) = \frac{1}{2d^3}\int_{\rm V_c} \mathbf{r}\times\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r}) d^3r,\ \mathbf{M}_0(\boldsymbol{\beta}, \omega) = \frac{1}{d^3}\int_{\rm V_c} \boldsymbol{\mathcal{M}}_\omega(\mathbf{r}) d^3r \tag{10b}$$

$$\overline{\mathbf{Q}}^e_0(\boldsymbol{\beta}, \omega) = \frac{i}{\omega d^3}\int_{\rm V_c} [\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})\mathbf{r} + \mathbf{r}\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})] d^3r = \frac{1}{d^3}\int_{\rm V_c} \rho^p_\omega(\mathbf{r})\mathbf{r}\mathbf{r} d^3r. \tag{10c}$$

Multiplying equations (1)–(2) by $e^{i(\boldsymbol{\beta}\cdot\mathbf{r} - \omega t)}$, then inserting the expressions in (8)–(10) for the fields and polarization densities into these equations, and lastly taking the four-fold $(\boldsymbol{\beta}, \omega)$ Fourier transform shows that to first order in $|\boldsymbol{\beta} d|$ the macroscopic fields of the continuum array satisfy the following Maxwell macroscopic space-time continuum equations

$$\nabla\times\boldsymbol{\mathcal{E}}_{\rm ave}(\mathbf{r}, t) + \frac{\partial\boldsymbol{\mathcal{B}}_{\rm ave}(\mathbf{r}, t)}{\partial t} = 0 \tag{11a}$$

$$\nabla\times\boldsymbol{\mathcal{H}}_{\rm ave}(\mathbf{r}, t) - \frac{\partial\boldsymbol{\mathcal{D}}_{\rm ave}(\mathbf{r}, t)}{\partial t} = \boldsymbol{\mathcal{J}}_{\rm a,ave}(\mathbf{r}, t) \tag{11b}$$

$$\nabla\cdot\boldsymbol{\mathcal{B}}_{\rm ave}(\mathbf{r}, t) = 0 \tag{11c}$$

$$\nabla\cdot\boldsymbol{\mathcal{D}}_{\rm ave}(\mathbf{r}, t) = \rho_{\rm a,ave}(\mathbf{r}, t) \tag{11d}$$

with

$$\boldsymbol{\mathcal{D}}_{\rm ave}(\mathbf{r}, t) \approx \epsilon_0\boldsymbol{\mathcal{E}}_{\rm ave}(\mathbf{r}, t) + \boldsymbol{\mathcal{P}}^e_{0\rm ave}(\mathbf{r}, t) - \frac{1}{2}\nabla\cdot\overline{\boldsymbol{\mathcal{Q}}}^e_{0\rm ave}(\mathbf{r}, t) \tag{12a}$$

$$\boldsymbol{\mathcal{H}}_{\rm ave}(\mathbf{r}, t) \approx \boldsymbol{\mathcal{B}}_{\rm ave}(\mathbf{r}, t)/\mu_0 - \boldsymbol{\mathcal{M}}^e_{0\rm ave}(\mathbf{r}, t) - \boldsymbol{\mathcal{M}}_{0\rm ave}(\mathbf{r}, t) \tag{12b}$$

for $\boldsymbol{\mathcal{J}}_{\rm a,ave}(\mathbf{r}, t)$ within the spatial and temporal bandwidths ($\Delta\boldsymbol{\beta}$ and $\Delta\omega$) of the largest sufficiently small $|\boldsymbol{\beta} d|$ and $|k_0 d|$ for the approximations in (7)–(8) to hold and all multipole polarization densities of higher order than $\boldsymbol{\mathcal{P}}^e_{0\rm ave}(\mathbf{r}, t)$, $\boldsymbol{\mathcal{M}}^e_{0\rm ave}(\mathbf{r}, t) + \boldsymbol{\mathcal{M}}_{0\rm ave}(\mathbf{r}, t)$, and $\overline{\boldsymbol{\mathcal{Q}}}^e_{0\rm ave}(\mathbf{r}, t)$ (the ordinary electric-dipole, magnetic-dipole, and electric quadrupole space-time polarization densities) to be negligible, where from (8) we have

