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AN ADAPTIVE FINITE ELEMENT METHOD FOR THE WAVE SCATTERING BY A PERIODIC CHIRAL STRUCTURE*

Zhoufeng Wang
School of Mathematics and Statistics, Henan University of Science and Technology, Henan 471023 and Department of Mathematics, Nanjing University, Nanjing 210093, China
Email: zfwang801003@126.com
Peiqi Huang
Department of Applied Mathematics, Nanjing Forestry University, Nanjing 210037, China
Email: pqhuang1979@163.com

Abstract

The electromagnetic wave propagation in the chiral medium is governed by Maxwell's equations together with the Drude-Born-Fedorov (constitutive) equations. The problem is simplified to a two-dimensional scattering problem, and is formulated in a bounded domain by introducing two pairs of transparent boundary conditions. An a posteriori error estimate associated with the truncation of the nonlocal boundary operators is established. Based on the a posteriori error control, a finite element adaptive strategy is presented for computing the diffraction problem. The truncation parameter is determined through sharp a posteriori error estimate. Numerical experiments are included to illustrate the robustness and effectiveness of our error estimate and the proposed adaptive algorithm.

Mathematics subject classification: 35Q61, 65N15, 65N30, 78A45.
Key words: Maxwell's equations, A posteriori error analysis, Adaptive algorithm, Scattering.

1. Introduction

Consider a time-harmonic electromagnetic plane wave incident on a periodic chiral structure in $\mathbb{R}^3$. The medium inside the structure is chiral and nonhomogeneous. In particular, two homogeneous regions are separated by the periodic structure. In this paper, we restrict ourselves to the special case, i.e., by assuming that the chiral structure is periodic in x_1 direction and invariant in x_2 direction, the scattering problem may be simplified to a two-dimensional one. The more general diffraction problem by chiral gratings in $\mathbb{R}^3$ will be discussed in a separate work.

Recently, chiral materials have been studied intensively in the electromagnetic theory literature. In general, the electromagnetic fields inside the chiral medium are governed by Maxwell equations and a set of constitutive equations known as the Drude-Born-Fedorov constitutive equations, in which the electric and magnetic fields are coupled. The property of the chiral media is completely characterized by the electric permittivity ε, the magnetic permittivity μ and the chirality admittance β. On the other hand, periodic structures(grating) have received considerable attention in the past several years because of important applications in integrated optics, optical lenses, antireflective structures, lasers, etc. For the model equations, the

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physical background and computational aspects, there exist lots of results in the literature for the electromagnetic scattering problem in periodic and non-periodic chiral structures. we refer to [3, 4, 15, 27, 30, 41] and the references therein. It should be noted that a good introduction and review on the electromagnetic diffractive in chiral medias can be found in Lakhtakia [30] and Lakhtakia, Varadan and Varadan [31]. Recently, thin chiral coatings and the low frequency behavior of the scatting problems in chiral media are studied by Ammari and Nédélec [2] and Ammari et al [5]. The existence and uniqueness of solutions to the scattering problem are established for biperiodic chiral media in Ammari and Bao [1] and for nonperiodic chiral media in Ammari and Nédélec [3]. The related work on the variational formulations and the numerical analysis for the scattering problems in chiral environment can found in Ammari and Bao [1], Zhang and Ma [43], and Zhang et al [42, 44]. Also see [6, 9, 10, 12, 13, 20, 22, 23, 25, 26] for other related mathematical results and practical applications of Maxwell's equation in general media.

A posteriori error estimates, which measure the actual discrete errors without knowledge of the limit solutions, is computable quantities in terms of discrete solution. Ever since the pioneering work of Babuška and Rheinboldt [8], the adaptive finite element methods based on the a posteriori error estimates have become a class of important numerical tools for solving many model equations, especially for those which have physical features of multiscale phenomenon. We refer to [11, 17, 24, 33–35, 40] for numerical analysis and scientific computations. For the convergence and the quasi-optimality of adaptive finite element methods, some typical works can be found in Dörfler [24], Verfürth [40], Monk, Nochetto, and Siebert [35, 36], Binev, Dahmen and DeVore [16], Mekchay and Nochetto [32], Stevenson [39], Cascon, Kreuzer, Nochetto, and Siebert [17] and Stevenson [39]. In particular, Chen and Wu [20] proposed a new numerical approach with combinations of adaptive finite element method and perfectly matched layer(PML) technique for a 1D grating problem. Based on this numerical tool, great progress has been made in convergence analysis as well as algorithm design for a large class of the scattering problems. We can refer to [11, 14, 18, 19, 21, 28, 29, 45] and the references therein. This approach is very attractive in the scattering problems, mainly because PML can be used to deal with the difficulty in truncating the unbounded domain and the adaptive finite element method can very efficiently capture the local singularities.

