Computation of Eigenmodes in 2-Layer Waveguide with a Curved Interface

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1 Basic equation

We start from the two-dimensional Helmholtz equation with a stratified waveguide, and the domain is separated into two parts by an curved interface which is described by $x = h(z)$. The refractive index function

$$n(x) = \begin{cases} n_0 \text{ for } x < h(z) \\ n_1 \text{ for } x > h(z) \end{cases}$$

The Helmholtz equations of optical wave propagation under this case is:

$$\begin{cases} \mathcal{U}_{xx} + \mathcal{U}_{zz} + \kappa_0^2 n^2(x)\mathcal{U} = 0, \quad x \neq h(z) \\ \lim\limits_{x\to+\infty} \mathcal{U} = 0, \quad \mathcal{U}(0) = 0, \\ \lim\limits_{x\to h(z)^-} \mathcal{U} = \lim\limits_{x\to h(z)^+} \mathcal{U}, \\ \dfrac{1}{\rho_0} \lim\limits_{x\to h(z)^-} \dfrac{\partial \mathcal{U}}{\partial \mathbf{n}} = \dfrac{1}{\rho_1} \lim\limits_{x\to h(z)^+} \dfrac{\partial \mathcal{U}}{\partial \mathbf{n}}, \end{cases} \tag{1}$$

$$\rho_0 = \begin{cases} 1 & \text{for TE case,} \\ \frac{1}{n_0^2} & \text{for TM case,} \end{cases} \qquad \rho_1 = \begin{cases} 1 & \text{for TE case,} \\ \frac{1}{n_1^2} & \text{for TM case,} \end{cases}$$

where $\kappa_0 = \frac{2\pi}{\lambda_0}$ is called the vacuum wave number, and $\mathbf{n}$ represents the normal vector of the interface $x = h(z)$ $\kappa_0 = \frac{2\pi}{\lambda_0}$ is the vacuum wave number. We mainly consider TM case in this paper.

Local orthogonal coordinate transform and equation transform

By the local orthogonal coordinate transformation, (1) can be transformed to a new coordinate system $\hat{x}, \hat{z}$. In the new coordinate system,the curved interface $x = h(z)$ is transformed into $\hat{x} = 1$; $x = 0$ and $x = D$ are transformed into $\hat{x} = 0$ and $\hat{x} = D$. For $x \geq D$,the local orthogonal coordinate transform takes a simple form $\hat{x} = x$.

After the coordinate transform, an equation transform $\mathcal{U} = w\mathcal{V}$ is introduced to eliminate $\mathcal{U}_{\hat{x}}$, and w can be solved from this condition. The Helmholtz equation in(1) is transformed to a nonlinear PDE: $\mathcal{V}_{\hat{z}\hat{z}} + \mathcal{A}\mathcal{V}_{\hat{x}\hat{x}} + \mathcal{B}\mathcal{V}_{\hat{x}} + \mathcal{G}\mathcal{V} = 0$

Perfect matched layer

Further, a Perfectly Matched Layer (PML) is applied within the third layer, to truncate the open domain along $\hat{x}$ at $\hat{z} = D_1$.

It can be derived by a complex coordinate stretching,

$$\check{x} = \hat{x} + i\int_0^{\hat{x}} \sigma(s)ds$$

Here $\sigma(s) > 0$ for $D < s < D_1$. This stretching leads to:

$$\frac{d}{d\check{x}} = \frac{1}{1 + i\sigma(\hat{x})}\frac{d}{d\hat{x}}$$

Figure.1 illustrates the of the coordinate transformation and the PML region: the coordinate transform is divided into three layers, with each ranges from $[0, 1], [1, D], [D, D_1]$. We denote values associated with certain layer by superscripts ℓ, where $\ell = 0, 1, 2$ represents the first, second, and third layer transformations.

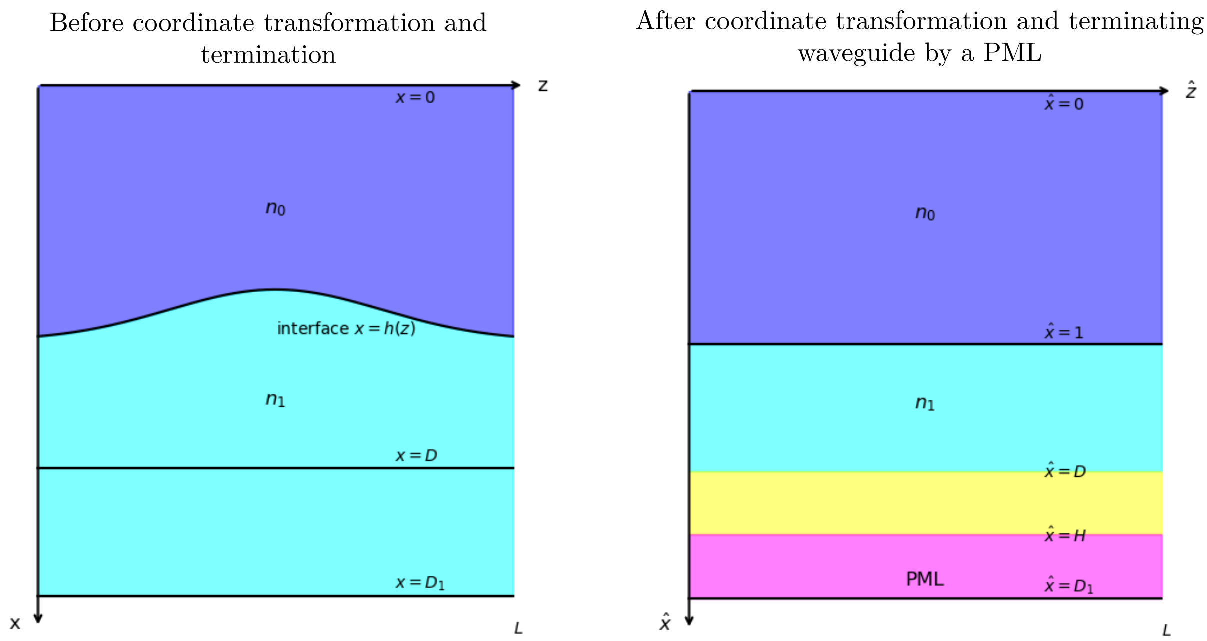

Figure 1: Sketch of the problem.

For more details about the coordinate transform, equation transform and PML, see Refs[3]. After the these three steps, the Helmholtz equation(1) becomes:

$$
\begin{cases}
\mathcal{V}_{\hat{z}\hat{z}} + \mathcal{A}\mathcal{V}_{\hat{x}\hat{x}} + \mathcal{B}\mathcal{V}_{\hat{x}} + \mathcal{G}\mathcal{V} = 0, \quad \hat{x} \in [0,1), (1, D) \\
\mathcal{V}_{\hat{z}\hat{z}} + \dfrac{\mathcal{A}}{1+i\sigma(\hat{x})}\left(\dfrac{1}{1+i\sigma(\hat{x})}\mathcal{V}_{\hat{x}}\right)_{\hat{x}} + \mathcal{G}\mathcal{V} = 0, \quad \hat{x} \in (D, D_1] \\
(w\mathcal{V})\Big|_{\hat{x}=1^-} = (w\mathcal{V})\Big|_{\hat{x}=1^+} \\
\dfrac{1}{\rho_0} w \left\{\dfrac{1}{2}\left[h''(z) - 2\dfrac{h'(z)^2}{h(z)}\right]\mathcal{V} - \dfrac{1+h'(z)^2}{h(z)}\mathcal{V}_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^-} \\
= \dfrac{1}{\rho_1} w \left\{\dfrac{1}{2}\left[h''(z) + 2\dfrac{h'(z)^2}{D-h(z)}\right]\mathcal{V} - \dfrac{D-1}{D-h(z)}\left[1+h'(z)^2\right]\mathcal{V}_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^+}, \\
(w\mathcal{V})\Big|_{\hat{x}=D^-} = (w\mathcal{V})\Big|_{\hat{x}=D^+} \\
w\left(\dfrac{1-D}{h(z)-D}\mathcal{V}_{\hat{x}}\right)\Bigg|_{\hat{x}=D^-} = w\mathcal{V}_{\hat{x}}\Big|_{\hat{x}=D^+}, \\
\mathcal{V}|_{\hat{x}=0} = 0, \quad \mathcal{V}|_{\hat{x}=D_1} = 0.
\end{cases}
\tag{2}
$$

$\mathcal{B} = 0$ in the third layer, thus the terms with $\mathcal{B}$ is does not appear in PML region $[D, D_1]$.

The explicit expressions for $\mathcal{A}, \mathcal{B}, \mathcal{G}$ are in the Ref.[3]. They depend on $\hat{x}$ and $\hat{z}$.