$$\boldsymbol{\mathcal{E}}_{\rm ave}(\mathbf{r}, t) = \int_{-\Delta\omega}^{+\Delta\omega}\int_{-\Delta\beta_z}^{+\Delta\beta_z}\int_{-\Delta\beta_y}^{+\Delta\beta_y}\int_{-\Delta\beta_x}^{+\Delta\beta_x} \mathbf{E}(\boldsymbol{\beta}, \omega) e^{i(\boldsymbol{\beta}\cdot\mathbf{r} - \omega t)} d^3\beta d\omega \tag{13}$$

and similarly for the other space-time averages. If the multipole polarization densities of higher order than $\boldsymbol{\mathcal{P}}^e_{0\rm ave}(\mathbf{r}, t)$, $\boldsymbol{\mathcal{M}}^e_{0\rm ave}(\mathbf{r}, t) + \boldsymbol{\mathcal{M}}_{0\rm ave}(\mathbf{r}, t)$, and $\overline{\boldsymbol{\mathcal{Q}}}^e_{0\rm ave}(\mathbf{r}, t)$ are not all negligible over the continuum bandwidths ($\Delta\boldsymbol{\beta}$ and $\Delta\omega$), then the integrals in (3) could be further expanded as in (9) beyond the first-order $|\boldsymbol{\beta} d|$ terms, similarly to what is done in [2], to obtain ordinary multipole densities in (12) of higher order than the dipolar and electric quadrupolar polarization densities.

With the expressions in (9)–(10), the total current is given to first order in $\boldsymbol{\beta}$ as

$$\begin{aligned}\mathbf{J}^{\rm tot}(\boldsymbol{\beta}, \omega) = &-i\omega\mathbf{P}^e_0(\boldsymbol{\beta}, \omega) - \omega\boldsymbol{\beta}\cdot\overline{\mathbf{Q}}^e_0(\boldsymbol{\beta}, \omega)/2 \\ &+ i\boldsymbol{\beta}\times[\mathbf{M}^e_0(\boldsymbol{\beta}, \omega) + \mathbf{M}_0(\boldsymbol{\beta}, \omega)] + O(|\boldsymbol{\beta} d|^2)\,.\end{aligned} \tag{14}$$

Because the microscopic current and charge densities, $\boldsymbol{\mathcal{J}}^p_\omega(\mathbf{r})$ and $\rho^p_\omega(\mathbf{r})$, induced on polarizable or perfectly conducting inclusions are absolutely integrable (so that all the multipole-moment densities are finite), we see from (9a) that for $|\boldsymbol{\beta} d|$ small enough the electric quadrupole-moment density contributes negligibly to the electric polarization and both the electric and magnetic polarizations in (2) become equal to the ordinary electric and magnetic dipole moments per unit-cell volume. Higher order multipole moments do not have to be taken into account in order to determine the macroscopic permittivity for $|\boldsymbol{\beta} d|$ sufficiently small (unless the electric dipole polarization $\mathbf{P}^e_0(\boldsymbol{\beta},\omega)$ is negligible for $|\boldsymbol{\beta} d|$ less than some finite value).

However, both the electric quadrupole-moment density and magnetic dipole-moment density contribute to order $\boldsymbol{\beta}$ in (14) as $\boldsymbol{\beta} \to 0$ and thus generally both have to be taken into account (at higher temporal frequencies ω) in determining the macroscopic permeability as $\boldsymbol{\beta} \to 0$ [3, p. 61], [4]. However, as $\boldsymbol{\beta} \to 0$, the permeability does not explicitly reveal the contribution to the fields from the electric-quadrupole polarization for an applied magnetic field. Nonetheless, for $|k_0 d| = |\omega d/c|$ sufficiently small, we see from (14) that the contribution of the electric quadrupole-moment density becomes negligible compared to that of a nonzero magnetic dipole-moment density.

