Homogenization of 3D-dielectric photonic crystals and artificial magnetism.

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Maxwell System in harmonic regime: $\exp(-i\omega t)$

ω : angular frequency: $\frac{\omega}{c} = \frac{2\pi}{\lambda} = k_0$ (wave number)

$\varepsilon(\omega)$: permittivity (nonnegative imaginary part)

$\mu(\omega)$: permeability (real close to 1)

Optical Index: $n(\omega) = \sqrt{\varepsilon\mu} = n' + i\, n''$

where $n' =$ refraction index , $n'' =$ absorption index.

Case of disconnected dielectric inclusions

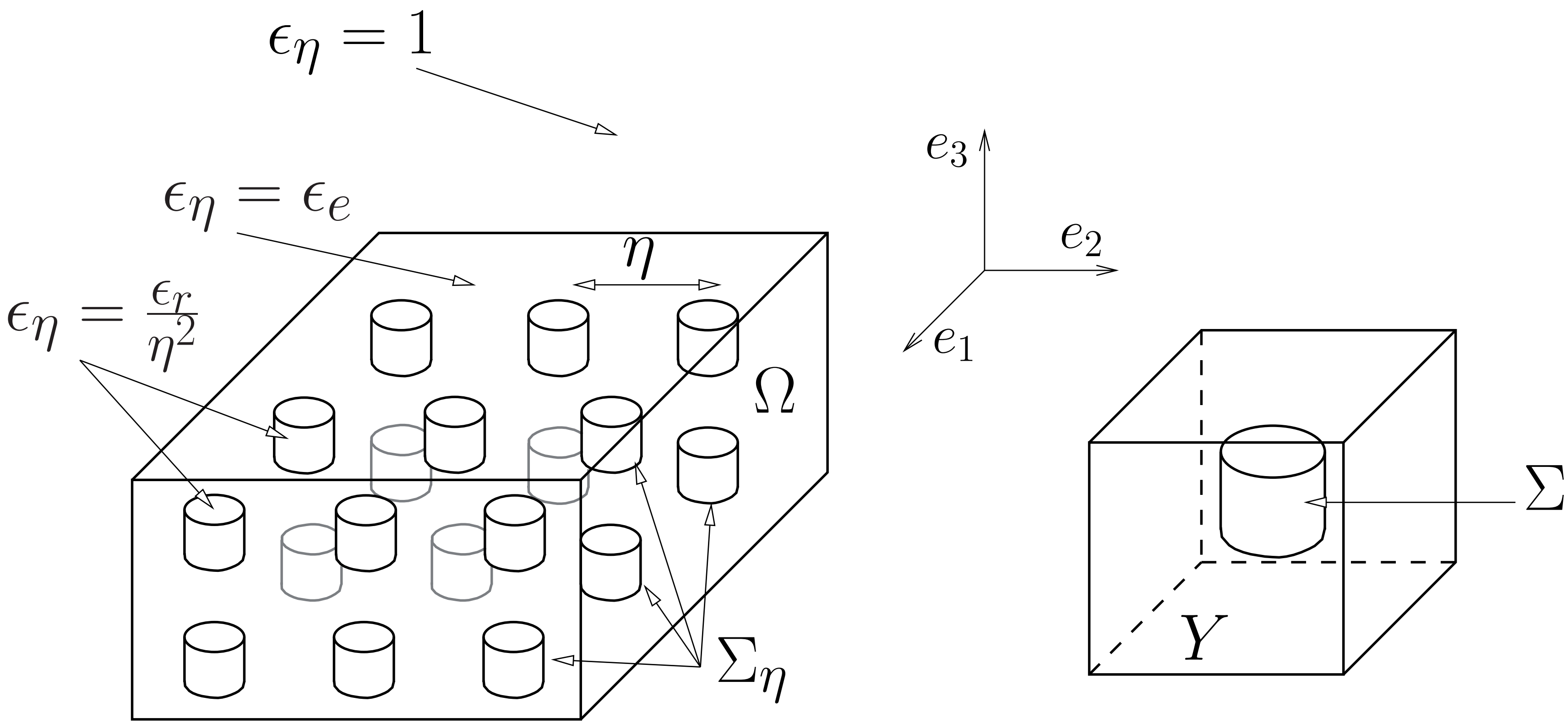

Figure 1: Sketch of the geometry, showing one layer of rings.