The purpose of this paper is to extend our previous work on 1D linear grating problem(cf., [46]) to 1D chiral grating problem. In our approach, the first step is to reduce the problem from an infinite domain into a bounded domain by introducing nonlocal boundary operators, the so-called DtN operators. Then the nonlocal boundary operators are approximately truncated by taking sufficiently many terms of the corresponding infinite series expansions. A finite element formulation with the truncation operators is established for solving the diffractive problem. Finally, we obtain an a posteriori error estimate between the exact solution and finite element solution. The a posteriori error estimate consists of two parts, finite element discretization error and the truncation error of boundary operators. It is easy to see that the truncation error is exponentially decaying when the parameter N with being dependent on the truncation is increased. The adaptive finite element algorithm is also designed to determine the parameter N and choose elements for refinement. The numerical examples are included to show the feasibility and effectiveness of our adaptive algorithm. In the future, we hope that the algorithm can be applied to solve other scientific problems defined on unbounded domain, even those problems that could not be solved with the PML techniques can be solved with our algorithm.

The organization of this paper is as follows. In Section 2, we introduce some notation used in this paper and give the variational formulation for the model problem with the transparent boundary condition. In Section 3 we introduce the truncation approximation of the nonlocal boundary operator and the finite element discretization. A crucial a posteriori estimate is also stated. Section 4, we derive the a posteriori error estimate which includes the finite element discretization error and the truncation error. In Section 5 we describe our adaptive algorithm and present several examples to illustrate the performance of our adaptive method.

2. The Variational Formulation

The electromagnetic fields are governed by the following time-harmonic Maxwell equations(time dependence $e^{-i\omega t}$):

$$\nabla \times \mathbf{E} - i\omega \mathbf{B} = 0, \tag{2.1}$$

$$\nabla \times \mathbf{H} + i\omega \mathbf{D} = 0, \tag{2.2}$$

where **E**, **H**, **D** and **B** denote the electric field, the magnetic field, the electric and magnetic displacement vectors in $\mathbb{R}^3$, respectively. In addition, **E**, **H**, **D** and **B** satisfy the following Drude-Born-Fedorov constitutive equations:

$$\mathbf{D} = \varepsilon(x)(\mathbf{E} + \beta(x)\nabla \times \mathbf{E}), \tag{2.3}$$

$$\mathbf{B} = \mu(x)(\mathbf{H} + \beta(x)\nabla \times \mathbf{H}), \tag{2.4}$$

where $x = (x_1, x_2, x_3)$, ε is electric permittivity, μ is the magnetic permeability, and β is the chirality admittance. By eliminating **D** and **B**, the Maxwell equations may be rewritten as

$$\nabla \times \mathbf{E} = (\gamma(x))^2 \beta(x)\mathbf{E} + i\omega\mu(x)\Big(\frac{\gamma(x)}{k(x)}\Big)^2 \mathbf{H}, \tag{2.5}$$

$$\nabla \times \mathbf{H} = (\gamma(x))^2 \beta(x)\mathbf{H} - i\omega\varepsilon(x)\Big(\frac{\gamma(x)}{k(x)}\Big)^2 \mathbf{E}, \tag{2.6}$$

where

$$k(x) = \omega\sqrt{\varepsilon(x)\mu(x)}, \quad (\gamma(x))^2 = \frac{(k(x))^2}{1-(k(x)\beta(x))^2}.$$

Throughout, we always assume that $(k(x)\beta(x))^2 \neq 1$, $x \in \mathbb{R}^3$. In addition, it is assumed that the structure is periodic in the x_1 direction with period L and invariant in the x_2 direction. Therefore, we have

$$\varepsilon(x_1+nL, x_3) = \varepsilon(x_1, x_3), \quad \mu(x_1+nL, x_3) = \mu(x_1, x_3), \quad \beta(x_1+nL, x_3) = \beta(x_1, x_3),$$

and **E** and **H** only depend on x_1 and x_3.

