A High-Order Perturbation of Surfaces Method for Electromagnetic Scattering by multiply Layered Periodic Crossed Gratings *

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- Seismic imaging
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- Plasmonic nano-structures

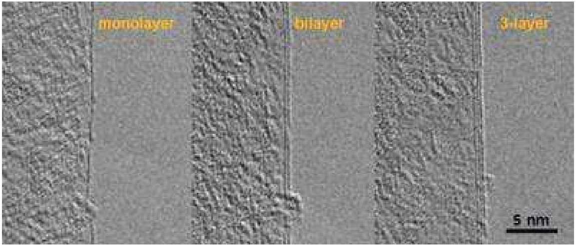
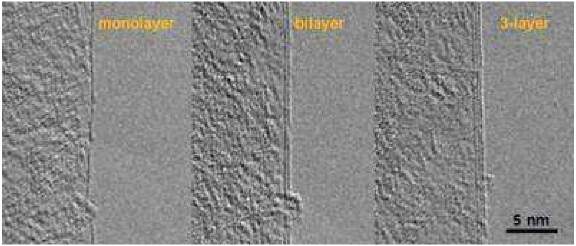


Figure: Examples of multiple layered structures (graphene films with different number of layers)‡

‡Nature Nanotechnology (doi:10.1038/nnano.2010.132)



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Rmk: Numerical simulations are very useful since building device is complicated and expensive.

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Maxwell's equations

The Maxwell's equations state that the field variables and sources occupied by the electromagnetic field: Using the constitutive equations, consider the time-harmonic Maxwell system:

$$\nabla \times \mathbf{E} = ik\mu_r \mathbf{H}, \qquad \nabla \cdot (\varepsilon_{\mathbf{r}} \mathbf{E}) = -\frac{1}{k^2} \nabla \cdot \mathbf{F}$$

$$\nabla \times \mathbf{H} = -ik\varepsilon_r \mathbf{E} - \frac{1}{ik} \mathbf{F}, \qquad \nabla \cdot (\mu_r \mathbf{H}) = 0,$$

where

$$F = ik\mu_0^{1/2} \mathbf{J_a}, \quad \varepsilon_r = \frac{1}{\varepsilon_0}(\varepsilon + \frac{i\sigma}{w}), \quad m_r = \frac{\mu}{\mu_0},$$

and

ω : temporal frequency, $\quad \varepsilon_0$: electric permittivity,

μ_0 : m$agneticpermeability$, $\quad \sigma$: c$onductivity$, $\quad k$: w$avenumber$,

$\mathbf{J_a}$: applied current density.

Aim and methodology

Aim: find a high order numerical method for electromagnetic waves interacting with periodic gratings separating several layers of materials (a small perturbation on the interface).

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Method: high order perturbation of surfaces (HOPS) and modified spectral element (Legendre-Galerkin) method.

Governing equations: Two layers

In 2D setting, the time-harmonic Maxwell equations decouple into two scalar Helmholtz equations. We seek outgoing α-quasiperiodic solutions of

$$\begin{cases} \Delta u + k_u^2 u = 0, \quad y > g(x), \\ \Delta v + k_v^2 v = 0, \quad y < g(x), \\ u - v = -u^{inc} = -e^{i\alpha x - i\beta g(x)}, \quad \text{on} \quad y = g(x) \\ \partial_N u - \partial_N v = -\partial_N u^{inc} \\ \qquad\qquad = -(i\beta + i\alpha \partial_x g(x)) e^{i\alpha x - i\beta g(x)}, \quad \text{on } y = g(x), \\ \text{OWC}[u] = 0, \quad y \longrightarrow \infty, \\ \text{OWC}[v] = 0, \quad y \longrightarrow -\infty, \end{cases}$$

where $u^{inc} = e^{i\alpha x - i\beta y}$ is an incident plane wave. Here, we assume that $g(x)$ stands for a small perturbation; for example,

$$g(x) = \varepsilon f(x),$$

where $f(x) = O(1)$.

For the far-field boundary conditions, consider the hyperplane $y = a$ and $y = -b$

$$
\begin{aligned}
&\Delta u + k_u^2 u = 0, \quad g(x) < y < a,\\
&\partial_y u = \partial_y \nu^+, \quad y = a,\\
&u = \nu^+, \quad y = a,\\
&\Delta \nu^+ + k_u^2 \nu^+ = 0, \quad y > a,\\
&\mathrm{OWC}[\nu^+] = 0, \quad y \longrightarrow \infty,\\
&\Delta v + k_v^2 v = 0, \quad -b < y < g(x),\\
&\partial_y v = \partial_y \nu^-, \quad y = -b,\\
&v = \nu^-, \quad y = -b,\\
&\Delta \nu^- + k_v^2 \nu^- = 0, \quad y < -b,\\
&\mathrm{OWC}[\nu^-] = 0, \quad y \longrightarrow -\infty,\\
&u - v = -e^{i\alpha x - i\beta g(x)}, \quad y = g(x),\\
&\partial_N u - \partial_N v = -(i\beta + i\alpha \partial_x g(x)) e^{i\alpha x - i\beta g(x)}, \quad y = g(x).
\end{aligned}
$$

The Rayleigh Expansions

John William Strutt, Third Baron Rayleigh (Lord Rayleigh) wrote down periodic, outgoing solutions of the Helmholtz equation in 1907. These are the foundation of our High-Order Perturbation of Surfaces (HOPS) algorithms. Setting

$$\alpha_p = \alpha + 2\pi p/d, \quad \beta_p^{u,v} = \begin{cases} \sqrt{(k_{u,v})^2 - \alpha_p^2}, & p \in U^{u,v}, \\ i\sqrt{\alpha_p^2 - (k_{u,v})^2}, & p \notin U^{u,v}, \end{cases}$$

$$U^{u,v} = \{p \in \mathbb{Z} : (k_{u,v})^2 - \alpha_p^2 > 0\},$$

the Rayleigh's expansions:

$$\nu^+ = \sum_{p=-\infty}^{\infty} \hat{\psi}_p e^{i\alpha_p x + i\beta_p^u (y-a)}, \quad \nu^- = \sum_{p=-\infty}^{\infty} \hat{\zeta}_p e^{i\alpha_p x + i\beta_p^v (y+b)},$$

where

$$\psi(x) := u(x,a) = \sum_{p=-\infty}^{\infty} \hat{\psi}_p e^{i\alpha_p x}, \quad \zeta(x) := v(x,-b) = \sum_{p=-\infty}^{\infty} \hat{\zeta}_p e^{i\alpha_p x}.$$