The macroscopic domain $\Omega \subset \mathbb{R}^3$ contains $O(\eta^{-3})$ periodic inclusions of diameter $O(\eta)$ filled with high permittivity dielectric (with positive filling ratio)

Geometry and scaling

The heterogeneous structure is placed in a bounded domain $\Omega \subset \mathbb{R}^3$. It consists of periodic high permittivity inclusions (period η) embedded in a lossless dielectric matrix. The inclusions occupy a subregion

$$\Sigma_\eta := \bigcup_{i \in I_\eta} \eta(i + \Sigma) \ , \ I_\eta = \{i \in \mathbb{Z}^2 : \eta(i+\Sigma) \subset\subset \Omega\}.$$

Here $\Sigma \subset\subset Y := (-1/2, 1/2)^3$ is a regular connected domain whose complement $Y^* := Y \setminus \Sigma$ is assumed to be simply connected. The structure, whose relative permeability is assumed to be equal to 1, is characterized by its relative permittivity ε_η given by:

$$\varepsilon_\eta(x) := \begin{cases} \dfrac{\varepsilon_r}{\eta^2} & \text{if } \ x \in \Sigma_\eta \\ \varepsilon_e & \text{if } \ x \in \Omega \setminus \Sigma_\eta \\ 1 & \text{if } \ x \in \mathbb{R}^3 \setminus \Omega \end{cases} \tag{1}$$

We assume that $\varepsilon_r = \varepsilon_r' + i\,\varepsilon_r''$ with $\varepsilon_r' > 0$ and ε_r'' ‘small”

Two scale approach

We start with the energy bound

$$\sup_{\eta} \int_{\mathcal{B}} (|H^{\eta}|^2 + |\varepsilon_\eta||E_\eta|^2) \ < \ +\infty \tag{2}$$

where B is a big ball containing Ω.

Then

- $\{E_\eta, H\eta\}$ is unformly bounded in $L^2(B)$
- The rescaled displacement vectors $J_\eta := \ \eta\varepsilon_\eta \, E_\eta$ is also bounded $L^2(B)$.

We are going to identfy the zero order tem in the expansions

$$\begin{aligned} E_\eta(x) &= E_0(x, x/\eta) \ + \ \eta \, E_1(x, x/\eta) \ + \ \eta^2 \, E_2(x, x/\eta) \\ H_\eta(x) &= H_0(x, x/\eta) \ + \ \eta \, H_1(x, x/\eta) \ + \ \eta^2 \, H_2(x, x/\eta) \\ J_\eta(x) &= J_0(x, x/\eta) \ + \ \eta \, J_1(x, x/\eta) \ + \ \eta^2 \, J_2(x, x/\eta) \end{aligned}$$

Cell problem for $E_0(x,\cdot)$

From It is easy to show that for $x \in \Omega$ the periodic field $E_0(x,\cdot)$ satisfies the equations

$$\mathrm{curl}_y\ E_0 \ = \ 0 \quad \text{in } Y \quad , \quad \mathrm{div}_y\ E_0 \ = \ 0 \quad \text{in } Y \setminus \bar{\Sigma} \quad , \quad E_0 \ = \ 0 \quad \text{in } \Sigma. \quad (3)$$

By the curl-free condition and letting $E(x) = \int_Y E_0(x,y)\,dy$, we search a solution $E_0(x,y) = E(x) + \nabla_y \chi$ for a suitable periodic $\chi \in W^{1,2}_\sharp(Y)$. We are led to:

$$E_0(x,y) = \sum_{i=1}^{3} E_i(x)\, E^i(y)\,, \quad E^i(y) = e_i + \nabla_y \chi_i\,, \quad \Delta\chi_i = 0 \quad \text{on } Y^*\,, \quad \chi_i = -y_i \quad \text{on } \Sigma \quad (4)$$

Note that $E_0(x,y) = E(x)$ for $x \notin \Omega$.