The problem geometry in one period L is defined as:

$$\Omega = \Big\{(x_1, x_3) : 0 < x_1 < L,\ b_2 < x_3 < b_1\Big\},$$

for some positive constants b_2 and b_1.

Fig. 2.1 shows the structure of the domain Ω, where s_1 and s_2 are two simple curves imbedded in the region Ω. The space above the curve s_1 and below the curve s_2 is filled with chiral and homogeneous medium , and the medium in the region Ω between s_1 and s_2 is chiral or achiral. Based on the characteristics of the medium, it is assumed that these exist positive constants d_1 and d_2 such that

$$\begin{aligned} &\varepsilon(x_1,x_3)=\varepsilon_1, \quad \mu(x_1,x_3)=\mu_1, \quad \beta(x_1,x_3)=0 \ \text{ for } \ x_3\geq b_1-d_1, \\ &\varepsilon(x_1,x_3)=\varepsilon_2, \quad \mu(x_1,x_3)=\mu_2, \quad \beta(x_1,x_3)=0 \ \text{ for } \ x_3\leq b_2+d_2, \end{aligned}$$

where ε_1, ε_2, μ_1 and μ_2 are positive constants.

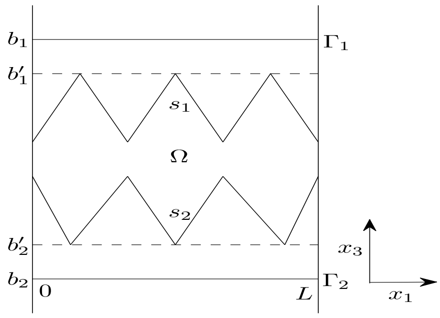

Fig. 2.1. Geometry of the grating problem.

As in [43], we also make the following general assumptions:

(1) $\varepsilon(x)$, $\mu(x)$ and $\beta(x)$ are all real valued L^∞ functions, $\varepsilon(x)\geq\varepsilon_0$, $\mu(x)\geq\mu_0$ and $\beta(x)\geq 0$, where ε_0 and μ_0 are positive constants;

(2) $d=1-k\beta\geq d_0>0$, for some positive constant d_0.

Note that the second assumption is essential in the following numerical analysis. Fortunately, it appears to be common in the literature and justified since β is generally small. The first assumption is a technical one.

Next, we will briefly introduce some notation. Based on these notation, we will introduce the weak formulation of the scattering problem. Let $(\mathbf{E}_\mathrm{I},\mathbf{H}_\mathrm{I})$ be the incoming plane waves that are incident on Ω:

$$\mathbf{E}_\mathrm{I}=\tilde{s}e^{i\tilde{q}.x}, \quad \mathbf{H}_\mathrm{I}=\tilde{p}e^{i\tilde{q}.x}, \quad \tilde{s}=\frac{\tilde{p}\times\tilde{q}}{\omega\varepsilon_1}, \quad \tilde{q}\cdot\tilde{q}=\omega^2\varepsilon_1\mu_1, \quad \tilde{p}\cdot\tilde{q}=0,$$

where $\tilde{q}=(\alpha,-\beta_1,0)^\mathrm{T}=\omega\sqrt{\varepsilon_1\mu_1}(\sin\theta,-\cos\theta,0)^\mathrm{T}$ is the incident wave vector, and θ is the incidence angle satisfying $0\leq\theta<\pi$.

We are interested in quasi-periodic solutions, i.e., solutions $(\mathbf{E},\mathbf{H})$ such that $(\mathbf{E}_\alpha,\mathbf{H}_\alpha)=e^{-i\alpha x_1}(\mathbf{E},\mathbf{H})$ are periodic in the x_1 direction of period L . According to the radiation condition imposed on the scattering problem, we shall insist that the electromagnetic fields $(\mathbf{E}$,$\mathbf{H})$ is composed of bounded outgoing plane wave, plus the incident wave $(\mathbf{E}_\mathrm{I}$,$\mathbf{H}_\mathrm{I})$ above the structure.