In addition, we compute the Neumann data

$$\partial_y \nu^+(x,a) = \sum_{p=-\infty}^{\infty} (i\beta_p^u)\hat{\psi}_p e^{i\alpha_p x} =: T^u[\psi(x)] = T^u[u(x,a)],$$

$$\partial_y \nu^-(x,-b) = \sum_{p=-\infty}^{\infty} (-i\beta_p^v)\hat{\zeta}_p e^{i\alpha_p x} =: T^v[\zeta(x)] = T^v[v(x,-b)],$$

Hence, we finally study the reduced equations (but equivalent to the governing equations):

$$\begin{aligned}
&\Delta u + k_u^2 u = 0, \quad g(x) < y < a,\\
&\partial_y u - T^u[u] = 0, \quad y = a,\\
&\Delta v + k_v^2 v = 0, \quad -b < y < g(x),\\
&\partial_y v - T^v[v] = 0, \quad y = -b,\\
&u - v = \phi(x), \quad y = g(x),\\
&\partial_N u - \partial_N v = (i\beta + i\alpha\partial_x g(x))\phi(x), \quad y = g(x),\\
&u(x+d, y) = e^{i\alpha d} u(x, y),\\
&v(x+d, y) = e^{i\alpha d} v(x, y),
\end{aligned}$$

where

$$\phi(x) := -e^{i\alpha x - i\beta g(x)}$$

Transformed fields expansions

Domain flattening through a change of variables (σ coordinates or C-method):

$$
\begin{aligned}
x' &= x, \\
y_1 &= a\frac{y-g}{a-g}, \quad g < y < a, \\
y_2 &= b\frac{y-g}{b+g}, \quad -b < y < g.
\end{aligned}
$$

Rewrite the equations

$$
\begin{aligned}
&(\partial_{x'}^2 + \partial_{y_1}^2)u(x', y_1) + (k_u)^2 u(x', y_1) = F^u(x', y_1), \quad 0 < y_1 < a, \\
&\partial_{y_1} u(x', a) - T^u[u(x', a)] = J_u(x'), \\
&(\partial_{x'}^2 + \partial_{y_2}^2)v(x', y_2) + (k_v)^2 v(x', y_2) = F^v(x', y_2), \quad -b < y_2 < 0, \\
&\partial_{y_2} v(x', -b) - T^v[v(x', -b)] = J_v(x'), \\
&u(x', 0) - v(x', 0) = \phi(x'), \\
&\partial_{y_1} u(x', 0) - \partial_{y_2} v(x', 0) = Q(x', 0).
\end{aligned}
$$

Here we define

$$F^u(x', y_1) = \partial_{x'} F^u_x(x', y_1) + \partial_{y_1} F^u_y(x', y_1) + F^u_h(x', y_1),$$

where

$$F^u_x = \frac{2}{a} g \partial_{x'} u - \frac{1}{a^2} g^2 \partial_{x'} u + \frac{a - y_1}{a} (\partial_{x'} g) \partial_{y_1} u - \frac{a - y_1}{a^2} g (\partial_{x'} g) \partial_{y_1} u,$$

$$F^u_y = \frac{a - y_1}{a} (\partial_{x'} g) \partial_{x'} u - \frac{a - y_1}{a^2} g (\partial_{x'} g) \partial_{x'} u - \frac{(a - y_1)^2}{a^2} (\partial_{x'} g)^2 \partial_{y_1} u,$$

$$F^u_h = -\frac{1}{a} (\partial_{x'} g) \partial_{x'} u + \frac{1}{a^2} g (\partial_{x'} g) \partial_{x'} u + \frac{a - y_1}{a^2} (\partial_{x'} g)^2 + \frac{2}{a} k_u^2 g u - \frac{1}{a^2} k_u^2 u,$$

and

$$J_u = -\frac{1}{a} g T^u[u],$$

$$Q = \frac{1}{ab} \{ (ab + ag - bg - g^2)(i\alpha(\partial_{x'} g) + i\beta)\phi(x') - ag \partial_{y_1} u + (\partial_{x'} g)(b + g)(a - g)\partial_{x'} u - (\partial_{x'} g)^2 a(b + g)\partial_{y_1} u - bg \partial_{y_2} v - (\partial_{x'} g)(b + g)(a - g)\partial_{x'} v + (\partial_{x'} g)^2 b(a - g)\partial_{y_2} v \}.$$

Boundary perturbation

Setting $g = \varepsilon f$, we can write

$$u(x, y, \varepsilon) = \sum_{n=0}^{\infty} u_n(x, y)\varepsilon^n,$$
$$v(x, y, \varepsilon) = \sum_{n=0}^{\infty} v_n(x, y)\varepsilon^n.$$

We then derive

$$\begin{aligned}
&\partial_{x'}^2 + \partial_{y_1}^2 u_n(x', y_1) + (k_u)^2 u_n(x', y_1) = F_n^u(x', y_1), \quad 0 < y_1 < a,\\
&\partial_{y_1} u_n(x', a) - T^u[u_n(x', a)] = (J_u)_n(x'),\\
&\partial_{x'}^2 + \partial_{y_2}^2 v_n(x', y_2) + (k_v)^2 v_n(x', y_2) = F_n^v(x', y_2), \quad -b < y_2 < 0,\\
&\partial_{y_2} v_n(x', -b) - T^v[v_n(x', -b)] = (J_v)_n(x'),\\
&u_n(x', 0) - v_n(x', 0) = \phi_n(x'),\\
&\partial_{y_1} u_n(x', 0) - \partial_{y_2} v_n(x', 0) = Q_n(x', 0).
\end{aligned}$$

Note that

$$F^u_n(x', y_1) = \partial_{x'} F^u_{x,n}(x', y_1) + \partial_{y_1} F^u_{y,n}(x', y_1) + F^u_{h,n}(x', y_1),$$

where

$$F^u_{x,n}, F^u_{y,n}, F^u_{h,n} = \text{consist of the terms with } u_{n-1},\ u_{n-2}.$$

