Supplementary Material for Proc. R. Soc. A 20190220 — Homogenization of plasmonic crystals: Seeking the epsilon-near-zero effect

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The supplementary material contains a derivation of compatibility conditions (2.3) from Gauss' and Ampère's law (Section SM 1), a derivation of all interface and internal boundary conditions starting from a weak formulation of the problem (Section SM 2).

SM 1. Derivation of compatibility conditions from Gauss' and Ampère's law

In this section, we give a short derivation of the internal compatibility condition (2.3).

For an arbitrary volume V in Ω, the integral over the *electric displacement in normal direction* has to be equal to the integral over the total charge density contained in V,

$$i\omega \int_V \rho \,\mathrm{d}x = \int_{\partial V} \boldsymbol{n}_{\partial V} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right) \mathrm{d}o_x.$$

We now choose V to be an arbitrary rectangular box containing a part of the edge $\partial\Sigma^d$. We extend the sheet over the edge parallel in $\boldsymbol{n}$-direction, and assume $\sigma^d = 0$ in the extension. The box shall be of vanishing length and height, and with top and bottom faces parallel to the extended sheet Σ^d_*; see Figure 1. Then,

$$\begin{aligned}
\lim_{\text{height}\to 0} i\omega \int_V \rho \,\mathrm{d}x &= \lim_{\text{height}\to 0} \int_{\partial V} \boldsymbol{n}_{\partial V} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right) \mathrm{d}o_x \\
&= \lim_{\text{height}\to 0} \int_{\text{top}} \boldsymbol{\nu} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right)^{\text{above}} \mathrm{d}o_x - \int_{\text{bottom}} \boldsymbol{\nu} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right)^{\text{below}} \mathrm{d}o_x \\
&= + \int_{V\cap\Sigma^d_*} \boldsymbol{\nu} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right)^{\text{above}} \mathrm{d}o_x - \int_{V\cap\Sigma^d_*} \boldsymbol{\nu} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right)^{\text{below}} \mathrm{d}o_x.
\end{aligned}$$

Here, $\boldsymbol{n}_{\partial V}$ denotes the outward pointing unit normal on faces of the volume V and $\boldsymbol{\nu}$ is the normal field on Σ^d_*. Now, utilizing the third jump condition in (2.2) we conclude that

$$\begin{aligned}
\lim_{\text{height}\to 0} i\omega \int_V \rho \,\mathrm{d}x &= \int_{V\cap\Sigma^d_*} \left[\boldsymbol{\nu} \cdot \left(\varepsilon^d \boldsymbol{E}^d\right)\right]_{\Sigma^d} \mathrm{d}o_x \\
&= \int_{V\cap\Sigma^d_*} \nabla \cdot \left(\sigma^d \boldsymbol{E}^d\right) \mathrm{d}o_x \\
&= \int_{\partial V\cap\Sigma^d_*} \boldsymbol{n} \cdot \left(\sigma^d \boldsymbol{E}^d\right) \mathrm{d}o_x.
\end{aligned}$$

Here, $\boldsymbol{n}$ is the outward pointing normal on the edge, see Figure 1. By keeping the width (dimension parallel to the edge $\partial\Sigma^d$) fixed and in the limit of vanishing height and length, we conclude that the volume integral over the charge density ρ reduces to

$$\lim_{\text{height}\to 0} \lim_{\text{length}\to 0} i\omega \int_V \rho \,\mathrm{d}x = \int_{V\cap\partial\Sigma^d} \nabla \cdot \left(\lambda^d(\boldsymbol{x}) \boldsymbol{E}^d(\boldsymbol{x})\right) \mathrm{d}s.$$

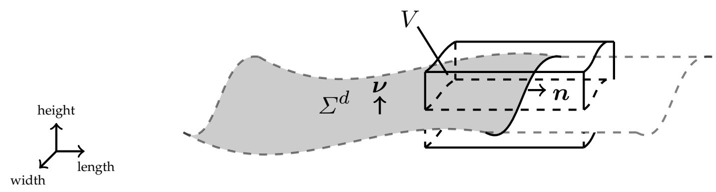

Figure 1: Choice of rectangular box V; a curved, rectangular box containing a part of the edge $\partial\Sigma^d$. We extend the sheet over the edge parallel in $\boldsymbol{n}$-direction, and assume $\sigma^d = 0$ in the extension. The box shall be of vanishing length and height, and with top and bottom faces parallel to the extended sheet Σ^d.