Define the boundaries

$$\Gamma_1=\Big\{(x_1,x_3):0<x_1<L,x_3=b_1\Big\}, \qquad \Gamma_2=\Big\{(x_1,x_3):0<x_1<L,x_3=b_2\Big\}.$$

Let Ω^* denote the component of the domain Ω between the curves s_1 and s_2. Introduce

$$\Gamma_1' = \Big\{(x_1,x_3) : 0 < x_1 < L,\ x_3 = b_1'\Big\}, \qquad \Gamma_2' = \Big\{(x_1,x_3) : 0 < x_1 < L,\ x_3 = b_2'\Big\},$$

with $b_2 < b_2' < b_1' < b_1$ and $|b_j - b_j'| \le d_j$, j=1,2, such that $\Omega^* \subseteq \{(x_1,x_3) : 0 < x_1 < L,\ b_2' < x_3 < b_1'\}$ and

$$\begin{aligned} &\varepsilon(x_1,x_3) = \varepsilon_1, \quad \mu(x_1,x_3) = \mu_1, \quad \beta(x_1,x_3) = 0 \qquad \text{for } x_3 \ge b_1', \\ &\varepsilon(x_1,x_3) = \varepsilon_2, \quad \mu(x_1,x_3) = \mu_2, \quad \beta(x_1,x_3) = 0 \qquad \text{for } x_3 \le b_2'. \end{aligned}$$

Define for $j = 1,2$ the coefficients

$$\beta_j^n(\alpha) = \begin{cases} (k_j^2 - (\alpha_n + \alpha)^2)^{1/2} & \text{if } k_j^2 \ge (\alpha_n+\alpha)^2, \\ i((\alpha_n+\alpha)^2 - k_j^2)^{1/2} & \text{if } k_j^2 < (\alpha_n+\alpha)^2, \end{cases} \tag{2.7}$$

where $\alpha_n = 2\pi n/L$ for all $n \in Z$. Note that $\beta_1^0 = \beta$ by definition. For any quasi-periodic function $f \in H^{1/2}(\Gamma_j)$, define the Dirichlet-to-Neumann(DtN) operator $T^{(j)}$ by

$$T^{(j)} f(x_1) = \sum_{n\in Z} i\beta_j^n f^{(n)} e^{i(\alpha_n+\alpha)x_1}, \qquad 0 < x_1 < L,\ j = 1,2, \tag{2.8}$$

where

$$f^{(n)} = L^{-1} \int_0^L f(x) e^{-i(\alpha_n+\alpha)x_1} dx_1. \tag{2.9}$$

Let $\mathbf{E} = (E_1, E_2, E)^{\mathrm{T}}$, $\mathbf{H} = (H_1, H_2, H)^{\mathrm{T}}$. It is easily obtained that E_1, E_2, H_1 and H_2 can be expressed in terms of E and H. Then, two coupled equations for E and H can be achieved. Denoting by ϕ the component E or H, it follows from the Fourier series expansion of ϕ and the method of separation of variables that ϕ has the following Rayleigh expansion:

$$\phi = \phi_I + \sum_{n\in Z} A_1^n e^{i(\alpha_n+\alpha)x_1 + i\beta_1^n x_3}, \quad \text{for } x_3 \ge b_1, \tag{2.10}$$

$$\phi = \sum_{n\in Z} A_2^n e^{i(\alpha_n+\alpha)x_1 - i\beta_2^n x_3}, \qquad \text{for } x_3 \le b_2. \tag{2.11}$$

Based on (2.10) and (2.11), we can readily derive the boundary condition on Γ_j for E and H. Then the scattering problem can be simplified to the following problem:

$$\begin{aligned} &-\nabla\cdot(\frac{1}{\mu}\nabla E) + i\omega\nabla\cdot(\beta\nabla H) - i\omega\gamma^2\beta H - \frac{\gamma^2}{\mu}E = 0, && \text{in } \Omega, \\ &-\nabla\cdot(\frac{1}{\varepsilon}\nabla H) - i\omega\nabla\cdot(\beta\nabla E) + i\omega\gamma^2\beta E - \frac{\gamma^2}{\varepsilon}H = 0, && \text{in } \Omega, \\ &\Big(T^{(1)} - \frac{\partial}{\partial n}\Big)E = 2i\beta_1 E_I, \quad \Big(T^{(1)} - \frac{\partial}{\partial n}\Big)H = 2i\beta_1 H_I, && \text{on } \Gamma_1, \\ &\Big(T^{(2)} - \frac{\partial}{\partial n}\Big)E = 0, \quad \Big(T^{(2)} - \frac{\partial}{\partial n}\Big)H = 0, && \text{on } \Gamma_2, \end{aligned} \tag{2.12}$$

where $E_I = \tilde{s}_3 e^{i\alpha x_1 - i\beta_1 b_1}$ and $H_I = \tilde{p}_3 e^{i\alpha x_1 - i\beta_1 b_1}$.