Moreover,

$$Q_n = \text{consist of the terms with } u_{n-1},\ u_{n-2},\ u_{n-3}, v_{n-1},\ v_{n-2},\ v_{n-3},$$
$$J^u_n = -\frac{1}{a} f T^u[u_{n-1}],$$
$$J^v_n = \frac{1}{b} f T^v[v_{n-1}],$$
$$\phi_n = (-1)^{n+1} \frac{(i\beta f)^n}{n!} e^{i\alpha x}.$$

Considering

$$u_n(x,y) = \sum_{p=-\infty}^{\infty} u_{n,p} e^{i\alpha_p x}, \quad F_n^u(x,y) = \sum_{p=-\infty}^{\infty} F_{n,p}^u e^{i\alpha_p x},$$

$$Q_n(x) = \sum_{p=-\infty}^{\infty} Q_{n,p} e^{i\alpha_p x}, \quad \phi_n(x) = \sum_{p=-\infty}^{\infty} \phi_{n,p} e^{i\alpha_p x},$$

and also apply the similar expansion on v terms, we obtain a sequence of equations

$$\begin{aligned}
&\partial_{y_1}^2 u_{n,p}(y_1) + (k_u^2 - \alpha_p^2) u_{n,p}(y_1) = F_{n,p}^u(y_1), \quad 0 < y_1 < a, \\
&\partial_{y_1} u_{n,p}(a) - i\beta_p^u u_{n,p}(a) = J_{n,p}^u, \\
&\partial_{y_2}^2 v_{n,p}(y_2) + (k_v^2 - \alpha_p^2) v_{n,p}(y_2) = F_{n,p}^v(y_2), \quad -b < y_2 < 0, \\
&\partial_{y_2} v_{n,p}(-b) + i\beta_p^v v_{n,p}(-b) = J_{n,p}^v, \\
&u_{n,p}(0) - v_{n,p}(0) = \phi_{n,p}, \\
&\partial_{y_1} u_{n,p}(0) - \partial_{y_2} v_{n,p}(0) = Q_{n,p},
\end{aligned}$$

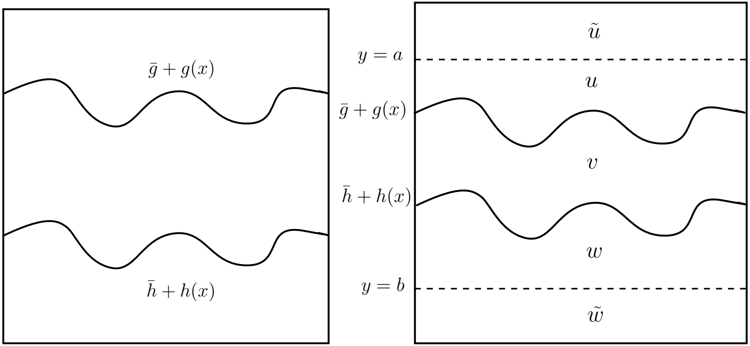
which is a 1D problem.

Governing equations: Three layers

$$\begin{cases} \Delta u + k_u^2 = 0, \quad \text{in } y > \overline{g} + g(x), \\ \Delta v + k_v^2 = 0, \quad \text{in } \overline{h} + h(x) < y < \overline{g} + g(x), \\ \Delta w + k_w^2 = 0, \quad \text{in } y < \overline{h} + h(x), \\ u + u^i = v, \quad \text{on } y = \overline{g} + g(x), \\ \partial_{N_g}(u + u_i) = \tau^2 \partial_{N_g} v, \quad \text{on } y = \overline{g} + g(x), \\ v = w, \quad \text{on } y = \overline{h} + h(x), \\ \partial_{N_h} v = \sigma^2 \partial_{N_h} w, \quad \text{on } y = \overline{h} + h(x), \end{cases}$$

where $\overline{g}$ and $\overline{h}$ are constants (base line) and $u^i = e^{i\alpha x - i\beta y}$ is an incident plane wave. Here, we assume that $g(x)$ and $h(x)$ are small perturbations

Description of artificial boundaries



(a) (b)

Reformulate the equations

Introduce artificial boundaries and boundary conditions to solve the governing equations:

$$
\begin{cases}
\Delta \tilde{u} + k_u^2 \tilde{u} = 0, & \text{in } y > a, \\
\Delta u + k_u^2 u = 0, & \text{in } \overline{g} + g(x) < y < a, \\
\Delta v + k_v^2 v = 0, & \text{in } h + h(x) < y < \overline{g} + g(x), \\
\Delta w + k_w^2 w = 0, & \text{in } b < y < \overline{h} + h(x), \\
\Delta \tilde{w} + k_w^2 \tilde{w} = 0, & \text{in } y < b,
\end{cases}
$$

and the boundary conditions are

$$
\begin{cases}
\tilde{u} = u \quad \text{ on } y = a, \\
\partial_y \tilde{u} = \partial_y u \quad \text{ on } y = a, \\
\mathrm{OWC}[\tilde{u}], \quad \text{ as } y \to \infty, \\
u - v = -e^{i\alpha x - i\beta y} \quad \text{ on } y = \overline{g} + g(x), \\
\partial_{N_g} u - \tau^2 \partial_{N_g} v = (i\alpha \partial_x g(x) + i\beta) e^{i\alpha x - i\beta y} \quad \text{ on } y = \overline{g} + g(x), \\
v = w \quad \text{ on } y = \overline{h} + h(x), \\
\partial_{N_h} v = \sigma^2 \partial_{N_h} w \quad \text{ on } y = \overline{h} + h(x), \\
w = \tilde{w} \quad \text{ on } y = b, \\
\partial_y w = \partial_y \tilde{w} \quad \text{ on } y = b, \\
\mathrm{OWC}[\tilde{w}], \quad \text{ as } y \to -\infty.
\end{cases}
$$