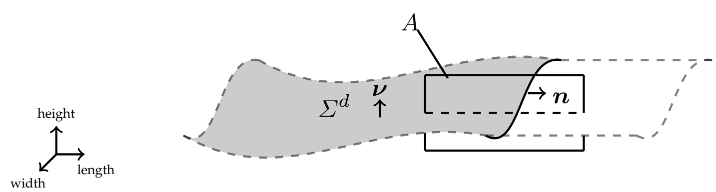

Figure 2: Choice of area element A; a curved, rectangular rectangle enclosing a point of the edge $\partial\Sigma^d$. We extend the sheet over the edge parallel in $\boldsymbol{n}$-direction, and assume $\sigma^d = 0$ in the extension. The area shall be of vanishing length and height, and with top and bottom lines parallel to the extended sheet Σ^d.

Consequently,

$$\int_{V\cap\partial\Sigma^d} \nabla\cdot\left(\lambda^d(\boldsymbol{x})\boldsymbol{E}^d(\boldsymbol{x})\right)\mathrm{d}s = \int_{V\cap\partial\Sigma^d}\Big[\boldsymbol{n}\cdot\left(\sigma^d\boldsymbol{E}^d\right)\Big]_{\Sigma^d}\,\mathrm{d}o_x.$$

Due to the fact that V was chosen arbitrarily, we conclude that

$$\Big[\boldsymbol{n}\cdot\left(\sigma^d\boldsymbol{E}^d\right)\Big]_{\Sigma^d} = \nabla\cdot\left(\lambda^d(\boldsymbol{x})\boldsymbol{E}^d(\boldsymbol{x})\right)$$

has to hold true pointwise on $\partial\Sigma^d$. But σ^d vanishes outside of Σ^d, thus

$$\boldsymbol{n}\cdot\left(\sigma^d\boldsymbol{E}^d\right) = \nabla\cdot\left(\lambda^d(\boldsymbol{x})\boldsymbol{E}^d(\boldsymbol{x})\right) \quad \text{on } \partial\Sigma^d.$$

In a similar vain, let A be an arbitrary area element perpendicular to the edge; see Figure 2. By virtue of Ampère's law we have

$$\int_{\partial A}\boldsymbol{H}^d\cdot\mathrm{d}\boldsymbol{s} = \int_A \boldsymbol{J}\cdot\boldsymbol{\tau}\,\mathrm{d}o_x, \tag{SM 1.1}$$

where $\boldsymbol{\tau}$ is the unit vector in edge direction, orthogonal to $\boldsymbol{n}$ and $\boldsymbol{\nu}$. In the limit of vanishing length, we can rewrite the left-hand side:

$$\begin{aligned}\lim_{\text{length}\to 0}\int_{\partial A}\boldsymbol{H}^d\cdot\mathrm{d}\boldsymbol{s} &= \lim_{\text{length}\to 0}\left\{\int_{\text{left,right}}(\boldsymbol{n}\times\boldsymbol{H}^d)\cdot\boldsymbol{\tau}\,\mathrm{d}s + \int_{\text{top,bottom}}(\pm\boldsymbol{\nu}\times\boldsymbol{H}^d)\cdot\boldsymbol{\tau}\,\mathrm{d}s\right\}\\ &= \lim_{\text{length}\to 0}\int_{\text{left,right}}(\boldsymbol{n}\times\boldsymbol{H}^d)\cdot\boldsymbol{\tau}\,\mathrm{d}s.\end{aligned}$$

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Exploiting the fact that $\boldsymbol{J} = \boldsymbol{J}_a + \delta_{\Sigma^d}\sigma^d\boldsymbol{E}^d + \delta_{\partial\Sigma^d}\lambda^d\boldsymbol{E}^d$ and by taking the limit of vanishing length we conclude that:

$$\lambda^d \boldsymbol{E}^d\Big|_{\partial\Sigma^d\cap A} \cdot \boldsymbol{\tau} \,=\, \lim_{\text{length}\to 0}\int_{\text{left,right}} (\boldsymbol{n}\times\boldsymbol{H}^d)\cdot\boldsymbol{\tau}\,\mathrm{d}s. \tag{SM 1.2}$$

This implies that the jump over $\boldsymbol{n}\times\boldsymbol{H}^d$ must have a singular point contribution:

$$\left\{\boldsymbol{n}\times\boldsymbol{H}^d\right\}_{\partial\Sigma^d}\cdot\boldsymbol{\tau} \,=\, \lambda^d\boldsymbol{E}^d\Big|_{\partial\Sigma^d\cap A}\cdot\boldsymbol{\tau}.$$

Here, we defined $\{.\}_{\partial\Sigma^d}$ rigorously as the corresponding limit in (SM 1.2). Note that the height of the area element A was arbitrarily chosen. Indeed, the actual value of $\left\{\boldsymbol{n}\times\boldsymbol{H}^d\right\}_{\partial\Sigma^d}$ does not depend on the particular choice of the area element A because it corresponds directly to a residue of an analytic function $(\boldsymbol{n}\times\boldsymbol{H}^d)\cdot\boldsymbol{\tau}$. In thise sense, Definition (2.3) is an equivalent, sligthly less technical definition.