The characteristic problem of the above equation (2) is

$$\begin{cases} \mathcal{A}\phi_{\hat{x}\hat{x}} + \mathcal{B}\phi_{\hat{x}} + \mathcal{G}\phi = \beta^2\phi, \quad \hat{x} \in [0,1),(1,D) \\ \dfrac{\mathcal{A}}{1+i\sigma(\hat{x})}\left(\dfrac{1}{1+i\sigma(\hat{x})}\phi_{\hat{x}}\right)_{\hat{x}} + \mathcal{G}\phi = \beta^2\phi, \quad \hat{x} \in (D, D_1] \\ (w\phi)\Big|_{\hat{x}=1^-} = (w\phi)\Big|_{\hat{x}=1^+} \\ \dfrac{1}{\rho_0}w\left\{\dfrac{1}{2}\left[h''(z) - 2\dfrac{h'(z)^2}{h(z)}\right]\phi - \dfrac{1+h'(z)^2}{h(z)}\phi_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^-} \\ = \dfrac{1}{\rho_1}w\left\{\dfrac{1}{2}\left[h''(z) + 2\dfrac{h'(z)^2}{D-h(z)}\right]\phi - \dfrac{D-1}{D-h(z)}\left[1+h'(z)^2\right]\phi_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^+}, \\ (w\phi)\Big|_{\hat{x}=D^-} = (w\phi)\Big|_{\hat{x}=D^+} \\ w\left(\dfrac{1-D}{h(z)-D}\phi_{\hat{x}}\right)\Bigg|_{\hat{x}=D^-} = w\phi_{\hat{x}}\Big|_{\hat{x}=D^+}, \\ \phi|_{\hat{x}=0} = 0, \quad \phi|_{\hat{x}=D_1} = 0. \end{cases} \tag{3}$$

where β^2 is the eigenvalue.

We are computing characteristic problem at a fixed $\hat{z}$, thus $\mathcal{A}, \mathcal{B}, \mathcal{G}$, and the eigenfunction ϕ now depends only on $\hat{x}$.

Standard form of the characteristic problem

To further convert this eigenvalue problem to standard form, we introduce a new function $\hat{\phi}$ by defining:

$$\phi(\hat{x}) = \hat{\phi}(\hat{x}) \cdot e^{\int_1^{\hat{x}} \mu(s)\,ds} \tag{4}$$

Substitute ϕ in (3), then solve for $\mu(s)$ by eliminating terms with $\hat{\phi}_{\hat{x}}$. We get:

$$\mu(\hat{x}) = -\frac{\mathcal{B}(\hat{x})}{2\mathcal{A}(\hat{x})} \tag{5}$$

And characteristic problem (3) is transformed to standard form:

$$\begin{cases} \mathcal{P}(\hat{x})\hat{\phi} + \mathcal{A}(\hat{x})\hat{\phi}_{\hat{x}\hat{x}} = \beta^2\hat{\phi}, \quad \text{for } \hat{x} \in [0,1),(1,D) \\ \dfrac{\mathcal{A}}{1+i\sigma}\left(\dfrac{1}{1+i\sigma}\hat{\phi}_{\hat{x}}\right)_{\hat{x}} + \mathcal{G}\hat{\phi} = \beta^2\hat{\phi}, \quad \text{for } \hat{x} \in (D, D_1] \\ \left(w\hat{\phi}\right)\Big|_{\hat{x}=1^-} = \left(w\hat{\phi}\right)\Big|_{\hat{x}=1^+} \\ \dfrac{1}{\rho_0}w\left\{\left[\dfrac{1}{2}h''(z) - \dfrac{h'(z)^2}{h(z)} - \dfrac{1+h'(z)^2}{h(z)}\mu\right]\hat{\phi} - \dfrac{1+h'(z)^2}{h(z)}\hat{\phi}_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^-} \\ = \dfrac{1}{\rho_1}w\left\{\left[\dfrac{1}{2}h''(z) + \dfrac{h'(z)^2}{D-h(z)} - \dfrac{D-1}{D-h(z)}\left(1+h'(z)^2\right)\mu\right]\hat{\phi} - \dfrac{D-1}{D-h(z)}\left(1+h'(z)^2\right)\hat{\phi}_{\hat{x}}\right\}\Bigg|_{\hat{x}=1^+}, \\ \left(w\hat{\phi}\right)\Big|_{\hat{x}=D^-} = \left(w\hat{\phi}\right)\Big|_{\hat{x}=D^+}, \\ w\left[\dfrac{1-D}{h(z)-D}\hat{\phi}_{\hat{x}}\right]\Bigg|_{\hat{x}=D^-} = w\hat{\phi}_{\hat{x}}\Big|_{\hat{x}=D^+}, \\ \hat{\phi}|_{\hat{x}=0} = 0, \quad \hat{\phi}|_{\hat{x}=D_1} = 0. \end{cases} \tag{6}$$

where

$$\mathcal{P}(\hat{x}) = \frac{\frac{1}{2}\left(-\mathcal{B}'(\hat{x})\mathcal{A}(\hat{x}) + \mathcal{B}(\hat{x})\mathcal{A}'(\hat{x})\right) - \frac{1}{4}\mathcal{B}^2(\hat{x})}{\mathcal{A}(\hat{x})} + \mathcal{G}(\hat{x}) \tag{7}$$

Here we use the property that $\mu = 0$ when $\hat{z} \geq D$.

2 Dispersion Relation Approximation

Rearranging the eigenvalue equation (6) in the first and second layer:

$$\hat{\phi}_{\hat{z}\hat{z}} + \frac{\mathcal{P}(\hat{x}) - \beta^2}{\mathcal{A}(\hat{x})}\hat{\phi} = 0, \quad \text{for } \hat{x} \in [0,1), (1, D)$$

which we denote as:

$$\hat{\phi}_{\hat{z}\hat{z}} + \mathcal{K}(\hat{x})\hat{\phi} = 0, \tag{8}$$

where $\mathcal{K}(\hat{x}) = \frac{\mathcal{P}(\hat{x})-\beta^2}{\mathcal{A}(\hat{x})}$.

The following derivation is similar to [1]. The function $\mathcal{K}(\hat{x})$ can be approximated by a piecewise polynomial of degree two. We divide the interval $[0, 1]$ into m_0 sub-intervals $[(j-1)l_0, jl_0]$ for $j = 1, 2, \ldots, m_0$, and the interval $[1, D]$ into m_1 sub-intervals $[1 + (j - m_0 - 1)l_1, 1 + (j - m_0)l_1]$ for $j = m_0 + 1, m_0 + 2, \ldots, m_0 + m_1$. These sub-intervals are denoted as $I_j = (\hat{z}_{j-1}, \hat{z}_j)$, where:

$$\hat{x}_j = \begin{cases} jl_0, & \text{if } 1 \le j \le m_0, \\ 1 + (j - m_0)l_1, & \text{if } m_0 + 1 \le j \le m_0 + m_1. \end{cases}$$

On each sub-interval, $\mathcal{K}$ is interpolated using a polynomial of degree two with three nodes chosen at the endpoints and the midpoint.

By approximating $\mathcal{K}$, equation (8) becomes:

$$\frac{d^2 y_j}{d\hat{x}^2} + (a_j\hat{x}^2 + b_j\hat{x} + c_j)y_j = 0, \quad \hat{x} \in I_j \tag{9}$$

where y_j approximates $\hat{\phi}$ on the interval I_j, and the coefficients a_j, b_j, and c_j are defined for each sub-interval. The interpolate coefficients in the first and second layer of coordinate transformation are in the appendixA.

The solution to equation (9) for each interval is given by confluent hyper-geometric functions. Let $\{u_j(\hat{x}), v_j(\hat{x})\}$ be the fundamental solutions on the j-th interval, then:

$$y_j(\hat{x}) = A_j u_j(\hat{x}) + B_j v_j(\hat{x}), \quad \hat{x} \in I_j,$$

for $j = 1, 2, \ldots, m_0 + m_1$.

For the basis solution between $\hat{x} \in [D, D_1]$, using variable $\check{x}$, the equation of the second layer in (6) can be written as:

$$\mathcal{A}\hat{\phi}_{\check{x}\check{x}} + \mathcal{G}\hat{\phi} = \beta^2\hat{\phi}, \quad \text{for } \hat{x} \in (D, D_1] \tag{10}$$

where $\mathcal{A}$ and $\mathcal{G}$ are constants. Denoting $\gamma^{(2)} = \sqrt{\frac{\mathcal{G}-\beta^2}{\mathcal{A}}}$, the solution of (10) is simply:

$$\hat{\phi} = C_1 e^{-i\gamma^{(2)}\check{x}} + C_2 e^{i\gamma^{(2)}\check{x}}, \quad \hat{x} \in (D, D_1]. \tag{11}$$

To maintain consistent notation, we can also express (11) as:

$$y_{m_0+m_1+1}(\hat{x}) = A_{m_0+m_1+1}u_{m_0+m_1+1}(\hat{x}) + B_{m_0+m_1+1}v_{m_0+m_1+1}(\hat{x}),$$

note that we use $\hat{x}$ as variables, instead of $\check{x}$.