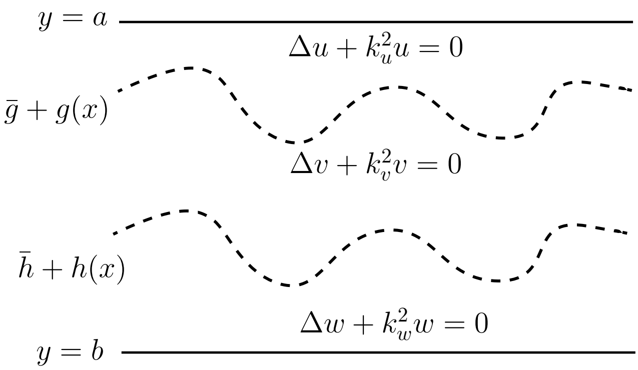
Regarding the similar simplifications as in the two layers case, the governing equation read

$$\begin{cases} \Delta u + k_u^2 u = 0, \quad \text{in } \overline{g} + g(x) < y < a, \\ \partial_y u = T_1[u], \quad \text{on } y = a, \\ \Delta v + k_v^2 v = 0, \quad \text{in } \overline{h} + h(x) < y < \overline{g} + g(x), \\ u - v = -e^{i\alpha x - i\beta y}, \quad \text{on } y = \overline{g} + g(x), \\ \partial_{N_g} u - \tau^2 \partial_{N_g} v = (i\alpha \partial_x g(x) + i\beta) e^{i\alpha x - i\beta y}, \quad \text{on } y = \overline{g} + g(x), \\ \Delta w + k_w^2 w = 0, \quad \text{in } b < y < \overline{h} + h(x), \\ \partial_y w = T_3[w], \quad \text{on } y = b, \\ w = v, \quad \text{on } y = \overline{h} + h(x), \\ \sigma^2 \partial_{N_h} w = \partial_{N_h} v, \quad \text{on } y = \overline{h} + h(x), \end{cases}$$

where

$$\begin{cases} T_1[u] := \sum_{p=-\infty}^{\infty} (i\beta_p^u) \hat{u}_p e^{i\alpha_p x}, \\ T_3[w] := \sum_{p=-\infty}^{\infty} (-i\beta_p^w) \hat{w}_p e^{i\alpha_p x}. \end{cases}$$

Description of reduced domain



TFE revisted

Consider the domain flattening methods via a change of variables.

$$x' = x,$$

$$y_1 = a\Big(\frac{y-(\overline{g}+g)}{a-(\overline{g}+g)}\Big) + \overline{g}\Big(\frac{a-y}{a-(\overline{g}+g)}\Big), \quad \text{where } \overline{g}+g < y < a,$$

$$y_2 = \overline{h}\Big(\frac{y-(\overline{g}+g)}{(\overline{h}+h)-(\overline{g}+g)}\Big) + \overline{g}\Big(\frac{(\overline{h}+h)-y}{(\overline{h}+h)-(\overline{g}+g)}\Big), \quad \text{where } \overline{h}+h <$$

$$y_3 = b\Big(\frac{y-(\overline{h}+h)}{b-(\overline{h}+h)}\Big) + \overline{h}\Big(\frac{b-y}{b-(\overline{h}+h)}\Big), \quad \text{where } b < y < \overline{h}+h.$$

Then, as before the underlying equations becomes

$$\partial_{x'}^2 u_i + \partial_{y_i}^2 u_i + k^2 u_i = \partial_{x'} R_i^x + \partial_{y_i} R_i^y + R_i, \quad 1 \le i \le 3.$$

Introduce the fields expansion

$$u_i = \sum_{n=-\infty}^{\infty} u_{i,n}(x,y)\varepsilon^n,$$

Rearrange in terms of ε orders:

$$\begin{aligned}
&\Delta_{x',y_i} u_{i,n} + k_i^2 u_{i,n} = R_{i,n},\\
&\partial_{y_1} u_n - T_1[u_n] = -\frac{f_g}{a-\overline{g}} T_1[u_{n-1}], \quad \text{on } y_1 = a,\\
&\partial_{y_3} w_n - T_3[u_n] = -\frac{f_h}{b-\overline{h}} T_3[w_{n-1}], \quad \text{on } y_3 = b,\\
&u_n - v_n = -e^{i\alpha x'} e^{-i\beta\overline{g}} \frac{(-i\beta f_g)^n}{n!}, \quad \text{at } y_1 = y_2 = \overline{g},\\
&w_n = v_n, \quad \text{at } y_2 = y_3 = \overline{h},\\
&\partial_{y_1} u_n - \tau^2 \partial_{y_2} v_n = J_{1,n}, \quad \text{at } y_1 = y_2 = \overline{g},\\
&\partial_{y_2} v_n - \sigma^2 \partial_{y_3} w_n = J_{2,n}, \quad \text{at } y_2 = y_3 = \overline{h},
\end{aligned}$$

where $1 \leq i \leq 3$ and $n \geq 0$.

Considering Fourier expansions, we deduce the two point boundary value problem:

$$
\begin{aligned}
&\partial_y^2 u_n^p(y) + (k_u^2 - \alpha_p^2) u_n^p(y) = R_{1,n}^p, \quad \overline{g} < y < a,\\
&\partial_y^2 v_n^p(y) + (k_v^2 - \alpha_p^2) v_n^p(y) = R_{2,n}^p, \quad \overline{h} < y < \overline{g},\\
&\partial_y^2 w_n^p(y) + (k_w^2 - \alpha_p^2) w_n^p(y) = R_{3,n}^p, \quad b < y < \overline{h},\\
&\partial_y u_n^p - i\beta_p^u u_n^p = -\frac{f_g}{a-\overline{g}} T_1^p[u_{n-1}^p] =: \mathcal{B}_{1,n}^p, \qquad \text{at } y = a,\\
&\partial_y w_n^p + i\beta_p^w w_n^p = -\frac{f_h}{b-\overline{h}} T_2^p[w_{n-1}^p] =: \mathcal{B}_{2,n}^p, \qquad \text{at } y = b,\\
&u_n^p(\overline{g}) - v_n^p(\overline{g}) = -e^{-i\beta\overline{g}} \frac{(-i\beta f_g)^n}{n!} =: \zeta_n^p,\\
&w_n^p(\overline{h}) - v_n^p(\overline{h}) = 0,\\
&\partial_y u_n^p(\overline{g}) - \tau^2 \partial_y v_n^p(\overline{g}) = J_{1,n}^p,\\
&\partial_y v_n^p(\overline{h}) - \sigma^2 \partial_y w_n^p(\overline{h}) = J_{2,n}^p.
\end{aligned}
$$