In summary, as both $|\boldsymbol{\beta} d|$ and $|k_0 d|$ become small, the enforced and free-space wavelengths become much larger than the separation distance d between the inclusions, and the anisotropic formulation for the fundamental Floquet mode approaches that of an anisotropic continuum with ordinary electric-dipole, magnetic-dipole, and electric quadrupole polarization densities. *In addition, we have shown that a metamaterial array with inclusions having nonzero electric and/or magnetic dipole moments at low spatial and temporal frequencies (that is, for $|\boldsymbol{\beta} d|$ and $|k_0 d|$ sufficiently small) can be represented by an anisotropic dipolar continuum with negligible higher-order multipole-moment densities.* Since most molecules can be modeled by polarizable or perfectly conducting inclusions, this result also holds for most natural materials with electrically isolated molecules at sufficiently low spatial and temporal frequencies [5, p. 111]. The fields of the dipolar continuum satisfy the space-time Maxwellian equations in (11)–(12) with the electric quadrupole density $\overline{\boldsymbol{\mathcal{Q}}}^e_{0\text{ave}}(\mathbf{r},t) = 0$.

III. Boundary conditions for electric-quadrupolar continua

The Maxwellian macroscopic space-time continuum equations in (11)–(12) hold for applied current excitations with spatial and temporal bandwidths ($\Delta\boldsymbol{\beta}$ and $\Delta\omega$) determined by small enough $|\boldsymbol{\beta} d|$ and $|k_0 d|$, respectively, for the approximations in (7)–(10) to be sufficiently accurate that ordinary macroscopic averaging applies over macroscopic volumes ΔV containing many inclusions. The equations (11)–(12) were derived for infinite periodic arrays of separated inclusions with small enough $|\boldsymbol{\beta} d|$ and $|k_0 d|$ that all multipole-moment polarization densities of higher order than ordinary dipolar and electric quadrupolar polarization densities are negligible. In this section, we want to terminate the infinite array in a surface S that is effectively planar in the sense that any subsurface S_p of S extending a distance less than several lattice distances d is approximately planar. The surface S is assumed to be an interface between the array and free space or another array and we want to determine the boundary conditions across this interface.

The termination of the array(s) by the surface S introduces strong spatial variations of the fields and induced sources in the vicinity of S that invalidates the approximations in (7) and (8). Although averages of the microscopic fields and induced sources can still be performed using macroscopic volumes ΔV throughout all space, the resulting macroscopic fields will not generally satisfy (11)–(12) in a transition layer [6, p. 271] containing the interface surface S. For the original infinite continuum arrays characterized by $|\Delta\boldsymbol{\beta} d| \ll 1$ and $|\Delta k_0 d| = \Delta\omega d/c \ll 1$, the thickness δ of the transition layer is much smaller than the free-space and $2\pi/|\boldsymbol{\beta}|$ wavelengths; see discussion of evanescent eigenmodes in the previous section. The effect of this transition layer can be represented in equations (11) by additional transition-layer electric and magnetic current and charge densities on the right-hand sides of the equations in (11). For example, (11a) and (11b) become

$$\nabla \times \boldsymbol{\mathcal{E}}_{\text{ave}}(\mathbf{r},t) + \frac{\partial \boldsymbol{\mathcal{B}}_{\text{ave}}(\mathbf{r},t)}{\partial t} = -\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t) \tag{15a}$$

$$\nabla \times \boldsymbol{\mathcal{H}}_{\text{ave}}(\mathbf{r},t) - \frac{\partial \boldsymbol{\mathcal{D}}_{\text{ave}}(\mathbf{r},t)}{\partial t} = \boldsymbol{\mathcal{J}}_{\text{a,ave}}(\mathbf{r},t) + \boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t) \tag{15b}$$

where $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$ are transition-layer macroscopic electric and magnetic current densities, respectively, that are zero everywhere except within the transition layer of thickness δ. These equations in (15), along with the constitutive equations in (12), now hold throughout all space. The two divergence equations associated with (15) can be obtained by taking the divergence of the equations in (15). Note from (12a) that $\boldsymbol{\mathcal{P}}^e_{\text{ave}}(\mathbf{r},t) = \boldsymbol{\mathcal{P}}^e_{0\text{ave}}(\mathbf{r},t) - \nabla\cdot\overline{\boldsymbol{\mathcal{Q}}}^e_{0\text{ave}}(\mathbf{r},t)/2$ effectively contains a delta function across the thin transition layer if the electric quadrupole density is not negligible and differs in value on either side of the transition layer; specifically