Further we define the effective permittivity tensor $\varepsilon^{\mathrm{eff}}$:

$$A^{\mathrm{hom}}_{i,j} \ := \ \int_Y E^i \cdot E^j\, dy \ = \ \int_{Y^*} (e_i + \nabla_y \chi_i)\cdot(e_j + \nabla_y \chi_j)\, dy \quad , \quad \varepsilon^{\mathrm{eff}} \ := \ \varepsilon_e\, A^{\mathrm{hom}}\,. \quad (5)$$

NB: $\varepsilon^{\mathrm{eff}}$ is **real symmetric positive and independent of the frequency.**

Cell problem for $H_0(x,\cdot)$ and geometric averaging

By using equations Maxwell eq. (**??**), the periodic fields $H_0(x,\cdot)$ and $J_0(x,\cdot)$ satisfy

$$\mathrm{curl}_y\ H_0 + i\omega\varepsilon_0 J_0 = 0 \quad \text{in } Y \quad , \quad \mathrm{div}_y\, H_0 = 0 \quad \text{in } Y \tag{6}$$

$$\mathrm{curl}_y\ J_0 + i\varepsilon_r\omega\mu_0 H_0 = 0 \quad \text{in } \Sigma \quad , \quad J_0 = 0 \quad \text{in } Y\setminus\Sigma \tag{7}$$

By (6), $H_0(x,\cdot)$ belongs to the Sobolev space $W^{1,2}_\sharp(Y;\mathbb{C}^3)$ unlike $J_0(x,\cdot)$ (supported in Σ) which may have a tangential jump across $\partial\Sigma$. The analysis of the full system relies **on the simple connectedness of $Y\setminus\Sigma$.**

Geometric averaging Let $u \in W^{1,2}_\sharp(Y;\mathbb{C}^3)$ such that $\mathrm{curl}\, u = 0$ on $Y\setminus\Sigma$. We associate the *circulation vector* $\oint u \in \mathbb{C}^3$ which is characterized by the identity

$$\int_Y u\cdot\varphi\, dy = \left(\int_Y \varphi\, dy\right)\cdot\left(\oint u\right) \quad \text{if } \varphi \text{ periodic, } \mathrm{div}\,\varphi = 0 \text{ and } \varphi = 0 \text{ on } \Sigma. \tag{8}$$

When u is smooth, the components of $\oint u$ represents the circulation of u along any curve in Y^* connecting opposite points on the faces of ∂Y. In general we have $\oint u \neq \int_Y u dy$ (however equality holds if $\mathrm{curl}\, u = 0$ on all Y). On $Y\setminus\Sigma$ (simply connected), any $u \in X$ can be written in the form

$$u = z + \nabla_y w \quad , \quad z = \oint u \quad , \quad w \in W^{1,2}_\sharp(Y^*)\ .$$

Space of solutions $H_0(x,\cdot)$ is three dimensional

Claim 3. For $i \in \{1,2,3\}$ there is a unique solution $H^i(y)$ to (6)(7) with $\oint H^i = e_i$. Thus

$$H_0(x,) \;=\; \sum_{i=1}^{3} H_i(x)\, H^i(y) \quad \text{for } x \in \Omega \quad , \quad H_0(x,y) \;=\; H(x) \quad \text{for } x \in \mathcal{B} \setminus \Omega \tag{9}$$

The macroscopic field $H(x) = (H_i(x)) \in L^2(\mathcal{B};\mathbb{C}^3)$ is related to the weak limit $[H_0](x) := \int_Y H_0(x,\cdot)$ of (H_η) in $L^2(\mathcal{B};\mathbb{C}^3)$ by the tensorial relation

$$[H_0](x) \;=\; \mu^{\text{eff}}\, H(x) \quad , \quad \mu^{\text{eff}}_{i,j} := \int_Y (H^j \cdot e_i)\, dy \tag{10}$$