Spitting solutions

Decompose $\{u_n^p, v_n^p, w_n^p\}$ as

$$\{u_n^p, v_n^p, w_n^p\} = \{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\} + \{\check{u}_n^p, \check{v}_n^p, \check{w}_n^p\},$$

where $\{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\}$ homogeneous equations with the boundary conditions and $\{\check{u}_n^p, \check{v}_n^p, \check{w}_n^p\}$ nonhomogeneous equations with homogeneous boundary conditions. For simplicity, dropping $\{n, p\}$ indices, write homogeneous equations

$$\partial_y^2 \tilde{u}(y) + (k_u^2 - \alpha^2)\tilde{u} = 0, \quad \overline{g} < y < a$$

$$\partial_y^2 \tilde{v}(y) + (k_v^2 - \alpha^2)\tilde{v}(y) = 0, \quad \overline{h} < y < \overline{g}$$

$$\partial_y^2 \tilde{w}(y) + (k_w^2 - \alpha^2)\tilde{w} = 0, \quad b < y < \overline{h}$$

$$\partial_y \tilde{u} - i\beta^u \tilde{u} = \mathcal{B}_1, \qquad \text{at } y = a,$$

$$\partial_y \tilde{w} + i\beta^w \tilde{w} = \mathcal{B}_2, \qquad \text{at } y = b,$$

$$\tilde{u}(\overline{g}) - \tilde{v}(\overline{g}) = \zeta, \quad \tilde{w}(\overline{h}) - \tilde{v}(\overline{h}) = 0,$$

$$\partial_y \tilde{u}(\overline{g}) - \tau^2 \partial_y \tilde{v}(\overline{g}) = J_1,$$

$$\partial_y \tilde{v}(\overline{h}) - \sigma^2 \partial_y \tilde{w}(\overline{h}) = J_2.$$

Homogeneous equations

Utilizing the decomposition, the set of solutions $\{\tilde{u}_n^p, \tilde{v}_n^p, \tilde{w}_n^p\}$ can be found explicitly, and the spectral elements methods can be applied to $\{\breve{u}_n^p, \breve{v}_n^p, \breve{w}_n^p\}$.

We first find explicit solutions of $\{\tilde{u}, \tilde{v}, \tilde{w}\}$ by setting

$$
\begin{aligned}
\tilde{u} &= M_1 e^{i\beta^u y} + N_1 e^{-i\beta^u y}, \\
\tilde{v} &= M_2 e^{i\beta^v y} + N_2 e^{-i\beta^v y}, \\
\tilde{w} &= M_3 e^{i\beta^w y} + N_3 e^{-i\beta^w y}
\end{aligned}
$$

By direct computations, we find explicit form of M_i and N_i.

Inhomogeneous equations

To study $\{\check{u}_n^p, \check{v}_n^p, \check{w}_n^p\}$, it requires to use numerical treatments.

$$
\begin{aligned}
&\partial_y^2 \check{u}(y) + (k_u^2 - \alpha^2)\check{u} = R_1, \quad \overline{g} < y < a \\
&\partial_y^2 \check{v}(y) + (k_v^2 - \alpha^2)\check{v}(y) = R_2, \quad \overline{h} < y < \overline{g} \\
&\partial_y^2 \check{w}(y) + (k_w^2 - \alpha^2)\check{w} = R_3, \quad b < y < \overline{h} \\
&\partial_y \check{u} - i\beta^u \check{u} = 0, \qquad \text{at } y = a, \\
&\partial_y \check{w} + i\beta^w \check{w} = 0, \qquad \text{at } y = b, \\
&\check{u}(\overline{g}) - \check{v}(\overline{g}) = 0, \\
&\check{v}(\overline{h}) - \check{w}(\overline{h}) = 0, \\
&\partial_y \check{u}(\overline{g}) - \tau^2 \partial_y \check{v}(\overline{g}) = 0, \\
&\partial_y \check{v}(\overline{h}) - \sigma^2 \partial_y \check{w}(\overline{h}) = 0.
\end{aligned}
\tag{1}
$$

Weak formumation

The weak formulation is: To find $U \in H^1$ such that

$$(\tilde{k}^2 U, \varphi) - (\partial_y U, \partial_y \varphi) + (1-\tau^2)\partial_y v(\bar{g})\overline{\varphi}(\bar{g}) + (\sigma^{-2}-1)\partial_y v(\bar{h})\overline{\varphi}(\bar{h})$$
$$= (R, \varphi) - i\beta_u u(a)\overline{\varphi}(a) - i\beta_w w(b)\overline{\varphi}(b), \quad \forall \varphi \in H^1,$$

where

$$U = \begin{cases} u_N, & y \in I_1, \\ v_N, & y \in I_2, \\ w_N, & y \in I_3, \end{cases} \qquad R = \begin{cases} R_1, & y \in I_1, \\ R_2, & y \in I_2, \\ R_3, & y \in I_3, \end{cases}$$

and

$$I_1 = \{\overline{g} < y < a\}, \quad I_2 = \{\overline{h} < y < \overline{g}\}, \quad I_3 = \{\overline{h} < y < d\}.$$

Discretization

Define the functional space X_N to consider the Legendre-Galerkin method,

$$X_N := \{\varphi \in P_N(I_1), P_N(I_2), P_N(I_3) |\ \partial_y \varphi(a) - i\beta^u \varphi(a) = 0,$$
$$\partial_y \varphi(b) - i\beta^w \varphi(b) = 0\}.$$

Then the Legendre-Galerkin formulation is derived

$$(\tilde{k}^2 U_N, \varphi_N) - (\partial_y U_N, \partial_y \varphi_N) + (1-\tau^2)\partial_y v_N(\bar{g})\overline{\varphi}_N(\bar{g})$$
$$+ (\sigma^{-2} - 1)\partial_y v_N(\bar{h})\overline{\varphi}_N(\bar{h})$$
$$= (I_N R, \varphi_N) - i\beta_u u_N(a)\overline{\varphi}_N(a) - i\beta_w u_N(b)\overline{\varphi}_N(b), \quad \forall \varphi_N \in X_N.$$

By integration by parts on each subdomain, we obtain

$$(\partial_y^2 U_N, \varphi_N) + \tilde{k}^2(U_N, \varphi_N) + \partial_y u_N(\overline{g})\bar{\varphi}_N(\overline{g}) - \tau^2 \partial_y v_N(\overline{g})\bar{\varphi}_N(\overline{g})$$
$$+ \sigma^{-2}\partial_y v_N'(\overline{h})\bar{\varphi}_N(\overline{h}) - \partial_y w_N(\overline{h})\bar{\varphi}_N(\overline{h}) = (I_N R, \varphi_N).$$