$$\begin{aligned} \boldsymbol{\mathcal{P}}^e_{\text{ave}}(\mathbf{r},t) &= \boldsymbol{\mathcal{P}}^e_{0\text{ave}}(\mathbf{r},t) \\ &-\frac{1}{2}\left[\nabla\cdot\overline{\boldsymbol{\mathcal{Q}}}^e_{0\text{ave}}(\mathbf{r},t)\right]_{\text{dfr}} - \frac{1}{2}\hat{\mathbf{n}}\cdot(\overline{\boldsymbol{\mathcal{Q}}}^{e2}_{0\text{ave}} - \overline{\boldsymbol{\mathcal{Q}}}^{e1}_{0\text{ave}})\delta(n) \end{aligned} \tag{16}$$

in which $\hat{\mathbf{n}}$ is the unit normal to the surface S pointing from the side "1" to side "2" of the transition layer, and $\delta(n)$ is the delta function in the normal coordinate n. The subscript "$_{\text{dfr}}$" means "delta function removed" from the divergence of the electric quadrupole dyadic, so that $\left[\nabla\cdot\overline{\boldsymbol{\mathcal{Q}}}^e_{0\text{ave}}(\mathbf{r},t)\right]_{\text{dfr}}$ can be discontinuous but otherwise nonsingular across the thin transition layer. We are assuming that there are no effective delta functions in the macroscopic dipolar and electric-quadrupolar polarization densities, $\boldsymbol{\mathcal{P}}^e_{0\text{ave}}(\mathbf{r},t)$, $\boldsymbol{\mathcal{M}}^e_{0\text{ave}}(\mathbf{r},t) + \boldsymbol{\mathcal{M}}_{0\text{ave}}(\mathbf{r},t)$, and $\overline{\boldsymbol{\mathcal{Q}}}^{e}_{0\text{ave}}(\mathbf{r},t)$, represented by $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$ within the thin transition layer.[1]

Boundary conditions on the tangential components of the macroscopic $\boldsymbol{\mathcal{E}}_{\text{ave}}$ and $\boldsymbol{\mathcal{H}}_{\text{ave}}$ fields and on the normal components of the macroscopic $\boldsymbol{\mathcal{D}}_{\text{ave}}$ and $\boldsymbol{\mathcal{B}}_{\text{ave}}$ fields across the transition layer can be determined by applying the integral forms of (15) and the corresponding divergence equations to thin rectangular closed curves and closed surfaces (pillboxes) with their long dimensions of length ℓ on either side of the transition layer so that their short sides are of width $\delta \ll \ell$ (taking into account the effective delta functions in $\nabla \cdot \overline{\boldsymbol{\mathcal{Q}}}^{e}_{0\text{ave}}$ across the transition layer). Although $\ell \gg \delta$, it is assumed that ℓ is short enough that the macroscopic fields and sources along the length of ℓ do not change appreciably. This determination of boundary conditions for the equations in (15) with the constitutive relations in (12) and (16) has been done in [7] but without the transition current densities, $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$. However, the additional integrals over $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$ become insignificant for δ sufficiently small, or equivalently, for $|\Delta\beta d|$ and $|\Delta k_0 d|$ sufficiently small, provided, as discussed in Footnote 1, that $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$ do not contain delta functions. Thus, we can apply the boundary conditions derived in [7][2] with the surface polarization $\mathbf{P}^\delta$ in [7] replaced by $-\hat{\mathbf{n}} \cdot (\overline{\boldsymbol{\mathcal{Q}}}^{e2}_{0\text{ave}} - \overline{\boldsymbol{\mathcal{Q}}}^{e1}_{0\text{ave}})/2$ given in (16), to get

$$\boldsymbol{\mathcal{E}}^{2s}_{\text{ave}} - \boldsymbol{\mathcal{E}}^{1s}_{\text{ave}} \approx \frac{1}{2\epsilon_0}\nabla_s \left[\hat{\mathbf{n}} \cdot (\overline{\boldsymbol{\mathcal{Q}}}^{e2}_{0\text{ave}} - \overline{\boldsymbol{\mathcal{Q}}}^{e1}_{0\text{ave}}) \cdot \hat{\mathbf{n}}\right] \tag{17a}$$