Next, we will derive the iterative relations for A_j and B_j by the connection conditions at the interfaces of subinterval. The zero boundary condition $\hat{\phi}(0) = 0$ gives the first relation:

$$A_1 u_1(0) + B_1 v_1(0) = 0 \tag{12}$$

The approximation of $\hat{\phi}$ should be continuous until first order across interpolate sub-intervals, and this condition gives a iterative relation of A_j, B_j within a layer.

And the interface conditions in(6) also lead to relations across interfaces.

Finally, the zero boundary condition at D_1 implies:

$$0 = A_{m_0+m_1+1}e^{-i\gamma^{(2)}\check{D}_1} + B_{m_0+m_1+1}e^{i\gamma^{(2)}\check{D}_1}, \tag{13}$$

where $\check{D}_1 = D_1 + i\int_0^{D_1}\sigma(s)ds$.

A linear system of A_j, B_j can be derived. by combining the above relations:

$$
\begin{cases}
A_1 u_1(0) + B_1 v_1(0) = 0 \\
\\
u_{j+1}(\hat{z_j})A_{j+1} + v_{j+1}(\hat{z_j})B_{j+1} = u_j(\hat{z_j})A_j + v_j(\hat{z_j})B_j, \\
u'_{j+1}(\hat{z_j})A_{j+1} + v'_{j+1}(\hat{z_j})B_{j+1} = u'_j(\hat{z_j})A_j + v'_j(\hat{z_j})B_j. \\
j = 1, \dots, m_0 - 1 \quad \text{and} \quad j = m_0 + 1, \dots, m_0 + m_1 - 1, \\
\\
u_{m_0+1}(1)A_{m_0+1} + v_{m_0+1}(1)B_{m_0+1} = t_{11}\left[u_{m_0}(1)A_{m_0} + v_{m_0}(1)B_{m_0+1}\right], \\
u'_{m_0+1}(1)A_{m_0+1} + v'_{m_0+1}(1)B_{m_0+1} = \\
\left[t_{21}u_{m_0}(1) + t_{22}u'_{m_0}(1)\right]A_{m_0} + \left[t_{21}v_{m_0}(1) + t_{22}v'_{m_0}(1)\right]B_{m_0}, \\
\\
u_{m_0+m_1+1}(D)A_{m_0+m_1+1} + v_{m_0+m_1+1}(D)B_{m_0+m_1+1} = \\
\dot{t}_{11}\left[u_{m_0+m_1}(D)A_{m_0+m_1} + v_{m_0+m_1}(D)B_{m_0+m_1}\right], \\
\\
u'_{m_0+m_1+1}(D)A_{m_0+m_1+1} + v_{m_0+m_1+1}(D)'B_{m_0+m_1+1} = \\
\dot{t}_{22}\left[u'_{m_0+m_1}(D)A_{m_0+m_1} + v'_{m_0+m_1}(D)B_{m_0+m_1}\right], \\
\\
A_{m_0+m_1+1}e^{-i\gamma^{(2)}\bar{D}_1} + B_{m_0+m_1+1}e^{i\gamma^{(2)}\bar{D}_1} = 0
\end{cases}
\tag{14}
$$

denote:

$$
T_{1^-} = \begin{bmatrix} w & 0 \\ \frac{1}{\rho_0}w\left(\frac{1}{2}h''(x) - \frac{h'(x)^2}{h(z)} - \frac{1+h'(x)^2}{h(z)}\mu\right) & -\frac{1}{\rho_0}w\frac{1+h'(x)^2}{h(z)} \end{bmatrix}\Bigg|_{\hat{x}=1^-}
$$

$$
T_{1^+} = \begin{bmatrix} w & 0 \\ \frac{1}{\rho_1}w\left(\frac{1}{2}h''(x) + \frac{h'(x)^2}{D-h(z)} - \frac{D-1}{D-h(z)}\left(1+h'(x)^2\right)\mu\right) & -\frac{1}{\rho_1}w\frac{D-1}{D-h(z)}\left(1+h'(x)^2\right) \end{bmatrix}\Bigg|_{\hat{x}=1^+}
$$

and t_{ij} in the linear system (14) are the elements of $T_{1^+}^{-1}T_{1^-}$:

$$
T_{1^+}^{-1}T_{1^-} = \begin{bmatrix} t_{11} & 0 \\ t_{21} & t_{22} \end{bmatrix}. \tag{15}
$$

Similarly, denote

$$
T_{D^-} = \begin{bmatrix} w & 0 \\ 0 & \frac{(D-1)w}{D-h(z)} \end{bmatrix}\Bigg|_{\hat{x}=D^-}, \quad T_{D^+} = \begin{bmatrix} w & 0 \\ 0 & w \end{bmatrix}\Bigg|_{\hat{x}=D^+} \tag{16}
$$

and $\dot{t}_{ij}$ in (14) are the elements of $T_{D^+}^{-1}T_{D^-}$:

$$
T_{D^+}^{-1}T_{D^-} = \begin{bmatrix} \dot{t}_{11} & 0 \\ 0 & \dot{t}_{22} \end{bmatrix}. \tag{17}
$$

The above linear system for A_j, B_j leads to an algebraic equation for λ, by eliminating all the A_j and B_j. Denote $R_j = \frac{A_j}{B_j}$, $(j = 1, 2, \dots, m_0 + m_1 + 1)$:

$$
R_1 = -\frac{v_1(0)}{u_1(0)}, \tag{18}
$$

$$
R_{j+1} = \frac{R_j\left(u'_j(\hat{z}_j)v_{j+1}(\hat{z}_j) - u_j(\hat{z}_j)v'_{j+1}(\hat{z}_j)\right) - v_j(\hat{z}_j)v'_{j+1}(\hat{z}_j) + v_{j+1}(\hat{z}_j)v'_j(\hat{z}_j)}{R_j\left(u'_{j+1}(\hat{z}_j)u_j(\hat{z}_j) - u'_j(\hat{z}_j)u_{j+1}(\hat{z}_j)\right) + u'_{j+1}(\hat{z}_j)v_j(\hat{z}_j) - u_{j+1}(\hat{z}_j)v'_j(\hat{z}_j)}, \tag{19}
$$

for $j = 1, \dots, m_0 - 1$, and $j = m_0 + 1, \dots, m_0 + m_1 - 1$.

$$
\begin{aligned}
R_{m_0+1} = & \\
& \Big\{ R_{m_0} \left[u'_{m_0}(1) v_{m_0+1}(1) t_{22} + u_{m_0}(1) v_{m_0+1}(1) t_{21} - u_{m_0}(1) v'_{m_0+1}(1) t_{11} \right] + \ldots \\
& v_{m_0}(1) v_{m_0+1}(1) t_{21} - v_{m_0}(1) v'_{m_0+1}(1) t_{11} + v_{m_0+1}(1) v'_{m_0}(1) t_{22} \Big\} \Big/ \\
& \Big\{ R_{m_0} \left[u'_{m_0+1}(1) u_{m_0}(1) t_{11} - u'_{m_0}(1) u_{m_0+1}(1) t_{22} - u_{m_0}(1) u_{m_0+1}(1) t_{21} \right] + \ldots \\
& u'_{m_0+1}(1) v_{m_0}(1) t_{11} - u_{m_0+1}(1) v_{m_0}(1) t_{21} - u_{m_0+1}(1) v'_{m_0}(1) t_{22} \Big\} \qquad (20)
\end{aligned}
$$

$$
\begin{aligned}
R_{m_0+m_1+1} = & \\
& \Big\{ R_{m_0+m_1} \left[\dot{t}_{22}\, v_{m_0+m_1+1}(D)\, u'_{m_0+m_1}(D) - \dot{t}_{11}\, u_{m_0+m_1}(D)\, v'_{m_0+m_1+1}(D) \right] - \ldots \\
& \dot{t}_{11}\, v_{m_0+m_1}(D)\, v'_{m_0+m_1+1}(D) + \dot{t}_{22}\, v_{m_0+m_1+1}(D)\, v'_{m_0+m_1}(D) \Big\} \Big/ \\
& \Big\{ R_{m_0+m_1} \left[\dot{t}_{11}\, u_{m_0+m_1}(D)\, u'_{m_0+m_1+1}(D) - \dot{t}_{22}\, u_{m_0+m_1+1}(D)\, u'_{m_0+m_1}(D) \right] + \ldots \\
& \dot{t}_{11}\, v_{m_0+m_1}(D)\, u'_{m_0+m_1+1}(D) - \dot{t}_{22}\, u_{m_0+m_1+1}(D)\, v'_{m_0+m_1}(D) \Big\} \qquad (21)
\end{aligned}
$$

$$
R_{m_0+m_1+1} = -e^{2i\gamma^{(2)}\check{D}_1}, \qquad (22)
$$

The values of u_j and v_j depend on β^2, so the dispersion relation is expressed as a function of β^2. Recursively solving for $R_{m_0+m_1+1}$ through (18), (19), (20), and (21), we get the final dispersion relation:

$$
g(\beta^2) = R_{m_0+m_1+1} + e^{2i\gamma^{(2)}\check{D}_1} = 0. \qquad (23)
$$