The tensor μ^{eff} is symmetric and will be written explicitly by means of a suitable spectral problem (see (16)). Eventually applying (8) to $u = H^i$ and $\varphi = E^j \wedge z$ with E^j given in (4) ($z \in \mathbb{R}^3$), we infer

$$\int_Y (H^i \wedge E^j)\, dy \quad = \quad e^i \wedge e^j \quad , \quad \text{for every } i,j \in \{1,2,3\} \tag{11}$$

The homogenization result

Recalling (5) and (10), we introduce the tensors valued functions

$$\boldsymbol{\mu}(\omega, x) = \begin{cases} \mu^{\text{eff}}(\omega) & \text{for } x \in \Omega \\ I_3 & \text{for } x \in \mathbb{R}^3 \setminus \Omega \end{cases} \quad , \quad \boldsymbol{\varepsilon}(x) = \begin{cases} \varepsilon^{\text{eff}} & \text{for } x \in \Omega \\ I_3 & \text{for } x \in \mathbb{R}^3 \setminus \Omega \end{cases} \tag{12}$$

The limit diffraction problem as $\eta \to 0$ consists in finding $(E, H) \in L^2_{\text{loc}}(\mathbb{R}^3; \mathbb{C}^3)$ such that

$$\begin{cases} curl\, E & = \quad i\omega\mu_0\, \boldsymbol{\mu}(\omega, x)\, H \\ curl\, H & = \quad -i\omega\varepsilon_0\, \boldsymbol{\varepsilon}(x)\, E \\ (E - E^i, H - H^i) & \text{satisfies the O.W.C} \end{cases} \tag{13}$$

NB: 1. The problem (13) is well posed provided ε_r has a positive imaginary part.
2. The field H satifies the usual transmission conditin on $\partial\Omega$. It does not coincide with the weak limit of $H_\eta \sim H_0(x, x/\eta)$

The TM- case

If we consider cylindrical dielectric inclusions (for instance e_3 parallel long rods $\Sigma = D \times \mathbb{R}$) illuminated by a TM polarized incident wave, the situation becomes much simpler:

$$H_0 = u_0(x, y_1, y_2)\, e_3 \quad , \quad u_0(x, \cdot) = u(x) \quad \text{on } Y \setminus \Sigma \quad , \quad H(x) = u(x) e_3$$

(the constancy of $u_0(x, \cdot)$ corresponds to the curl free condition of H_0 on $Y \setminus \Sigma$).

The H_0 cell problem reduces to $u_0(x, y) = u(x)\, w(y)$ where $w \in W^{1,2}_\sharp$ solves

$$\Delta_y w + k^2\, w = 0 \text{ on } D \quad , \quad w = 1 \text{ on } Y_2 \setminus D$$

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Variational formulation of the cell problem

The field $H^i(y)$ solution of (6)(7) with $\oint H^i = e_i$ is searched as $H^i = e_i + u_i$ where u_i solves the variational equation

$$b_0(u_i, v) - k^2\,\varepsilon_r \int u_i \cdot \bar{v}\,dy \;=\; k^2\,\varepsilon_r \int e_i \cdot \bar{v}\,dy\ , \quad \forall v \in X_0\ . \tag{14}$$

where X_0 is the Hilbert space

$$\left\{ u \in W^{1,2}_\sharp(Y;\mathbb{C}^3)\ :\ \mathrm{curl}\ u = 0 \text{ on } Y \setminus \Sigma\ ,\ \oint u = 0 \right\}$$

(note that constant functions are ruled out) equipped with the scalar product:

$$b_0(u, v) \;:=\; \int_Y (\mathrm{curl}\,u \cdot \overline{\mathrm{curl}\,v} + \mathrm{div}\,u \cdot \overline{\mathrm{div}\,v})\,dy\ .$$

The operator B_0 on $L^2(Y;\mathbb{R}^3)$ associated with b_0 has a compact self adjoint resolvent (by the compact embedding of $W^{1,2}_\sharp(Y)$ in $L^2(Y)$)