Introduce the following space which includes all the quasi-periodic functions:

$$X(\Omega) = \Big\{ w \in H^1(\Omega) : w(0,x_3) = e^{-i\alpha L} w(L,x_3) \Big\}.$$

Let $u=(E,H)^{\mathrm{T}}$, $v=(p,q)^{\mathrm{T}}$ and $e=(s,t)^{\mathrm{T}}$. Introduce the following sesquilinear form

$$\begin{aligned} A(e,v)=&\int_\Omega \frac{1}{\mu}\nabla s\cdot\nabla\overline{p}+\int_\Omega\frac{1}{\varepsilon}\nabla t\cdot\nabla\overline{q}-i\omega\int_\Omega\beta\nabla t\cdot\nabla\overline{p}+i\omega\int_\Omega\beta\nabla s\cdot\nabla\overline{q}\\ &-\int_\Omega\frac{\gamma^2}{\mu}s\cdot\overline{p}-\int_\Omega\frac{\gamma^2}{\varepsilon}t\cdot\overline{q}-i\omega\int_\Omega\gamma^2\beta t\cdot\overline{p}+i\omega\int_\Omega\gamma^2\beta s\cdot\overline{q}\\ &-\sum_{j=1}^{2}\frac{1}{\mu_j}\int_{\Gamma_j}T^{(j)}s\cdot\overline{p}-\sum_{j=1}^{2}\frac{1}{\varepsilon_j}\int_{\Gamma_j}T^{(j)}t\cdot\overline{q}, \end{aligned} \tag{2.13}$$

$$\langle f_{\mathrm{I}},v\rangle=-\frac{1}{\mu_1}\int_{\Gamma_1}2i\beta_1E_I\overline{p}dx_1-\frac{1}{\varepsilon_1}\int_{\Gamma_1}2i\beta_1H_I\overline{q}dx_1. \tag{2.14}$$

A weak formulation of the scattering problem is as follows: Giving an incident plane wave (E_I,H_I), find $u\in X(\Omega)\times X(\Omega)$ such that

$$A(u,v)=\langle f_{\mathrm{I}},v\rangle,\qquad \forall v\in X(\Omega)\times X(\Omega). \tag{2.15}$$

See Zhang and Ma [43] for the proof of existence and uniqueness of the solution to (2.15). Throughout this paper, we assume that the variational problem has a unique solution for any frequency ω. The general theory in Babuška and Aziz [7] implies that there exists a constant $\gamma>0$ such that the following inf-sup condition holds:

$$\sup_{0\neq v\in X(\Omega)\times X(\Omega)}\frac{|A(e,v)|}{\|v\|_1}\geq\gamma\|e\|_1,\qquad\forall e\in X(\Omega)\times X(\Omega). \tag{2.16}$$

To simply the notation, $\|\cdot\|_{H^1(\Omega)\times H^1(\Omega)}$ and $\|\cdot\|_{L^2(\Omega)\times L^2(\Omega)}$ will be written as $\|\cdot\|_1$ and $\|\cdot\|_0$, respectively. And it can be shown that

$$\|u\|_1\leq C_0\Big(\|E_{\mathrm{I}}\|_{L^2(\Gamma_1)}+\|H_{\mathrm{I}}\|_{L^2(\Gamma_1)}\Big). \tag{2.17}$$

3. The Discrete Problem

To design a practicable algorithm, we do a truncation approximation to the nonlocal boundary operator $T^{(j)}(j=1,2)$, then the finite element formulation is presented by using new truncated operators. After introducing some notation, we will give the main conclusion in this paper.