3 Special Case: Flat Interface

When the waveguide interface is flat, with $h(z) \equiv 1$, the orthogonal coordinate transformation reduces to an identity mapping, i.e., $(\hat{x}, \hat{z}) = (x, z)$. And the equation coefficients in (2) are simplified to:

$$
\mathcal{A} = 1, \quad \mathcal{B} = 0, \quad \mathcal{G} = \kappa_0^2 n(x)^2,
$$

Therefore, the eigenvalue problem (6) is reduced to:

$$
\begin{cases}
\hat{\phi}_{\hat{x}\hat{x}} + \kappa_0^2 n(x)^2 \hat{\phi} = \beta^2 \hat{\phi}, \\
\hat{\phi}|_{\hat{x}=1^-} = \hat{\phi}|_{\hat{x}=1^+}, \\
\dfrac{1}{\rho_0} \hat{\phi}_{\hat{x}}|_{\hat{x}=1^-} = \dfrac{1}{\rho_1} \hat{\phi}_{\hat{x}}|_{\hat{x}=1^+}, \\
\hat{\phi}|_{\hat{x}=D^-} = \hat{\phi}|_{\hat{x}=D^+}, \\
\hat{\phi}_{\hat{x}}|_{\hat{x}=D^-} = \hat{\phi}_{\hat{x}}|_{\hat{x}=D^+}, \\
\hat{\phi}|_{\hat{x}=0} = 0, \quad \hat{\phi}|_{\hat{x}=D_1} = 0.
\end{cases} \qquad (24)
$$

with

$$
n(x) = \begin{cases} n_0, & \text{if } x \in [0, 1), \\ n_1, & \text{if } x \in (1, D_1], \end{cases}
$$

Again, we consider TM case only, so $\rho_0 = n_0^2, \rho_1 = n_1^2$

Define the following parameters:

$$
\gamma^{(0)} = \sqrt{\kappa_0^2 n_0^2 - \beta^2}, \quad \gamma^{(1)} = \sqrt{\kappa_1^2 n_1^2 - \beta^2}.
$$

The two basis solutions $\{u_j, v_j\}$ in each sub-interval of the first two layers $[0, 1)$ and $(1, D)$ are simply:

$$
u_j = e^{-i\gamma^{(\ell)}\hat{x}}, \quad v_j = e^{i\gamma^{(\ell)}\hat{x}}, \quad \hat{x} \in I_j, \qquad (25)
$$

$$
\ell = 0 \text{ if } j \leq m_0, \ell = 1 \text{ if } j \geq m_0 + 1
$$

They are already continuous at each sub-interval interfaces $\hat{z}_j$. Thus, the recursive relations for R_j within each layer is simplified to:

$$R_{j+1} = R_j, \quad j = 1, \ldots, m_0 - 1 \quad \text{and} \quad j = m_0 + 1, \ldots, m_0 + m_1 - 1. \tag{26}$$

From the zero boundary condition $\hat{\phi}(0) = 0$, we obtain:

$$R_1 = \frac{A_1}{B_1} = -1.$$

Thus, in the first layer,

$$R_j \equiv -1, \quad j = 1, 2, \ldots, m_0.$$

From the interface condition in (24), the interface condition matrices are reduced to:

$$T_{1^-} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\rho_0} \end{bmatrix}, \quad T_{1^+} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\rho_1} \end{bmatrix}.$$

Similarly, both T_{D^-} and T_{D^+} reduce to the identity matrix. Hence,

$$t_{11} = 1, t_{21} = 0, t_{22} = \frac{\rho_1}{\rho_0}, \quad \dot{t}_{11} = 1, \dot{t}_{22} = 1$$

The relation across the first interface $\hat{x} = 1$, based on (20), is now:

$$R_{m_0+1} = -e^{2i\gamma^{(1)}} \frac{e^{-i\gamma^{(0)}} \left[\gamma^{(0)} \frac{\rho_1}{\rho_0} + \gamma^{(1)}\right] + e^{i\gamma^{(0)}} \left[-\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right]}{e^{-i\gamma^{(0)}} \left[-\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right] + e^{i\gamma^{(0)}} \left[\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right]}. \tag{27}$$

And the relation across the second interface $\hat{x} = D$ is simply:

$$R_{m_0+m_1+1} = R_{m_0+m_1}.$$

Furthermore, since R_j is constant for $j = m_0 + 1, \ldots, m_0 + m_1$ so we have:

$$R_{m_0+m_1+1} = R_{m_0+m_1} = R_{m_0+1}.$$

In this case, $\gamma^{(1)} = \gamma^{(2)}$, so we substitute $\gamma^{(2)}$ with $\gamma^{(1)}$ in (27). The dispersion relation (23) is thus reduced to:

$$-e^{2i\gamma^{(1)}} \frac{e^{-i\gamma^{(0)}} \left[\gamma^{(0)} \frac{\rho_1}{\rho_0} + \gamma^{(1)}\right] + e^{i\gamma^{(0)}} \left[-\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right]}{e^{-i\gamma^{(0)}} \left[-\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right] + e^{i\gamma^{(0)}} \left[\gamma^{(1)} + \gamma^{(0)} \frac{\rho_1}{\rho_0}\right]} + e^{2i\gamma^{(1)} \check{D}_1} = 0. \tag{28}$$

Rearranging and expanding $e^{i\gamma}$ and $e^{-i\gamma}$ into trigonometric functions, we obtain:

$$\frac{i\gamma^{(0)} \frac{\rho_1}{\rho_0} \cos(\gamma^{(0)}) - i\gamma^{(1)} \sin(\gamma^{(0)})}{i\gamma^{(1)} \sin(\gamma^{(0)}) + \gamma^{(0)} \frac{\rho_1}{\rho_0} \cos(\gamma^{(0)})} = e^{2i\gamma^{(1)}(\check{D}_1 - 1)}. \tag{29}$$

Multiplying both the numerator and the denominator of the left-hand side by i, we arrive at the same dispersion relation as in Ref.[5]. This result confirms the theoretical validity of the dispersion relation we derived.

4 Asymptotic Solutions for TM Case

In numerical computation,to solve (23), initial values are needed. Here,asymptotic analysis is introduced to give initial guesses of the solutions.

The coefficients $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{G}$ in equation (2) are varying along the $\hat{x}$-direction, which is similar to the waveguide with varying refractive-index. Differential Transfer Matrix Method(DTMM) can be applied to derive an approximated dispersion relation, The detailed methods are referred to Ref.[4]. We only list some results here:

Let:

$$U = \begin{bmatrix} i\gamma'\hat{x} & 0 \\ 0 & -i\gamma'\hat{x} \end{bmatrix} \tag{30}$$

We have

$$T_{0 \to 1^-} \approx e^{\int_0^1 U \, d\hat{z}}, \quad T_{1^+ \to D^-} \approx e^{\int_1^D U \, d\hat{z}} \tag{31}$$

We denote $\gamma_{01} = \gamma(1^-), \gamma_{11} = \gamma(1^+), \gamma_{1D} = \gamma(D^-)$, and the transfer matrices across the interfaces $\hat{z} = 1$ and D are given below.

$$T_{1^-\to 1^+} = \begin{bmatrix} \frac{e^{-i(\gamma_{01}-\gamma_{11})}(\gamma_{01}t_{22}+\gamma_{11}t_{11}+it_{21})}{2\gamma_{11}} & \frac{e^{i(\gamma_{01}+\gamma_{11})}(-\gamma_{01}t_{22}+\gamma_{11}t_{11}+it_{21})}{2\gamma_{11}} \\ \frac{e^{-i(\gamma_{01}+\gamma_{11})}(-\gamma_{01}t_{22}+\gamma_{11}t_{11}-it_{21})}{2\gamma_{11}} & \frac{e^{i(\gamma_{01}-\gamma_{11})}(\gamma_{01}t_{22}+\gamma_{11}t_{11}-it_{21})}{2\gamma_{11}} \end{bmatrix} \tag{32}$$

The transfer matrix across $z = D$ is:

$$T_{D^-\to D^+} = \begin{bmatrix} \frac{e^{-i(\gamma_{1D}-\gamma^{(2)})}(\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} & \frac{e^{i(\gamma_{1D}+\gamma^{(2)})}(-\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} \\ \frac{e^{-i(\gamma_{1D}+\gamma^{(2)})}(-\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} & \frac{e^{i(\gamma_{1D}-\gamma^{(2)})}(\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} \end{bmatrix} \tag{33}$$

The values of t_{ij} and $\dot{t}_{ij}$ are defined in (15)(17).