Spectral problem on the unit cell

The eigenvalue problem in $L^2(Y;\mathbb{R}^3)$

$$b_0(\varphi, v) \;=\; \lambda \int \varphi \cdot \varphi' \, dy \quad , \quad \forall \varphi' \in X_0 \cap L^2(Y;\mathbb{R}^3). \tag{15}$$

has a sequence of real eigenvalues $0 < \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_n \leq \cdots$ $(\lambda_n \to +\infty)$ and we denote by $\{\varphi_n, n \in \mathbb{N}\}$ an orthonormal basis of $L^2(Y;\mathbb{R}^3)$ made of eigenfunctions in X_0. The solution u_i to (14) is given by

$$u_i = \sum_{n\in\mathbb{N}} c_{i,n}\, \varphi_n \quad , \quad c_{i,n} = \frac{\epsilon_r k^2}{\lambda_n - \epsilon_r k^2} \int_Y (e_i \cdot \varphi_n) \, dy$$

The tensor μ^{eff} defined in (10) can be therefore rewritten as an absolutely convergent series

$$\mu^{\text{eff}}_{ij}(\omega) = \delta_{ij} + \sum_{n\in\mathbb{N}} \frac{\varepsilon_r k^2}{\lambda_n - \varepsilon_r k^2} \left(e_j . \int_Y \varphi_n \right) \left(e_i . \int_Y \varphi_n \right) \; . \tag{16}$$

Numerical approach for the spectral problem

To compute eigenvectors φ_n related to (15), we transform into another spectral problem involving the unknown $f = \operatorname{curl} \varphi_n$ (supported in Σ) in the space

$$\mathcal{Z} = \left\{ f \in L^2(\Sigma, \mathbb{R}^3) \ / \ \operatorname{div} f = 0, \ f.n = 0 \text{ on } \partial\Sigma \right\}$$

Step 1. We have noticed that, in view of expansion (16) for μ^{eff}, we may restrict spectral equation (15) taking φ, φ' in $X_0^0 := X_0 \cap \{\operatorname{div} v = 0\}$ Such $\varphi \in X_0^0$ can be uniquely represented by using a periodic divergence free field ψ:

$$\varphi = \operatorname{curl} \psi - z \quad \text{with} \quad z = z(\psi) := \oint \operatorname{curl} \psi \quad (\operatorname{curl} \varphi = -\Delta \psi) \ .$$

Inserting this in (15) with $\varphi, \varphi' \in X_0^0$, we are led to

$$\int_\Sigma \Delta\psi \, \Delta\psi' = \lambda \left(- \int_\Sigma \psi \Delta\psi' + z(\psi).z(\psi') \right) \qquad (*)$$

Step 2. We rewrite (*) in term of $f := -\Delta\psi, \ g := -\Delta\psi'$ (seen as elements of $\mathcal{Z}$). Denote, for every $f \in Z$, the divergence free fields

- Hf the restriction to Σ of $\psi \in H^1_\sharp(Y)$ solution of $-\Delta\psi = f, \int_Y \psi = 0$.
- $\Gamma f(y) := \frac{1}{4} \left(\int_\Sigma y \wedge f(y) \, dy \right) \wedge y$.

Equivalent spectral problem on Σ

We define the operator $A : \mathcal{Z} \mapsto \mathcal{Z}$ by

$$A: \; f \in \mathcal{Z} \; \longrightarrow Hf + \Gamma f + Rf \; ,$$

where $Rf = \nabla\rho$, ρ being is the unique solution of

$$\Delta\rho = 0 \; , \; \frac{\partial\rho}{\partial n} = -(Hf + \Gamma f).n \text{ in } \partial\Sigma \; .$$