Standard Legendre-Galerkin basis

Choose standard combinations of Legendre polynomials

$$\phi_{s,j} := (1+i)L_j(z) + a_{1,j}L_{j+1}(z) + b_{1,j}L_{j+2}(z), \quad 1 \le s \le 3,$$

where $-1 \le z \le 1$ and

$$\begin{aligned}
&(\partial_y \phi_{1,j} - i\beta^u \phi_{1,j})(a) = 0, \qquad \phi_{1,j}(\overline{g}) = 0,\\
&\phi_{2,j}(\overline{g}) = 0, \qquad \phi_{2,j}(\overline{h}) = 0,\\
&\partial_y \phi_{3,j}(b) + i\beta^w \phi_{3,j}(b) = 0, \qquad \phi_{3,j}(\overline{h}) = 0.
\end{aligned}$$

Note that the Legedre-Galerkin basis function vanishes for the transition layers at $y = \overline{g}$ and $\overline{h}$. For this reason, we introduce an additional basis which has a nonzero value on $y = \overline{g}$ and $\overline{h}$.

Connecting (additional) basis

$$\eta_1(y) = \begin{cases} c_1(y - \overline{g}) + 1, \text{ for } \overline{g} \le y \le a, \\ c_2(y - \overline{g}) + 1, \text{ for } \overline{h} \le y \le \overline{g}, \\ 0, \text{ for } \text{ for } b \le y \le \overline{h}, \end{cases}$$

$$\eta_2(y) = \begin{cases} 0, \text{ for } \text{ for } \overline{g} \le y \le \overline{a}, \\ c_3(y - \overline{h}) + 1, \text{ for } \overline{h} \le y \le \overline{g}, \\ c_4(y - \overline{h}) + 1, \text{ for } b \le y \le \overline{h}, \end{cases}$$

such that

$$(\partial_y \eta_1 - i\beta^u \eta_1)(a) = 0, \quad \eta_1(\overline{h}) = 0,$$
$$(\partial_y \eta_2 + i\beta^w \eta_2)(b) = 0, \quad \eta_2(\overline{g}) = 0.$$

Hence, we easily find

$$c_1 = \frac{i\beta^u}{1 - i\beta^u(a - \overline{g})}, \quad c_2 = \frac{1}{\overline{g} - \overline{h}}, \quad c_3 = \frac{1}{\overline{h} - \overline{g}}, \quad c_4 = -\frac{i\beta^w}{1 + i\beta^w(b -$$

Modified LG basis

We define basis functions

$$\tilde{\phi}_j(y) = \begin{cases} \phi_{1,j}(y), & \text{where } \bar{g} < y < a, \\ 0, & \text{where } b < y < \bar{g}, \end{cases} \qquad j = 0, ..., N-2,$$

$$\tilde{\phi}_{N-1+j}(y) = \begin{cases} 0, & \text{where } \bar{g} < y < a \\ \phi_{2,j}(y), & \text{where } \bar{h} < y < \bar{g}, \\ 0, & \text{where } b < y < \bar{h}, \end{cases} \qquad j = 0, ..., N-2,$$

$$\tilde{\phi}_{2N-2+j}(y) = \begin{cases} 0, & \text{where } \bar{h} < y < a \\ \phi_{3,j}(y), & \text{where } \bar{b} < y < \bar{h}, \end{cases} \qquad j = 0, ..., N-2,$$

and

$$\tilde{\phi}_{3N-3}(y) = \eta_1(y), \quad \bar{h} < y < a,$$
$$\tilde{\phi}_{3N-2}(y) = \eta_2(y), \quad b < y < \bar{g}.$$

Modified LG method

Define

$$u^N(y) = \sum_{j=0}^{3N-2} \hat{u}_j \tilde{\phi}_j,$$

and

$$\mathbf{u} = (\hat{u}_0, ..., \hat{u}_{N-2})^T, \quad \mathbf{v} = (\hat{u}_{N-1}, ..., \hat{u}_{2N-3})^T,$$
$$\mathbf{w} = (\hat{u}_{2N-2}, ..., \hat{u}_{3N-4})^T, \quad \mathbf{f} = (\hat{f}_0, ..., \hat{f}_{3N-4})^T,$$

where

$$\hat{f}_j := (I_N f, \tilde{\phi}_j), \quad \text{where } j = 0, ..., 3N-2.$$

We also define the following block matrices

$$(A_{11})_{ij} = (\partial_y^2 \tilde{\phi}_j, \tilde{\phi}_i)_{I_1} + k^2 (\tilde{\phi}_j, \tilde{\phi}_i)_{I_1},$$
$$(C_{11})_{ij} = (\partial_y^2 \tilde{\phi}_{N-1+j}, \tilde{\phi}_{N-1+i})_{I_1} + k^2 (\tilde{\phi}_{N-1+j}, \tilde{\phi}_{N-1+i})_{I_2},$$
$$(B_{11})_{ij} = (\partial_y^2 \tilde{\phi}_{2N-2+j}, \tilde{\phi}_{2N-2+i})_{I_3} + k^2 (\tilde{\phi}_{2N-2+j}, \tilde{\phi}_{2N-2+i})_{I_3},$$

where $0 \leq i, j \leq N-2$.