When $|\beta^2|$ is large, the matrix (32) can be approximated as:

$$T_{1^-\to 1^+} \approx \begin{bmatrix} \frac{e^{-i(\gamma_{01}-\gamma_{11})}(\gamma_{01}t_{22}+\gamma_{11}t_{11})}{2\gamma_{11}} & \frac{e^{i(\gamma_{01}+\gamma_{11})}(-\gamma_{01}t_{22}+\gamma_{11}t_{11})}{2\gamma_{11}} \\ \frac{e^{-i(\gamma_{01}+\gamma_{11})}(-\gamma_{01}t_{22}+\gamma_{11}t_{11})}{2\gamma_{11}} & \frac{e^{i(\gamma_{01}-\gamma_{11})}(\gamma_{01}t_{22}+\gamma_{11}t_{11})}{2\gamma_{11}} \end{bmatrix} \tag{34}$$

Additionally, when the derivatives of the interface $h(z)$ are small, $\gamma_{1D}\dot{t}_{22} \approx \gamma^{(2)}\dot{t}_{11}$, as demonstrated in Appendix.B. Therefore, the matrix (33) can be approximated as:

$$T_{D^-\to D^+} \approx \begin{bmatrix} \frac{e^{-i(\gamma_{1D}-\gamma^{(2)})}(\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} & 0 \\ 0 & \frac{e^{i(\gamma_{1D}-\gamma^{(2)})}(\gamma_{1D}\dot{t}_{22}+\gamma^{(2)}\dot{t}_{11})}{2\gamma^{(2)}} \end{bmatrix} \tag{35}$$

From the boundary condition $\hat{\phi}(0) = 0$, and $\hat{\phi}(\check{D}_1) = 0$ an equation can be formed:

$$\begin{bmatrix} e^{-i\gamma^{(2)}\check{D}_1}, & e^{i\gamma^{(2)}\check{D}_1} \end{bmatrix} T_{D^-\to D^+} T_{1^+\to D^-} T_{1^-\to 1^+} T_{0\to 1^-} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0 \tag{36}$$

Plugging in the approximated transfer matrices (31), (34), and (35), and expanding the terms, we obtain the approximated dispersion relation:

$$\frac{\gamma_{11}t_{11}\left(-1+e^{2i\int_0^1 \gamma\, d\hat{x}}\right) - \gamma_{01}t_{22}\left(1+e^{2i\int_0^1 \gamma\, d\hat{x}}\right)}{\gamma_{01}t_{22}\left(1+e^{2i\int_0^1 \gamma\, d\hat{x}}\right) + \gamma_{11}t_{11}\left(-1+e^{2i\int_0^1 \gamma\, d\hat{x}}\right)} + e^{2i(\gamma^{(2)}(\check{D}_1-D)+\int_1^D \gamma\, d\hat{x})} \approx 0 \tag{37}$$

4.1 Leaky Mode

Of this kind of mode, the modal field is concentrated in the microstrip substrate, and the PML strongly attenuates the field, which means $|e^{2i\gamma^{(2)}(\check{D}_1-D)}| \approx 0$, the dispersion relation (37) simplifies to:

$$\frac{\gamma_{11}t_{11}+\gamma_{01}t_{22}}{\gamma_{11}t_{11}-\gamma_{01}t_{22}} \approx e^{2i\int_0^1 \gamma\, d\hat{x}} \tag{38}$$

Taking the logarithm on both sides, we get:

$$\ln\left(\frac{\gamma_{11}t_{11}+\gamma_{01}t_{22}}{\gamma_{11}t_{11}-\gamma_{01}t_{22}}\right) + 2m\pi i \approx 2i\int_0^1 \gamma\, d\hat{x}, \quad m \in \mathbb{Z} \tag{39}$$

Assuming $\int_0^1 \gamma\, d\hat{x} = \gamma(\xi_0)$, and define $\gamma_{0*} = \gamma(\xi_0)$, (In order to approximate ξ_0 in practice, it can be observed that, $\gamma = \sqrt{\frac{\mathcal{P}-\beta^2}{\mathcal{A}}} \approx \beta\sqrt{-\frac{1}{\mathcal{A}}}$ when $|\beta^2|$ is large. So the first approximation of ξ_0 is obtained by minimizing $\left|\int_0^1 \sqrt{-\frac{1}{\mathcal{A}}}\, d\hat{x} - \sqrt{-\frac{1}{\mathcal{A}(\xi)}}\right|$. Then, we can use the asymptotic solution to substitute β^2 in γ, and get a more accurate ξ_0.)

Next,we follow the similar derivation as in Ref.[2] to derive the asymptotic solutions. Define:

$$\sigma_{11} = \sqrt{\frac{\mathcal{A}(\xi_0)}{\mathcal{A}(1^+)}}, \quad \sigma_{01} = \sqrt{\frac{\mathcal{A}(\xi_0)}{\mathcal{A}(1^-)}}$$

$$\delta_{11} = \frac{\mathcal{P}(\xi_0)-\mathcal{P}(1^+)}{\mathcal{A}(\xi_0)}, \quad \delta_{01} = \frac{\mathcal{P}(\xi_0)-\mathcal{P}(1^-)}{\mathcal{A}(\xi_0)}$$

Then, we can express γ_{11} and γ_{01} in terms of γ_{0*}:

$$\gamma_{11} = \sigma_{11}\gamma_{0*}\sqrt{1 - \frac{\delta_{11}}{(\gamma_{0*})^2}}, \quad \gamma_{01} = \sigma_{01}\gamma_{0*}\sqrt{1 - \frac{\delta_{01}}{(\gamma_{0*})^2}}$$

Expand them into inverse power series of γ_{0*}, plug into (39), and then expand the left-hand side, we get:

$$2i\gamma_{0*} \approx L_0 + \frac{l_1}{(\gamma_{0*})^2} + \frac{L_4}{(\gamma_{0*})^4} + \dots \tag{40}$$

where:

$$\begin{aligned}
L_0 &= 2im\pi + \ln\left(\frac{\sigma_{11}t_{11} + \sigma_{01}t_{22}}{\sigma_{11}t_{11} - \sigma_{01}t_{22}}\right) \\
l_1 &= \frac{(-\delta_{01} + \delta_{11})\sigma_{01}\sigma_{11}t_{11}t_{22}}{(\sigma_{11}t_{11} - \sigma_{01}t_{22})(\sigma_{11}t_{11} + \sigma_{01}t_{22})} \\
L_4 &= \frac{(\delta_{01} - \delta_{11})\sigma_{01}\sigma_{11}t_{11}t_{22}\left(-(\delta_{01} + 3\delta_{11})\sigma_{11}^2t_{11}^2 + (3\delta_{01} + \delta_{11})\sigma_{01}^2t_{22}^2\right)}{4\left(\sigma_{11}^2t_{11}^2 - \sigma_{01}^2t_{22}^2\right)^2}
\end{aligned}$$

The asymptotic solutions for different orders $\tilde{\gamma}_{0*}^n$ are:

$$\begin{aligned}
\tilde{\gamma}_{0*}^0 &= L_0/2i \\
\tilde{\gamma}_{0*}^2 &= \left(L_0 + \frac{l_1}{(\tilde{\gamma}_{0*}^0)^2}\right)/2i \\
\tilde{\gamma}_{0*}^4 &= \left(L_0 + \frac{l_1}{(\tilde{\gamma}_{0*}^2)^2} + \frac{L_4}{(\tilde{\gamma}_{0*}^2)^4}\right)/2i
\end{aligned} \tag{41}$$

The approximations for $\tilde{\beta}^n$ can be solved from $\tilde{\gamma}_{0*}^n$ by:

$$\tilde{\beta}^n = \sqrt{\mathcal{P}(\xi_0) - \mathcal{A}(\xi_0)\left(\tilde{\gamma}_{0*}^n\right)^2}, \quad n = 0, 2, 4$$

4.2 Berenger Mode

For Berenger modes, the modal field is attenuated in microstrip substrate. Thus $e^{-2i\gamma^{(\ell)}} \approx 0, \ell = 0, 1$, the dispersion relation (37) reduces to:

$$-\frac{\gamma_{11}t_{11} - \gamma_{01}t_{22}}{\gamma_{11}t_{11} + \gamma_{01}t_{22}} \approx e^{2i(\gamma^{(2)}(\check{D}_1 - D) + \int_1^D \gamma\, d\hat{x})} \tag{42}$$