From (*) we are led to:

$$\int_\Sigma Af.g \; = \; \frac{1}{\lambda} \int_\Sigma f.g \; .$$

Summarizing, we need to compute the eigenvalues λ_n^{-1} and eigenfunctions of of the positive compact self adjoint operator A and the resulting μ^{eff} is recovered from (16) exploiting relation

$$\int_Y \varphi_n \; = \; \frac{1}{2} \int_\Sigma y \wedge f_n .$$

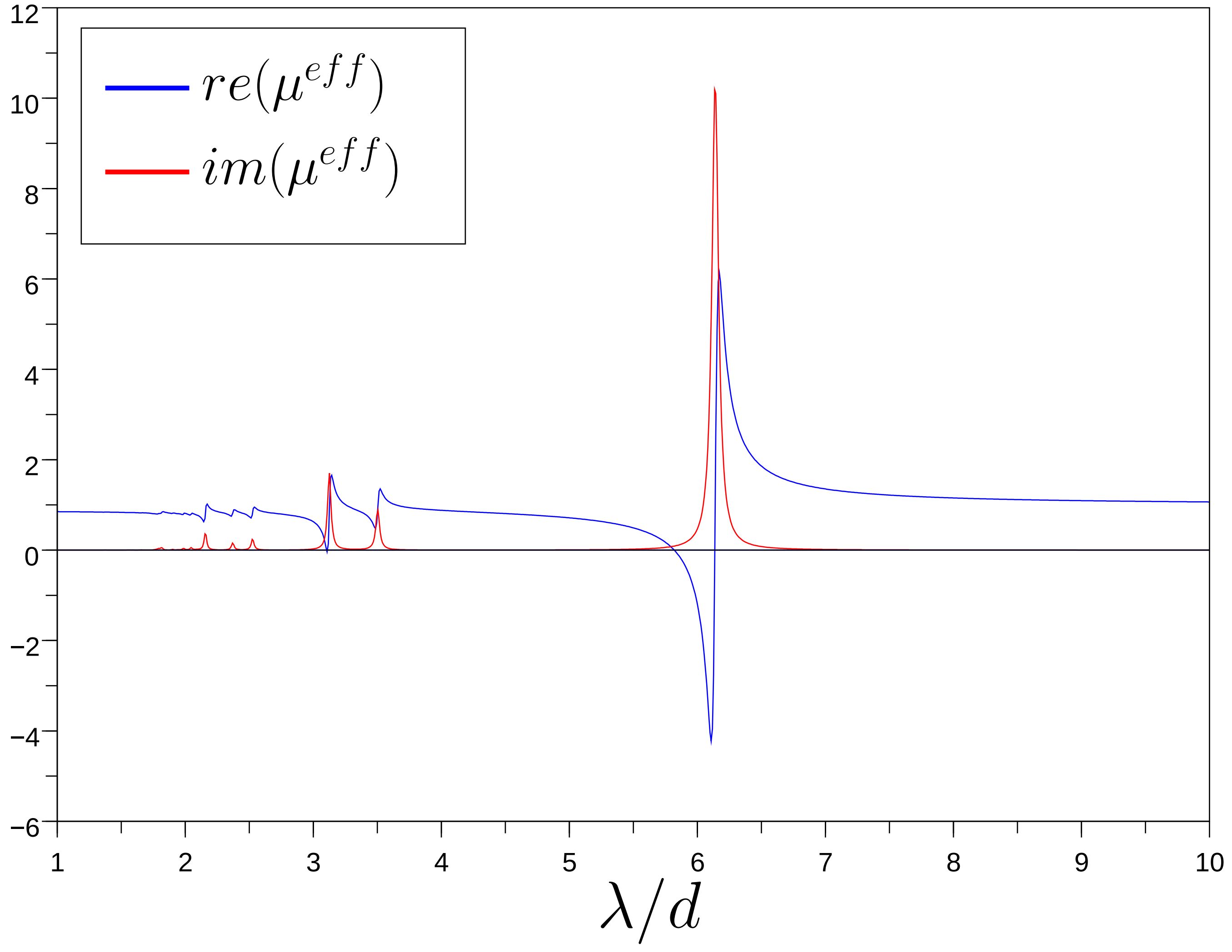

Figure 2: Case $\varepsilon_r := 100 + i$ and $\Sigma := [-0.25, 0.25]^3$.