Let $\mathcal{M}_h$ be a regular triangulation of the domain Ω. Every triangle $T\in\mathcal{M}_h$ is considered as closed. To deal with the quasi-periodic boundary condition, we require that if $(0,z)$ is a node on the left boundary, then (L,z) must be a node on the right boundary, and vice versa. Let $V_h\subset X(\Omega)$ denote a conforming linear finite element space, that is,

$$\begin{aligned} V_h:=\Big\{&q_h\in C(\overline{\Omega}):\, q_h|_T\in P_1(T),\forall T\in\mathcal{M}_h,\\ &q_h(0,x_3)=e^{-i\alpha L}q_h(L,x_3)\ \text{ for } b_2<x_3<b_1\Big\}, \end{aligned}$$

where $P_1(T)$ is the set of polynomials of degrees ≤ 1. The finite element approximation to the problem (2.15) reads as follows: Find $u_h=(E_h,H_h)^{\mathrm{T}}\in V_h\times V_h$ such that

$$A(u_h,v_h)=\langle f_{\mathrm{I}},v_h\rangle,\qquad\forall v_h=(p_h,q_h)^{\mathrm{T}}\in V_h\times V_h. \tag{3.1}$$

In practice, it is impossible that the non local operators $T^{(j)}$ in (2.8) is computed from the infinite series. Thus we need truncate the boundary operators by taking sufficiently many terms of the corresponding expansions so as to obtain our reliable and easily manipulated algorithm. Denote by $n_\alpha := \frac{\alpha L}{2\pi}$. For the quasic-periodic function f, the truncation operator $T^{(j,N_j)}$ is defined as

$$T^{(j,N_j)}f(x_1) = \sum_{|n+n_\alpha|\le N_j} i\beta_j^n f_\alpha^{(n)} e^{i(\alpha_n+\alpha)x_1}, \qquad j=1,2. \tag{3.2}$$

Now, we define the truncated finite element formulation for solving (2.15): Find $u_h^N = (E_h^N, H_h^N)^{\rm T} \in V_h \times V_h$ such that

$$A^N(u_h^N, v_h) = \langle f_{\rm I}, v_h\rangle, \qquad \forall v_h \in V_h \times V_h, \tag{3.3}$$

where the sesquilinear form

$$\begin{aligned} A^N(e,v) = &\int_\Omega \frac{1}{\mu}\nabla s\cdot\nabla\overline{p} + \int_\Omega \frac{1}{\varepsilon}\nabla t\cdot\nabla\overline{q} - i\omega\int_\Omega \beta\nabla t\cdot\nabla\overline{p} + i\omega\int_\Omega \beta\nabla s\cdot\nabla\overline{q} \\ &- \int_\Omega \frac{\gamma^2}{\mu} s\cdot\overline{p} - \int_\Omega \frac{\gamma^2}{\varepsilon} t\cdot\overline{q} - i\omega\int_\Omega \gamma^2\beta t\cdot\overline{p} + i\omega\int_\Omega \gamma^2\beta s\cdot\overline{q} \\ &- \sum_{j=1}^2 \frac{1}{\mu_j}\int_{\Gamma_j} T^{(j,N_j)} s\cdot\overline{p} - \sum_{j=1}^2 \frac{1}{\varepsilon_j}\int_{\Gamma_j} T^{(j,N_j)} t\cdot\overline{q}. \end{aligned} \tag{3.4}$$

Note that for sufficiently large N_j and sufficiently small h, the existence and uniqueness of solution of the problem (3.3) may be obtained by combing the argument of Schatz [37] with the general theory in [7]. In this paper, the discrete problem (3.3) is assumed to have a unique solution $u_h^N \in V_h \times V_h$. Also note that on the quasi-periodic boundary conditions, the quasi-periodic basis functions are not used in our implementation. In order to assemble the stiffness matrix for the quasi-periodic boundary condition, we assemble the system using the pure Neumann boundary condition first, then eliminate the degrees of freedom on the right (or left) side of the domain using the quasi-periodic boundary condition.