Similar to the discussion of Leaky modes, we assume $\int_1^D \gamma\, d\hat{x} = (D-1)\gamma(\xi_1)$, and denote $\gamma_{1*} = \gamma(\xi_1)$. Then express γ_{11}, γ_{01} and γ_{1*} in terms of γ_2 by defining:

$$\tau_{11} = \sqrt{\frac{\mathcal{A}^{(2)}}{\mathcal{A}(1^+)}}, \quad \tau_{01} = \sqrt{\frac{\mathcal{A}^{(2)}}{\mathcal{A}(1^-)}}, \quad \tau_{1*} = \sqrt{\frac{\mathcal{A}^{(2)}}{\alpha(\xi_1)}}$$

$$\epsilon_{11} = \frac{\mathcal{P}^{(3)} - \mathcal{P}(1^+)}{\mathcal{A}^{(2)}}, \quad \epsilon_{01} = \frac{\mathcal{P}^{(3)} - \mathcal{P}(1^-)}{\mathcal{A}^{(2)}}, \quad \epsilon_{1*} = \frac{\mathcal{P}^{(3)} - \mathcal{P}(\xi_1)}{\mathcal{A}^{(2)}}$$

In particular, as analyzed in Appendix.B, ϵ_{1*} is negligible with the assumption that the derivatives of the interface function $h(z)$ are small. Therefore, the zero-order expansion for γ_{1*} is sufficient:$\gamma_{1*} \approx \tau_{1*}\gamma^{(2)}$.

Take logarithm both sides to the approximated realtion for Berenger mode (42) then expand the left-hand side, we get:

$$2i\gamma^{(2)}\left[(\check{D}_1 - D) + \tau_{1*}(D-1)\right] \approx B_0 + \frac{B_2}{\left(\gamma^{(2)}\right)^2} + \frac{B_4}{\left(\gamma^{(2)}\right)^4} + \dots \qquad m \in \mathbb{Z} \tag{43}$$

where:

$$\begin{aligned}
B_0 &= 2im\pi + \ln\left(\frac{t_{22}\tau_{01} - t_{11}\tau_{11}}{t_{22}\tau_{01} + t_{11}\tau_{11}}\right) \\
B_2 &= \frac{(-\epsilon_{01} + \epsilon_{11})t_{11}t_{22}\tau_{01}\tau_{11}}{(t_{22}\tau_{01} - t_{11}\tau_{11})(t_{22}\tau_{01} + t_{11}\tau_{11})} \\
B_4 &= \frac{(\epsilon_{01} - \epsilon_{11})t_{11}t_{22}\tau_{01}\tau_{11}\left(-(3\epsilon_{01} + \epsilon_{11})t_{22}^2\tau_{01}^2 + (\epsilon_{01} + 3\epsilon_{11})t_{11}^2\tau_{11}^2\right)}{4\left(t_{22}^2\tau_{01}^2 - t_{11}^2\tau_{11}^2\right)^2}
\end{aligned}$$

The asymptotic solutions of different orders $\tilde{\gamma}^{(2)\,n}$are:

$$\tilde{\gamma}^{(2)\,0} = \frac{B_0}{2i\left[(\check{D}_1 - D) + \tau_{1*}(D-1)\right]}$$
$$\tilde{\gamma}^{(2)\,2} = \left(B_0 + \frac{B_2}{\left(\tilde{\gamma}^{(2)\,0}\right)^2}\right) \Big/ 2i\left[(\check{D}_1 - D) + \tau_{1*}(D-1)\right]$$
$$\tilde{\gamma}^{(2)\,4} = \left(B_0 + \frac{B_2}{\left(\tilde{\gamma}^{(2)\,2}\right)^2} + \frac{B_4}{\left(\tilde{\gamma}^{(2)\,2}\right)^4}\right) \Big/ 2i\left[(\check{D}_1 - D) + \tau_{1*}(D-1)\right] \tag{44}$$

The eigenvalue approximations $\tilde{\beta}^n$ can be solved by:

$$\tilde{\beta}^{(2)\,n} = \sqrt{\mathcal{P}^{(2)} - \mathcal{A}^{(2)}\left(\tilde{\gamma}^{(2)\,n}\right)^2} \quad n = 0, 2, 4$$

5 Numerical Example

Since the processes of finding roots for both TE and TM cases are similar,we only consider the TM caseas follows.

In this example, we set geometric parameter $D_1 = 2\mu m$, $D = 1.5\mu m$, and the refractive index in the first layer $n_0 = 2.1$, second layer $n_1 = 1.45$. The wave length $\lambda_0 = 9.6875\mu m$ We choose the curved interface as:

$$h(z) = 1 - 0.2e^{-10(z/10-0.5)^2}$$

The total z direction length is $10\mu m$, and compute the eigenvalues at $z = 6\mu m$.

The Perfectly Matched Layer (PML) parameter is:

$$\sigma(\hat{z}) = \begin{cases} 0, & 0 < \hat{z} \leq H \\ 16\eta^3/(1+\eta^2), & H < \hat{z} \leq D_1 \end{cases}$$

where $\eta = \frac{\hat{z}-H}{D_1-H}$ and $H = 1.75\mu m$. In order to verify the numerical results, we first compare our method with Finite Difference Methods (FDM). In FDM, we divide $[0, D_1]$ into 2000 equally spaced grids. In our new method, both the first and second layers $[0, 1]$ and $[1, D]$ are divided into $m_0 = 128, m_1 = 64$ intervals for interpolation. Müller's method is applied to solve the dispersion relation we derived (37), using eigenvalues from FDM as the initial guess. The termination condition is when $|g| \leq 10^{-10}$. For comparison purpose, the results of several scaled leaky modes β/κ_0 are listed in the table1. We consider Leaky modes only because Berenger modes converges with the similar scale. It can be seem that our methods agrees well with FDM, but requires significantly less computational efforts. Of all the chosen eigenmodes, Müller's method terminates with only 3 steps.

β/κ_0 (by FDM)	β/κ_0 (theoretical)	M	E_r (%)
1.0285563 + 11.4460713i	1.0286153 + 11.4465798i	3	0.0045
0.9977590 + 17.4514507i	0.9975235 + 17.4517659i	3	0.0023
0.9868451 + 23.4012859i	0.9866792 + 23.4012477i	3	0.0007
0.9818287 + 29.3285901i	0.9819297 + 29.3285354i	3	0.0004

Table 1: COMPARISON OF THE RESULTS FOR LEAKY MODES WITH THOSE OBTAINED BY FDM. THE THIRD COLUMN STORES THE STEP NUMBERS M USED IN MULLER'S METHOD

Next, we verify the asymptotic solutions derived in (41) and (44). We implimented Müller's method with $m_0 = 32, m_1 = 16$ and $m_0 = 128, m_1 = 64$ respectively, And the three initial guesses are obtained by the asymptotic solutions of different orders. The iteration stopping criteria is the same as above. Figures 2 demonstrate that the approximate propagation constant β converge very well as m increases