SM 2. Derivation of interface and internal boundary condition from weak formulation

In this appendix we derive the strong formulation with all jump and compatibility conditions starting from a varational formulation. The weak formulation reads, find a vector field E such that

$$\begin{aligned}\int_\Omega \mu_0^{-1}\nabla\times\boldsymbol{E}^d\cdot\nabla\times\overline{\boldsymbol{\psi}}\,\mathrm{d}x - \omega^2\int_\Omega \varepsilon\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x& \\ - i\omega\int_{\Sigma^d}\sigma^d\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x - i\omega\int_{\partial\Sigma^d}\lambda^d\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}s &= \int_\Omega i\omega\boldsymbol{J}_a\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x,\end{aligned} \tag{SM 2.1}$$

for all smooth, vector-valued test functions $\boldsymbol{\psi}$ with compact support in Ω. Let us now define

$$i\omega\mu_0\int_\Omega \boldsymbol{H}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x := \int_\Omega \boldsymbol{E}^d\cdot(\nabla\times\overline{\boldsymbol{\psi}})\,\mathrm{d}x. \tag{SM 2.2}$$

Integrating (SM 2.2) by parts yields

$$i\omega\mu_0\int_\Omega \boldsymbol{H}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x = \int_\Omega (\nabla\times\boldsymbol{E}^d)\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x - \int_{\Sigma^d}\left[\nu\times\boldsymbol{E}^d\right]_{\Sigma^d}\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}o_x.$$

Thus, testing with (a) a smooth, vector-valued test function $\boldsymbol{\psi}$ with $\boldsymbol{\psi}=0$ on Σ^d, and (b) a sequence $\boldsymbol{\psi}_h$ of test functions with vanishing support outside Σ^d gives

$$i\omega\mu_0\boldsymbol{H}^d = \nabla\times\boldsymbol{E}^d \quad \text{in } \Omega\setminus\Sigma^d, \qquad \left[\nu\times\boldsymbol{E}^d\right]_{\Sigma^d} = 0 \quad \text{on } \Sigma^d.$$

Similarly, integration by parts of (SM 2.1) and substituting $\boldsymbol{H}$:

$$\begin{aligned}i\omega\int_\Omega(\nabla\times\boldsymbol{H}^d)\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x - \omega^2\int_\Omega\varepsilon\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x - i\omega\int_\Omega\boldsymbol{J}_a\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}x& \\ = +i\omega\int_{\Sigma^d}\left[\boldsymbol{\nu}\times\boldsymbol{H}^d\right]_{\Sigma^d}\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}o_x + i\omega\int_{\partial\Sigma^d}\left\{\boldsymbol{n}\times\boldsymbol{H}^d\right\}_{\partial\Sigma^d}\overline{\boldsymbol{\psi}}\,\mathrm{d}s& \\ - i\omega\int_{\Sigma^d}\sigma^d\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}o_x - i\omega\int_{\partial\Sigma^d}\lambda^d\boldsymbol{E}^d\cdot\overline{\boldsymbol{\psi}}\,\mathrm{d}s.&\end{aligned}$$

The occurence of the jump term over $\partial\Sigma^d$ after the integration by parts has to be justified more precisely. Similarly, to the discussion in Appendix SM 1 we assume that the function space for $\boldsymbol{H}$

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admits singular distributions on the edge. More precisely, we define

$$\int_{\partial\Sigma^d} \{\boldsymbol{n}\times\boldsymbol{H}\}_{\partial\Sigma^d}\cdot\boldsymbol{\psi}\,\mathrm{d}s := \int_\Omega (\nabla\times\boldsymbol{H})\cdot\boldsymbol{\psi}\,\mathrm{d}x - \int_\Omega \boldsymbol{H}\cdot(\nabla\times\boldsymbol{\psi})\,\mathrm{d}x - \int_{\Sigma^d}[\boldsymbol{\nu}\times\boldsymbol{H}]_{\Sigma^d}\cdot\boldsymbol{\psi}\,\mathrm{d}o_x. \quad \text{(SM 2.3)}$$