For any $T \in \mathcal{M}_h$, denote by h_T its diameter. Introduce the residuals

$$R_T^{(1)} := -\nabla\cdot(\frac{1}{\mu}\nabla E_h^N) + i\omega\nabla\cdot(\beta\nabla H_h^N) - i\omega\gamma^2\beta H_h^N - \frac{\gamma^2}{\mu}E_h^N, \tag{3.5a}$$

$$R_T^{(2)} := -\nabla\cdot(\frac{1}{\varepsilon}\nabla H_h^N) - i\omega\nabla\cdot(\beta\nabla E_h^N) + i\omega\gamma^2\beta E_h^N - \frac{\gamma^2}{\varepsilon}H_h^N. \tag{3.5b}$$

For $j=1,2$, let $\mathcal{B}_h^j$ denotes the set of all the edges that lie on Γ_j, and $\mathcal{B}_h$ denotes the set of all the edges except $\mathcal{B}_h^j$ in Ω. For any $F \in \mathcal{B}_h$ or $F \in \mathcal{B}_h^j$, h_F stands for its length. For any interior edge $F \in \mathcal{B}_h$ which is the common edge of T_1 and $T_2 \in \mathcal{M}_h$, we define the jump residual across F as

$$J_F^{(1)} = \mu^{-1}(\nabla E_h^N|_{T_1} - \nabla E_h^N|_{T_2})\cdot n_F, \tag{3.6}$$

$$J_F^{(2)} = \varepsilon^{-1}(\nabla H_h^N|_{T_1} - \nabla H_h^N|_{T_2})\cdot n_F, \tag{3.7}$$

$$K_F^{(1)} = i\omega\beta(\nabla E_h^N|_{T_1} - \nabla E_h^N|_{T_2})\cdot n_F, \tag{3.8}$$

$$K_F^{(2)} = -i\omega\beta(\nabla H_h^N|_{T_1} - \nabla H_h^N|_{T_2})\cdot n_F. \tag{3.9}$$

Define $\Gamma_{left} = \{(x_1, x_3) : x_1 = 0, b_2 < x_3 < b_1\}$ and $\Gamma_{right} = \{(x_1, x_3) : x_1 = L, b_2 < x_3 < b_1\}$. If $F = \Gamma_{left} \bigcap \partial T$ for some element $T \in \mathcal{M}_h$ and F' be a corresponding edge on Γ_{right} which also belongs to some element T', then we define the jump residual as

$$
\begin{aligned}
J_F^{(1)} &= \mu^{-1}\Big(\frac{\partial E_h^N}{\partial x_1}|_{T_1} - e^{-i\alpha L}\frac{\partial E_h^N}{\partial x_1}|_{T_1'}\Big), &\quad J_F^{(2)} &= \varepsilon^{-1}\Big(\frac{\partial H_h^N}{\partial x_1}|_{T_1} - e^{-i\alpha L}\frac{\partial H_h^N}{\partial x_1}|_{T_1'}\Big),\\
K_F^{(1)} &= i\omega\beta\Big(\frac{\partial E_h^N}{\partial x_1}|_{T_1} - e^{-i\alpha L}\frac{\partial E_h^N}{\partial x_1}|_{T_1'}\Big), &\quad K_F^{(2)} &= -i\omega\beta\Big(\frac{\partial H_h^N}{\partial x_1}|_{T_1} - e^{-i\alpha L}\frac{\partial H_h^N}{\partial x_1}|_{T_1'}\Big),\\
J_{F'}^{(1)} &= \mu^{-1}\Big(e^{i\alpha L}\frac{\partial E_h^N}{\partial x_1}|_{T_1} - \frac{\partial E_h^N}{\partial x_1}|_{T_1'}\Big), &\quad J_{F'}^{(2)} &= \varepsilon^{-1}\Big(e^{i\alpha L}\frac{\partial H_h^N}{\partial x_1}|_{T_1} - \frac{\partial H_h^N}{\partial x_1}|_{T_1'}\Big),\\
K_{F'}^{(1)} &= i\omega\beta\Big(e^{i\alpha L}\frac{\partial E_h^N}{\partial x_1}|_{T_1} - \frac{\partial E_h^N}{\partial x_1}|_{T_1'}\Big), &\quad K_{F'}^{(2)} &= -i\omega\beta\Big(e^{i\alpha L}\frac{\partial H_h^N}{\partial x_1}|_{T_1} - \frac{\partial H_h^N}{\partial x_1}|_{T_1'}\Big).
\end{aligned}
\tag{3.10}
$$