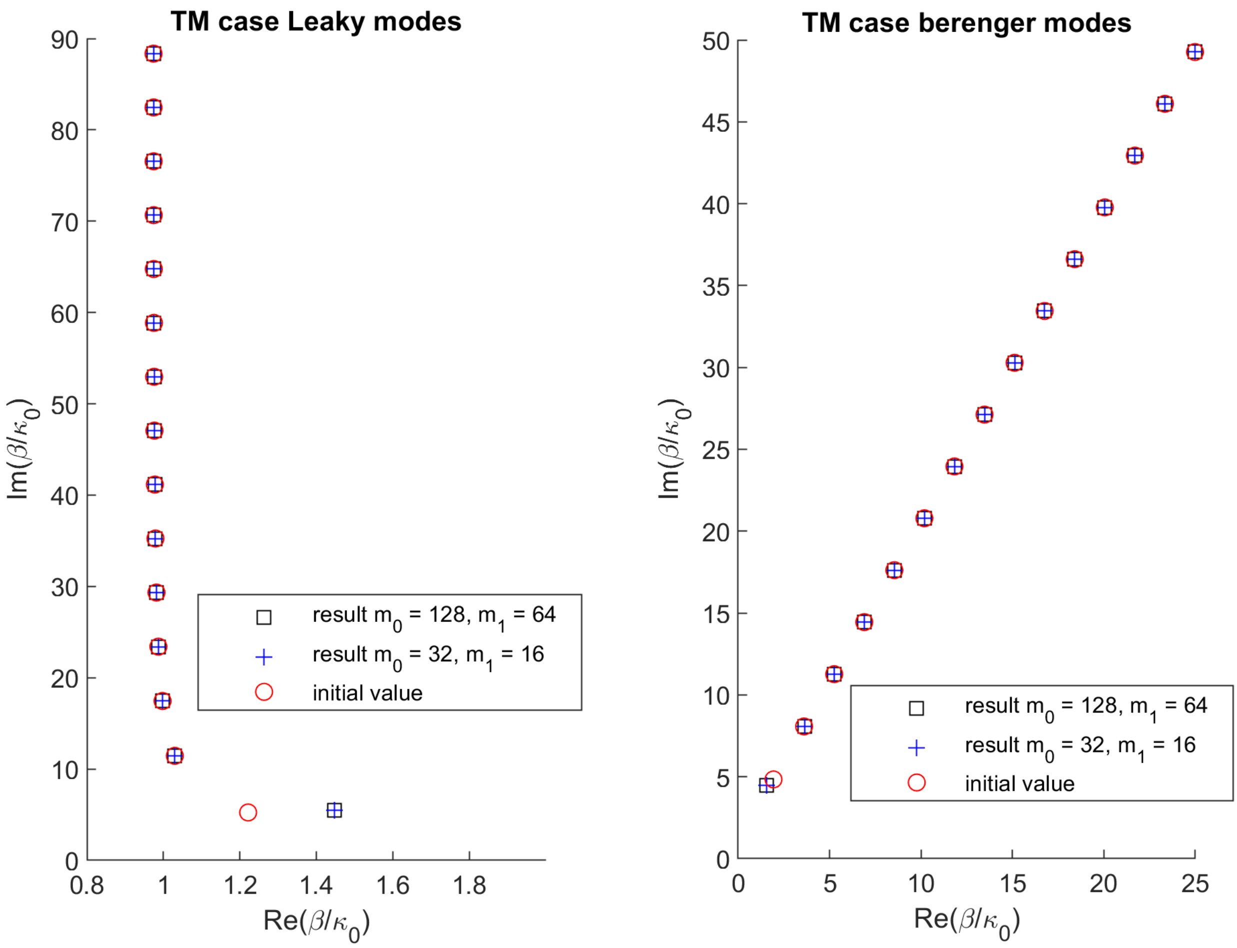

Figure 2: TM leaky modes and Berenger modes for this example, Left: leaky modes. Right: Berenger modes. 'o' stands for β obtained from the asymptotic solutions, '+' stands for the results of β with $m_0 = 32, m_0 = 16$ and '□' stands for the results of β with $m_0 = 128, m_0 = 64$

A interpolate coefficients

For the first layer:

$$\begin{cases} a_j = \dfrac{2K(t_0)}{l_0^2} - \dfrac{4K(t_1)}{l_0^2} + \dfrac{2K(t_2)}{l_0^2}, \\ b_j = \dfrac{(1-4j)K(t_0)}{l_0} + \dfrac{(8j-4)K(t_1)}{l_0} + \dfrac{(3-4j)K(t_2)}{l_0}, \\ c_j = \left(2j^2 - j\right) K(t_0) + \left(4j - 4j^2\right) K(t_1) + \left(2j^2 - 3j + 1\right) K(t_2), \\ t_0 = l_0(j-1), \quad t_1 = (j - 1/2) l_0, \quad t_2 = j l_0, \\ j = 1, 2, \dots, m_0. \end{cases} \tag{45}$$

In the second layer:

$$\begin{cases} a_j = \dfrac{2K(t_0)}{l_1^2} - \dfrac{4K(t_1)}{l_1^2} + \dfrac{2K(t_2)}{l_1^2} \\ b_j = \dfrac{K(t_0)(-4l_1 j + 4l_1 m_0 + l_1 - 4)}{l_1^2} \\ \qquad + \dfrac{K(t_1)(l_1(8j - 8m_0 - 4) + 8)}{l_1^2} \\ \qquad + \dfrac{K(t_2)(l_1(-4j + 4m_0 + 3) - 4)}{l_1^2}, \\ c_j = \dfrac{K(t_0)\left(l_1^2\left(2j^2 - 4jm_0 - j + 2m_0^2 + m_0\right) + l_1(4j - 4m_0 - 1) + 2\right)}{l_1^2} \\ \qquad + \dfrac{4K(t_1)(-l_1(j - m_0 - 1) - 1)(l_1(j - m_0) + 1)}{l_1^2} \\ \qquad + \dfrac{K(t_2)(-l_1(j - m_0 - 1) - 1)(-2l_1 j + 2l_1 m_0 + l_1 - 2)}{l_1^2}, \\ t_0 = 1 + (j - m_0 - 1) l_1, \quad t_1 = 1 + (j - m_0 - 1/2) l_1, \quad t_2 = 1 + (j - m_0) l_1 \\ j = m_0 + 1, m_0 + 1, \dots, m_1 + m_0 \end{cases} \tag{46}$$

B proof of $\gamma^{(1)}(D)\dot{t}_{22} \approx \gamma^{(2)}\dot{t}_{11}$

We will prove the following theorem:

$$\text{If } \max_{x \in [0,L]} \{|h'(x)|, |h''(x)|\} < \delta \tag{47}$$

$$\text{then} |\gamma^{(1)}(D)\dot{t}_{22} - \gamma^{(2)}\dot{t}_{11}| = O(\delta) \tag{48}$$

where $O(\delta)$ represents a small term of the same order as δ.

This theorem is used to simplify the transfer matrix across the second interface (33).

Firstly, we will show that $\mathcal{G}^{(1)}(D)$ and $\mathcal{G}^{(2)}$ from (2) are close when the condition (47) is satisfied. Their expressions are:

$$\begin{aligned} \mathcal{G}^{(1)}(\hat{x}, \hat{z}) = \Bigg\{ & \tfrac{[(D-h(z))/h'(z)]^2 + (D-z)^2}{[D-h(z^*)]^2} \Bigg[\tfrac{h^2(z^*)}{h^2(\hat{z})} \Bigg(-\tfrac{3}{4} \tfrac{\left(h'(\hat{z})\right)^4}{h^2(\hat{z})} \\ & + \tfrac{\left(h'(\hat{z})\right)^4 h''(\hat{z})}{h(\hat{z})} + \tfrac{1}{4}\left(h''(\hat{z})\right)^2 - \tfrac{1}{2} h'(\hat{z}) h_i'''(\hat{z}) \Bigg) + \tfrac{D\left(h'(z^*)\right)^2}{h(z^*)(D-h(z^*))\left[1+(h'(z^*))^2\right]^2} \\ & \times \Bigg(\tfrac{3}{4} \tfrac{\left(h'(z^*)\right)^2 (D-2h(z^*))}{h(z^*)(D-h(z^*))} - \tfrac{h''(z^*)}{1+(h'(z^*))^2} \Bigg) \Bigg] + \tfrac{2\left(h'(z)\right)^2}{(D-h(z))^2} + \tfrac{2h''(z)}{D-h(z)} + \tfrac{h'''(z)}{2h'(z)} \\ & - \tfrac{1}{4} \tfrac{\left(h''(z)\right)^2}{(h'(z))^2} + \kappa_0^2 n_1^2 \Bigg\} \tfrac{(h(\hat{z}))^2 (D-h(z^*))^2 \left(h'(z)\right)^2}{(h(z^*))^2 (h'(\hat{z}))^2 \left[(D-h(z))^2 + (h'(z))^2 (D-z)^2\right]}. \end{aligned} \tag{49}$$

$$
\begin{aligned}
\mathcal{G}^{(2)}(\hat{x},\hat{z}) = {} & \frac{h''(z)}{h(\hat{z})} - \frac{3}{4}\left[\frac{h'(\hat{z})}{h(\hat{z})}\right]^2 + \frac{1}{4}\left[\frac{h''(\hat{z})}{h'(\hat{z})}\right]^2 - \frac{1}{2}\frac{h'''(\hat{z})}{h'(\hat{z})} \\
& + \left\{\frac{h'(z^*)h(\hat{z})}{\left[1+(h'(z^*))^2\right]h'(\hat{z})h(z^*)}\right\}^2 \times \frac{D}{h(z^*)[D-h(z^*)]}\left\{\frac{3}{4}\frac{[D-2h(z^*)]\left[h'(z^*)\right]^2}{h(z^*)[D-h(z^*)]}\right. \\
& \left. - \frac{h''(z^*)}{1+[h'(z^*)]^2}\right\} + \left\{\frac{h'(z)h(\hat{z})[D-h(z^*)]}{h'(\hat{z})h(z^*)[D-h(z)]}\right\}^2 \times \left\{\kappa_0^2 n_1^2 + \frac{h''(z)}{2[D-h(z)]}\right. \\
& \left. + \frac{2h'''(z)h'(z)-\left[h''(z)\right]^2}{4[h'(z)]^2} + \frac{2h''(z)[D-h(z)]+3\left[h'(z)\right]^2}{4[D-h(z)]^2}\right\}.
\end{aligned}
\tag{50}
$$