We set column and row vectors

$$a_{12} = (\partial_y^2 \tilde{\phi}_{3N-3} + k^2 \tilde{\phi}_{3N-3}, \tilde{\phi}_j)_{I_1},$$
$$c_{12} = (\partial_y^2 \tilde{\phi}_{3N-3} + k^2 \tilde{\phi}_{3N-3}, \tilde{\phi}_{N-1+j})_{I_2},$$
$$d_{12} = (\partial_y^2 \tilde{\phi}_{3N-2} + k^2 \tilde{\phi}_{3N-2}, \tilde{\phi}_{N-1+j})_{I_2},$$
$$b_{12} = (\partial_y^2 \tilde{\phi}_{3N-2} + k^2 \tilde{\phi}_{3N-2}, \tilde{\phi}_{2N-2+j})_{I_3},$$

$$a_{21} = (\partial_y^2 \tilde{\phi}_j + k^2 \tilde{\phi}_j, \tilde{\phi}_{3N-3})_{I_1} + \partial_y \tilde{\phi}_j(\bar{g}),$$
$$c_{21} = (\partial_y^2 \tilde{\phi}_{N-1+j} + k^2 \tilde{\phi}_{N-1+j}, \tilde{\phi}_{3N-3})_{I_2} - \tau^2 \partial_y \tilde{\phi}_{N-1+j}(\bar{g}),$$
$$d_{21} = (\partial_y^2 \tilde{\phi}_{N-1+j} + k^2 \tilde{\phi}_{N-1+j}, \tilde{\phi}_{3N-2})_{I_2} + \sigma^{-2} \partial_y \tilde{\phi}_{N-1+j}(\bar{h}),$$
$$b_{21} = (\partial_y^2 \tilde{\phi}_{2N-2+j} + k^2 \tilde{\phi}_{2N-2+j}, \tilde{\phi}_{3N-2})_{I_3} - \partial_y \tilde{\phi}_{2N-2+j}(\bar{h}),$$

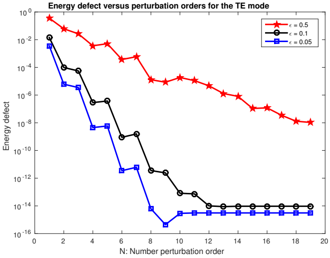
where $0 \leq j \leq N-2$. Moreover, we set

$$a_{22} = (\partial_y^2 \tilde{\phi}_{3N-3} + k^2 \tilde{\phi}_{3N-3}, \tilde{\phi}_{3N-3}) + \partial_y \tilde{\phi}_{3N-3}(\bar{g}^+) - \tau^2 \partial_y \tilde{\phi}_{3N-3}(\bar{g}^-),$$
$$a_{33} = (\partial_y^2 \tilde{\phi}_{3N-2} + k^2 \tilde{\phi}_{3N-2}, \tilde{\phi}_{3N-2}) + \sigma^{-2} \partial_y \tilde{\phi}_{3N-2}(\bar{h}^+) - \partial_y \tilde{\phi}_{3N-2}(\bar{h}^-),$$
$$a_{23} = (\partial_y^2 \tilde{\phi}_{3N-2} + k^2 \tilde{\phi}_{3N-2}, \tilde{\phi}_{3N-3}) + [\partial_y \tilde{\phi}_{3N-2}(\bar{g}^+) - \tau^2 \partial_y \tilde{\phi}_{3N-2}(\bar{g}^-)]\tilde{\phi}$$
$$a_{32} = (\partial_y^2 \tilde{\phi}_{3N-3} + k^2 \tilde{\phi}_{3N-3}, \tilde{\phi}_{3N-2}) + [\sigma^{-2} \partial_y \tilde{\phi}_{3N-3}(\bar{h}^+) - \partial_y \tilde{\phi}_{3N-3}(\bar{h}^-)]$$

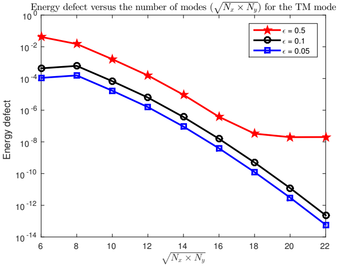
We then write the following system of $3N-1$ equations:

$$\begin{pmatrix} A_{11} & 0 & 0 & a_{12} & 0 \\ 0 & C_{11} & 0 & c_{12} & d_{12} \\ 0 & 0 & B_{11} & 0 & b_{12} \\ a_{21}^T & c_{21}^T & 0 & a_{22} & a_{23} \\ 0 & d_{21}^T & b_{21}^T & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \\ \mathbf{w} \\ \hat{u}_{3N-3} \\ \hat{u}_{3N-2} \end{pmatrix} = \begin{pmatrix} \\ \\ \mathbf{f} \\ \hat{f}_{3N-3} \\ \hat{f}_{3N-2} \end{pmatrix}.$$

Numerical Convergence †



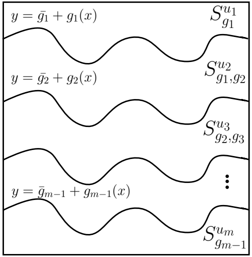
(a) Perturbation order



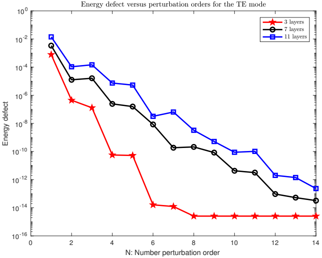
(b) Basis

†H.-Nicholls, J. Comput. Phys. (2017a)

Multiply layered media [†]



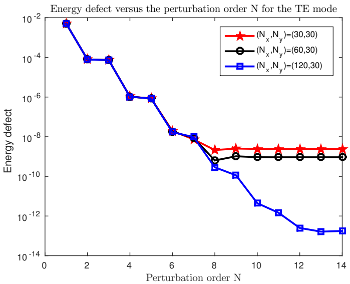
(a) A depiction of a multiply layered grating structure.



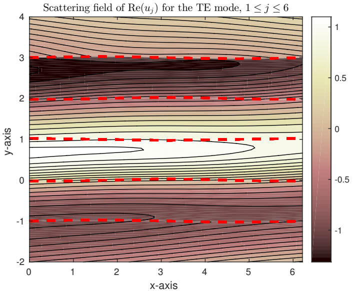
(b) Scattering solution with different numbers of layers.

[†]H.-Nicholls, J. Comput. Phys. (2017b)

Rough interfaces and 3D [†]



(a) Convergence of rough profiles with $\varepsilon = 0.05$



(b) Numerical solution at $x_2 = 0.5$ of the 3D problem

[†] H.-Nicholls, J. Comput. Phys. (2017b)

Maxwell equations in a layered medium*

The time-harmonic Maxwell equations revisited

$$
\begin{aligned}
\nabla \times \mathbf{E}_m &= ik\mu_m \mathbf{H}_m, \\
\nabla \times \mathbf{H}_m &= -ik\varepsilon_m \mathbf{E}_m, \\
\nabla \cdot (\varepsilon_m \mathbf{E}_m) &= 0, \\
\nabla \cdot (\mu_m \mathbf{H}_m) &= 0,
\end{aligned}
$$

with boundary conditions at the interface

$$
\begin{aligned}
\mathbf{n} \times [\mathbf{E}] &= 0, & z &= g(x, y), \\
\mathbf{n} \times [\mathbf{H}] &= \mathbf{J_s}, & z &= g(x, y), \\
\mathbf{n} \cdot [\varepsilon \mathbf{E}] &= 0, & z &= g(x, y), \\
\mathbf{n} \cdot [\mu \mathbf{H}] &= 0, & z &= g(x, y).
\end{aligned}
$$

Here, $[Z]$ is the jump at the interface $[Z] := Z_1 - Z_2$.