Utilizing the same sequences (a) and (b) of test functions yields a similar result:

$$\begin{aligned} \nabla\times\left(i\omega\boldsymbol{H}^d\right) - \omega^2\varepsilon\boldsymbol{E}^d - i\omega\boldsymbol{J}_a = 0 &\qquad \text{in } \Omega\setminus\Sigma^d,\\ i\omega\left[\boldsymbol{\nu}\times\boldsymbol{H}^d\right]_{\Sigma^d} = i\omega\sigma^d\boldsymbol{E}^d &\qquad \text{on } \Sigma^d\setminus\partial\Sigma^d,\\ i\omega\left\{\boldsymbol{n}\times\boldsymbol{H}^d\right\}_{\partial\Sigma^d} = i\omega\lambda^d\boldsymbol{E}^d &\qquad \text{on } \partial\Sigma^d. \end{aligned}$$

Now, let φ be an arbitrary scalar-valued test function with compact support and set $\boldsymbol{\psi}=\nabla\varphi$. And choose again (a) $\varphi=0$ on Σ^d, and (b) a sequence φ_h of test functions with vanishing support outside Σ^d. Testing (SM 2.2) and subsequent integration by parts results in

$$\nabla\cdot\boldsymbol{H}^d = 0 \quad \text{in } \Omega\setminus\Sigma^d, \qquad \left[\boldsymbol{\nu}\cdot\boldsymbol{H}^d\right]_{\Sigma^d} = 0 \quad \text{on } \Sigma^d.$$

In case of the first equation we start again at (SM 2.1). Utilizing the vector identity $\nabla\times(\nabla\varphi)=0$:

$$-\omega^2\int_\Omega \varepsilon\boldsymbol{E}^d\cdot\nabla\overline{\varphi}\,\mathrm{d}x - i\omega\int_{\Sigma^d}\sigma^d\boldsymbol{E}^d\cdot\nabla\overline{\varphi}\,\mathrm{d}o_x - i\omega\int_{\partial\Sigma^d}\lambda^d\boldsymbol{E}^d\cdot\nabla\overline{\varphi}\,\mathrm{d}s = i\omega\int_\Omega \boldsymbol{J}_a\cdot\nabla\overline{\varphi}\,\mathrm{d}x.$$

Integration by parts:

$$\begin{aligned} \omega^2\int_\Omega \nabla\cdot(\varepsilon\boldsymbol{E}^d)\overline{\varphi}\,\mathrm{d}x + i\omega\int_\Omega \nabla\cdot\boldsymbol{J}_a\overline{\varphi}\,\mathrm{d}x &\\ = -\omega^2\int_{\Sigma^d}\left[\nu\cdot(\varepsilon\boldsymbol{E}^d)\right]_{\Sigma^d}\overline{\varphi}\,\mathrm{d}o_x - i\omega\int_{\Sigma^d}\nabla\cdot(\sigma^d\boldsymbol{E}^d)\overline{\varphi}\,\mathrm{d}o_x &\\ + i\omega\int_{\partial\Sigma^d}\boldsymbol{n}\cdot(\sigma^d\boldsymbol{E}^d)\overline{\varphi}\,\mathrm{d}s - i\omega\int_{\partial\Sigma^d}\nabla\cdot(\lambda^d\boldsymbol{E}^d)\overline{\varphi}\,\mathrm{d}s. & \end{aligned}$$

Here, $\boldsymbol{n}$ denotes the outward-pointing unit vector tangential to Σ^d and normal to $\partial\Sigma^d$. We point out that for the integration by parts of the interface term $\int_{\Sigma^d}\sigma^d\boldsymbol{E}^d$ it is essential that σ^d projects onto the tangential space of Σ^d. We thus recover

$$\nabla\cdot\left(\varepsilon\boldsymbol{E}^d\right) = \frac{1}{i\omega}\nabla\cdot\boldsymbol{J}_a \quad \text{in } \Omega\setminus\Sigma^d, \qquad \left[\nu\cdot\left(\varepsilon\boldsymbol{E}^d\right)\right]_{\Sigma^d} = \frac{1}{i\omega}\nabla\cdot\left(\sigma^d\boldsymbol{E}^d\right) \quad \text{on } \Sigma^d,$$

and

$$\boldsymbol{n}\cdot\left(\sigma^d\boldsymbol{E}^d\right) = \nabla\cdot\left(\lambda^d\boldsymbol{E}^d\right) \quad \text{on } \partial\Sigma^d.$$