More numerical results

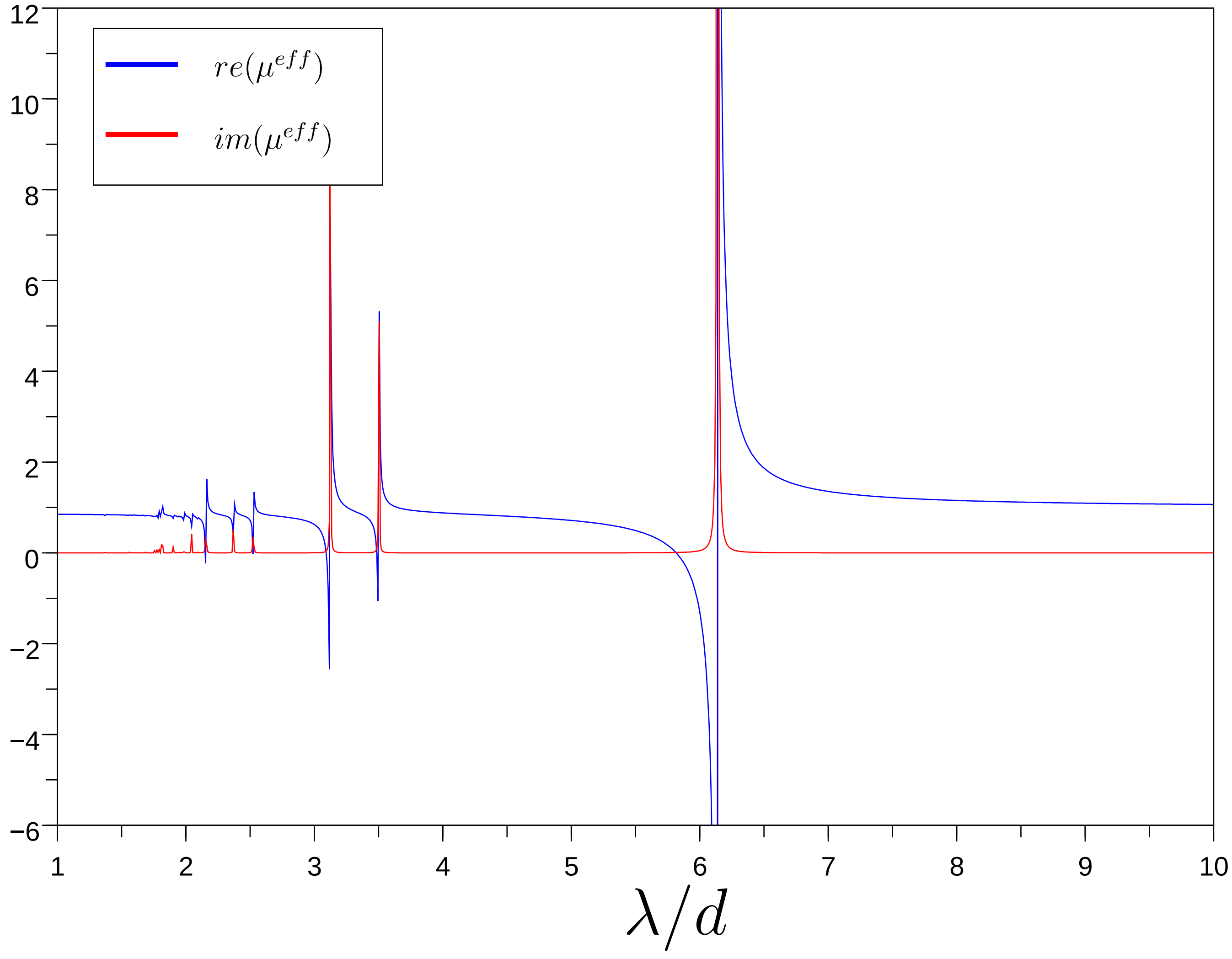

Figure 3: Case $\varepsilon_r := 100 + 0.1i$ and $\Sigma := [-0.25, 0.25]^3$.