$$\boldsymbol{\mathcal{H}}^{2s}_{\text{ave}} - \boldsymbol{\mathcal{H}}^{1s}_{\text{ave}} \approx \frac{1}{2}\hat{\mathbf{n}} \times \left[\partial(\hat{\mathbf{n}} \cdot \overline{\boldsymbol{\mathcal{Q}}}^{e2}_{0\text{ave}})^s/\partial t - \partial(\hat{\mathbf{n}} \cdot \overline{\boldsymbol{\mathcal{Q}}}^{e1}_{0\text{ave}})^s/\partial t\right] \tag{17b}$$

$$\mathcal{D}^{2n}_{\text{ave}} - \mathcal{D}^{1n}_{\text{ave}} \approx \frac{1}{2}\nabla_s \cdot \left[(\hat{\mathbf{n}} \cdot \overline{\boldsymbol{\mathcal{Q}}}^{e2}_{0\text{ave}})^s - (\hat{\mathbf{n}} \cdot \overline{\boldsymbol{\mathcal{Q}}}^{e1}_{0\text{ave}})^s\right] \tag{17c}$$

$$\mathcal{B}^{2n}_{\text{ave}} - \mathcal{B}^{1n}_{\text{ave}} \approx 0 \tag{17d}$$

where the superscripts "s" and "n" refer to vector components tangential and normal to the surface S, respectively, and we note that $\overline{\boldsymbol{\mathcal{Q}}}^{e}_{0\text{ave}}(\mathbf{r},t)$ is a symmetric dyadic because $\overline{\mathbf{Q}}^{e}_{0}(\boldsymbol{\beta},\omega)$ is a symmetric dyadic. These boundary conditions show that the change in electric quadrupole density across the thin transition layer produces discontinuities in the tangential components of $\boldsymbol{\mathcal{E}}_{\text{ave}}$ and $\boldsymbol{\mathcal{H}}_{\text{ave}}$ and in the normal component of $\boldsymbol{\mathcal{D}}_{\text{ave}}$. They agree with the boundary conditions of Raab and De Lange [4, eqs. (6.69)–(6.74)] if a term $\epsilon_0^{-1}\partial Q_{zz}/\partial z/2$ is added to the right-hand side of [4, eq. (6.71)]. In a private communication, Raab and De Lange have confirmed the necessity of this added term. Our expressions in (17) have also been confirmed in an unpublished independent derivation by M.G. Silveirinha using transverse averaging and assuming no delta-function contributions, as discussed in Footnote 1, from the effective polarizations in the transition layer [8].

[1] Delta-functions $\delta(n)$ in the polarizations as represented by $\boldsymbol{\mathcal{J}}_\delta(\mathbf{r},t)$ and $\boldsymbol{\mathcal{K}}_\delta(\mathbf{r},t)$ may exist if these polarizations are proportional to the derivatives of the fields, that is, if they display significant spatial dispersion. In that case, the boundary conditions in (17) would have to be modified.

[2] The field symbols on the left-hand sides of equations (13), (15), and (16) in [7] should be boldface, and the ∇ symbol one line below equation (12) of [7] should be ∇_s.

The results of several analyses and simulations of periodic arrays, for example those in [8]–[10], indicate that the effect of the boundary layer becomes negligible for spatial and temporal bandwidths, $|\Delta\beta d|$ and $|\Delta k_0 d|$, less than about 0.1. Thus, one would also expect that the boundary conditions in (17) are reliable approximations for $|\Delta\beta d|$ and $|\Delta k_0 d|$ less than about 0.1. If, as discussed in the previous section, these spatial and temporal bandwidths are small enough for the electric quadrupole density to be negligible compared to the dipolar polarization densities, then the electric quadrupole terms in (17) can be neglected and (17) predicts the usual continuity of the tangential $\boldsymbol{\mathcal{E}}_{\text{ave}}$ and $\boldsymbol{\mathcal{H}}_{\text{ave}}$ fields and the normal $\boldsymbol{\mathcal{D}}_{\text{ave}}$ field (as well as the normal $\boldsymbol{\mathcal{B}}_{\text{ave}}$ field) across the thin transition layer. Lastly, we mention the need for more analysis and simulations to investigate the possibility of additional delta functions, as discussed in Footnote 1, in the polarizations of more strongly spatially dispersive arrays and to determine additional boundary conditions (ABCs) for these arrays [11].

ACKNOWLEDGMENT

The paper benefited from many helpful discussions with Professors Mario G. Silveirinha and Andrea Alù. This research was supported by AFOSR through Dr. Arje Nachman.

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