When the condition (47) is satisfied, $\hat{z} \approx z \approx z^*$, and so we assume they are the same z. At $\hat{z} = D$, the expressions for $\mathcal{G}^{(1)}(D)$ and $\mathcal{G}^{(2)}$ can be simplified:

$$
\mathcal{G}^{(1)}(D) \approx -\frac{3}{4}\frac{h'^2}{h^2} + \frac{h'^2 h''}{h} + \frac{D}{h(D-h)(1+h'^2)^2}\left(\frac{3}{4}\frac{(D-2h)h'^2}{h(D-h)} - \frac{h''}{1+h'^2}\right) + \left(\frac{2h'}{D-h}\right)^2 + \frac{2h''}{D-h} + \kappa_0^2 n_1^2 \tag{51}
$$

$$
\mathcal{G}^{(2)} \approx \frac{h''}{h} - \frac{3}{4}\frac{h'^2}{h^2} + \frac{D}{h(D-h)(1+h'^2)^2}\left(\frac{3}{4}\frac{(D-2h)h'^2}{h(D-h)} - \frac{h''}{1+h'^2}\right) + \kappa_0^2 n_1^2 + \frac{h''}{(D-h)} + \frac{3h'}{4(D-h)^2} \tag{52}
$$

where:

$$
h = h(z), \quad h' = h'(z), \quad h'' = h''(z),
$$

and by subtracting the two, the remaining terms are all of the same order as $h'(z)$ and $h''(z)$. Therefore, we can conclude:

$$
|\mathcal{G}^{(2)} - \mathcal{G}^{(1)}(D)| = O(\delta) \tag{53}
$$

Additionally, at $\hat{x} = D$, the terms $\mathcal{B}, \mathcal{A}', \mathcal{B}'$ in equation (7) are all zero. Therefore, $\mathcal{P}^{(1)}(D) = \mathcal{G}^{(1)}(D)$ and $\mathcal{P}^{(2)} = \mathcal{G}^{(2)}$. By the definition of γ, we have:

$$
\gamma(D)^{(\ell)} = \sqrt{\frac{\mathcal{G}^{(\ell)}(D) - \beta^2}{\mathcal{A}^{(\ell)}(D)}}, \quad \ell = 2, 3
$$

Next, we will show that $\frac{\dot{t}_{11}}{\sqrt{\mathcal{A}^{(2)}}} = \frac{\dot{t}_{22}}{\sqrt{\mathcal{A}^{(1)}(D)}}$: Denote $w_D^{(1)} = w|_{D^-}, w^{(2)} = w|_{D^+}$. By (16):

$$
\dot{t}_{11} = \frac{w_D^{(1)}}{w^{(2)}}, \quad \dot{t}_{22} = \frac{(D-1)w_D^{(1)}}{(D-h(z))w^{(2)}}
$$

Substituting the expression for w, we get:

$$
w_D^{(1)} = \sqrt{\frac{h(\hat{z})}{h'(z)} \cdot \frac{D-h(z^*)}{h(z^*)} \cdot \frac{h'(z)}{(D-h(z))^2}}, \quad w^{(2)} = \sqrt{\frac{h(\hat{z})}{h'(z)} \cdot \frac{D-h(z^*)}{h(z^*)} \cdot \frac{h'(z)}{(D-h(z))}}
$$

Thus, we have:

$$
\dot{t}_{11} = \frac{1}{\sqrt{D-h(z)}}, \quad \dot{t}_{22} = \frac{D-1}{(D-h(z))^{\frac{3}{2}}} \tag{54}
$$

Furthermore, from the expressions for $\mathcal{A}$ and $\mathcal{A}^{(1)}$, we have:

$$
\mathcal{A} = (D-1)^2\frac{[D-h(z^*)]^2\,[h'(z)]^2\,[h(\hat{z})]^2}{(D-h(z))^4\,[h'(z)]^2\,[h(z^*)]^2}, \quad \mathcal{A}^{(1)} = \frac{[D-h(z^*)]^2\,[h'(z)]^2\,[h(\hat{z})]^2}{(D-h(z))^2\,[h'(z)]^2\,[h(z^*)]^2}
$$

It is straightforward to verify:

$$
\sqrt{\mathcal{A}(D)} = \frac{D-1}{D-h(z)}\sqrt{\mathcal{A}^{(1)}} \tag{55}
$$

From equations (54) and (55), it is easy to see that:

$$
\frac{\dot{t}_{11}}{\sqrt{\mathcal{A}^{(1)}}} = \frac{1}{\sqrt{(D-h(z))\mathcal{A}^{(1)}}} = \frac{\dot{t}_{22}}{\sqrt{\mathcal{A}(D)}} \tag{56}
$$

We are now ready to prove the main theorem (48):

$$
|\gamma^{(1)}(D)\dot{t}_{22} - \gamma^{(2)}\dot{t}_{11}| = \left|\frac{\dot{t}_{22}}{\sqrt{\mathcal{A}(D)}}\sqrt{\mathcal{G}^{(1)}(D) - \beta^2} - \frac{\dot{t}_{11}}{\sqrt{\mathcal{A}^{(1)}}}\sqrt{\mathcal{G}^{(2)} - \beta^2}\right|
$$

By the relation (56) and equation (53), the right-hand side of the above expression becomes:

$$\left|\frac{1}{\sqrt{(D-h(z))\mathcal{A}^{(1)}}}\left(\sqrt{\mathcal{G}^{(2)}+O(\delta)-\beta^2}-\sqrt{\mathcal{G}^{(2)}-\beta^2}\right)\right|$$

Expanding $O(\delta)$ to the first order gives $\sqrt{\mathcal{G}^{(2)}+O(\delta)-\beta^2} = \sqrt{\mathcal{G}^{(2)}-\beta^2}+O(\delta)$. Substituting this into the above expression, we obtain:

$$\left|\gamma^{(1)}(D)\dot{t}_{22}-\gamma^{(2)}\dot{t}_{11}\right| = \left|\frac{1}{\sqrt{(D-h(z))\mathcal{A}^{(1)}}}O(\delta)\right| = O(\delta)$$

This proves the theorem (48).

With this theorem, we can provide a brief explanation for $|\mathcal{P}^{(2)}-\mathcal{P}^{(1)}(\xi_1)| = O(\delta)$: one can observe that the derivatives of $\mathcal{A}$, $\mathcal{B}^{(1)}$, and $\mathcal{G}^{(1)}$ are bounded by the derivatives of $h(z)$, namely δ. Assuming $\mathcal{P}^{(1)\prime}(\hat{x})$ exist in $[1, D]$, and therefore, $\mathcal{P}^{(1)\prime}(\hat{x}) = O(\delta)$.

By the property for integral, we have $|\mathcal{P}^{(1)}(\hat{x})-\mathcal{P}^{(1)}(\xi_1)| \leq \sup_{\hat{x}\in(1,D)} |\mathcal{P}^{(1)\prime}(\hat{x})||\hat{x}-\xi_1| = O(\delta)$. Substituting $\hat{x}$ with D, we get $|\mathcal{P}^{(1)}(D)-\mathcal{P}^{(1)}(\xi_1)| = O(\delta)$. Applying the result of (48), we conclude $|\mathcal{P}^{(2)}-\mathcal{P}^{(1)}(\xi_1)| \leq |\mathcal{P}^{(2)}-\mathcal{P}^{(1)}(D)|+|\mathcal{P}^{(1)}(D)-\mathcal{P}^{(1)}(\xi_1)| = O(\delta)$.

References

[1] Jianxin Zhu and Yutian Li. A new approach of eigenmodes for varying refractive-index profile's waveguides. *IEEE Transactions on Microwave Theory and Techniques*, 64(10):3131–3138, 2016.

[2] Jianxin Zhu and Ya Yan Lu. Asymptotic solutions of eigenmodes in slab waveguides terminated by perfectly matched layers. *J. Opt. Soc. Am. A*, 30(10):2090–2095, Oct 2013.

[3] Jianxin Zhu and Guanjie Wang. Fast computation of wave propagation in the open acoustical waveguide with a curved interface. *Wave Motion*, 57:171–181, 2015.

[4] Jianxin Zhu and Yufang Wang. Exact analytical equations for eigenmodes in varying refractive-index profile's waveguides terminated by perfectly matched layers. *Journal of Lightwave Technology*, 33(2):324–332, 2015.

[5] Jianxin Zhu and Ying Zhang. Cross orthogonality between eigenfunctions and conjugate eigenfunctions of a class of modified helmholtz operator for pekeris waveguide. *Journal of Theoretical and Computational Acoustics*, 27(02):1850048, 2019.