*Joint work D. Nicholls (2018)

Assume μ and ε are continuous in the bulk. Using the identity

$$\nabla \times [\nabla \times Z] = -\Delta Z + \nabla(\nabla \cdot Z),$$

the magnetic field becomes

$$\Delta \mathbf{H}_m + \varepsilon_m \mu_m k^2 \mathbf{H}_m = 0,$$

which is the vector Helmholtz equations. At the interface, the transmission BCs are imposed:

$$\begin{cases} \nabla \cdot \mathbf{H}_m = 0, \quad m = 1, 2, \\ \mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = -\mathbf{n} \times \mathbf{H}^{inc}, \\ \mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = -\mathbf{n} \times \mathbf{E}^{inc}, \\ \mathbf{n} \cdot (\mathbf{H}_1 - \mathbf{H}_2) = -\mathbf{n} \cdot \mathbf{H}^{inc}, \end{cases}$$

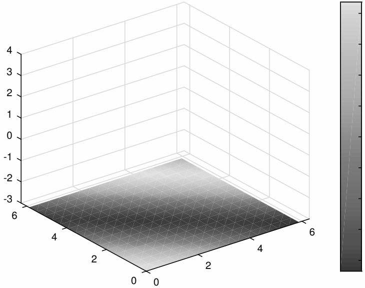
where $\mathbf{n} = (-\partial_x g, -\partial_y g, 1)$.

Then, the time-harmonic Maxwell equations read

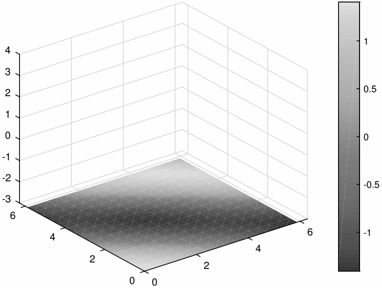
$$\begin{cases} \Delta \mathbf{H}_m + k_m \mathbf{H}_m = 0, \quad \text{in } \Omega_m, \\ \nabla \cdot \mathbf{H}_m = 0, \quad \text{at } \Gamma, \\ \mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = -\mathbf{n} \times \mathbf{H}^{inc}, \quad \text{at } \Gamma, \\ \mathbf{n} \times (\nabla \times (\mathbf{H}_1 - \tau \mathbf{H}_2)) = -\mathbf{n} \times (\nabla \times \mathbf{H}^{inc}), \quad \text{at } \Gamma, \\ \mathbf{n} \cdot (\mathbf{H}_1 - \mathbf{H}_2) = -\mathbf{n} \cdot \mathbf{H}^{inc}, \quad \text{at } \Gamma, \end{cases}$$

where $\tau = \varepsilon_1/\varepsilon_2$ and $\mathbf{H}^{inc} = \mathbf{A} \exp(i(\alpha x + \beta y - \gamma z))$ incidental plane wave.

Numerical results



scattering field of $\mathrm{Re}[H^x]$



scattering field of $\mathrm{Re}[H^z]$

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Journal of Computational Physics, Vol. 330, no. 1, pp. 1043-1068, 2017.

Thank you!!!

Appendix A: Pade approximation

Taylor approximation:

$$v(\varepsilon) = \sum_{n=0}^{N} c_n \varepsilon^n.$$

Pade approximation:

$$[L/M](\varepsilon) = \frac{a^L(\varepsilon)}{b^M(\varepsilon)} = \frac{\sum_{l=0}^{L} a_l \varepsilon^l}{1 + \sum_{m=1}^{M} b_m \varepsilon^m},$$

where

$$\begin{aligned}
a_0 &= c_0, \\
a_1 &= c_1 + c_0 b_1, \\
a_2 &= c_2 + c_1 b_1 + c_0 b_2, \\
a_3 &= c_3 + c_2 b_1 + c_1 b_2 + c_0 b_3, \\
&\ldots
\end{aligned}$$

Then, we find

$$v(\varepsilon) = [L/M](\varepsilon) + O(\varepsilon^{L+M+1}).$$

Appendix B: Energy defect

As an exact solution are unavailable for the governing problems, we use wildly-accepted diagnostic of energy defect to display the spectral accuracy.

Consider the Rayleigh expansions

$$u(x,y) = \sum_{-\infty}^{\infty} \hat{u}_p e^{i\beta_p^u y} e^{i\alpha_p x}, \qquad w(x,y) = \sum_{-\infty}^{\infty} \hat{w}_p e^{i\beta_p^w y} e^{i\alpha_p x},$$

and the "efficiencies" can be defined

$$e_p^u := \frac{\beta_p^u}{\beta} |\hat{u}_p|^2, \quad p \in U^u, \qquad e_p^w := \frac{\beta_p^w}{\beta} |\hat{w}_p|^2, \quad p \in U^w$$

The efficiencies measure the energy at wave mode p propagated away from the grating interface. More precisely,

$$\text{(TE mode):} \qquad \sum_{p \in U^u} e_p^u + \sum_{p \in U^w} e_p^w = 1,$$

$$\text{(TM mode):} \qquad \sum_{p \in U^u} e_p^u + \tau \sum_{p \in U^w} e_p^w = 1.$$

In particular, we can define the "energy defect" for TE and TM modes

$$\text{(TE mode):} \quad \delta_{TE} = 1 - \sum_{p \in U_u} e_p^u - \sum_{p \in U_w} e_p^w,$$

$$\text{(TM mode):} \quad \delta_{TM} = 1 - \sum_{p \in U_u} e_p^u - \tau \sum_{p \in U_w} e_p^w,$$

which should be zero for an exact solution.