For any $F \in \mathcal{B}_h^1$ and $F' \in \mathcal{B}_h^2$, define the jump residual as follows:

$$
\begin{aligned}
J_F^{(1)} &= 2\mu_1^{-1}\Big(\frac{\partial E_h^N}{\partial x_3}(x_1, b_1) - T^{(1,N_1)}E_h^N(x_1, b_1) + 2i\beta_1 E_I\Big),\\
J_F^{(2)} &= 2\varepsilon_1^{-1}\Big(\frac{\partial H_h^N}{\partial x_3}(x_1, b_1) - T^{(1,N_1)}H_h^N(x_1, b_1) + 2i\beta_1 H_I\Big),\\
J_{F'}^{(1)} &= 2\mu_2^{-1}\Big(\frac{\partial E_h^N}{\partial x_3}(x_1, b_2) - T^{(2,N_2)}E_h^N(x_1, b_2)\Big),\\
J_{F'}^{(2)} &= 2\varepsilon_2^{-1}\Big(\frac{\partial H_h^N}{\partial x_3}(x_1, b_2) - T^{(2,N_2)}H_h^N(x_1, b_2)\Big),\\
K_F^{(1)} &= 0, \quad K_F^{(2)} = 0, \quad K_{F'}^{(1)} = 0, \quad K_{F'}^{(2)} = 0.
\end{aligned}
\tag{3.11}
$$

For any $T \in \mathcal{M}_h$, denote by η_T the local error estimator, which is defined by:

$$
\begin{aligned}
\eta_T = & h_T\Big(\|R_T^{(1)}\|^2_{L^2(T)} + \|R_T^{(2)}\|^2_{L^2(T)}\Big)^{1/2}\\
&+ \Big(\frac{1}{2}\sum_{F\subset\partial T} h_F\big(\|J_F^{(1)}\|^2_{L^2(F)} + \|J_F^{(2)}\|^2_{L^2(F)} + \|K_F^{(1)}\|^2_{L^2(F)} + \|K_F^{(2)}\|^2_{L^2(F)}\big)\Big)^{1/2}.
\end{aligned}
\tag{3.12}
$$

The main theorem of this paper is the following:

Theorem 3.1. *Let u and u_h^N denote the solutions of* (2.15) *and* (3.3)*, respectively. Then there exist two integers $N_{j0}, j = 1, 2$ independent of h and satisfying $(2\pi N_{j0}/L)^2 > k_j^2$, such that for $N_j \geq N_{j0}$ the following a posteriori error estimate holds:*

$$
\|u - u_h^N\|_1 \leq \widetilde{C}\Big(\Big(\sum_{T\in\mathcal{M}_h}\eta_T^2\Big)^{\frac{1}{2}} + \sum_{j=1}^{2} e^{-|b_j - b_j'|\sqrt{(2\pi N_j/L)^2 - k_j^2}}\Big),
$$

where the constant $\widetilde{C}$ is independent of h, N_1 and N_2.

The first and second term on the right hand side of the above estimate are often called the finite element discretization error and truncation error of the DtN operators. We notice that the truncation error is exponentially decaying with respect to N_j and the distances from Γ_j $(j = 1, 2)$ to the grating.

4. A Posteriori Error Analysis

In this section we prove the posteriori error estimate in Theorem 3.1.

Define the error $\xi := u - u_h^N$. Let $w = (\varphi, \psi)^{\mathrm{T}}$ and $\xi = (\xi_E, \xi_H)^{\mathrm{T}}$. It is obvious that $\xi_E = E - E_h^N$ and $\xi_H = H - H_h^N$. Introduce the dual problem to the original problem (2.15): Find $w \in X(\Omega) \times X(\Omega)$ such that

$$A(v, w) = (v, \xi) \quad \forall v \in X(\Omega) \times X(\Omega), \tag{4.1}$$

After a series of complex calculations, we conclude that w is the weak solution of the following problem

$$-\nabla \cdot (\frac{1}{\mu}\nabla\varphi) + i\omega\nabla \cdot (\beta\nabla\psi) - \frac{\gamma^2}{\mu}\varphi - i\omega\gamma^2\beta\psi = \xi_E, \qquad \text{in } \Omega, \tag{4.2}$$

$$-\nabla \cdot (\frac{1}{\varepsilon}\nabla\psi) - i\omega\nabla \cdot (\beta\nabla\varphi) - \frac{\gamma^2}{\varepsilon}\psi + i\omega\gamma^2\beta\varphi = \xi_H, \qquad \text{in } \Omega, \tag{4.3}$$

$$\frac{\partial\varphi}{\partial n} - T^{(1,*)}\varphi = 0, \ \frac{\partial\psi}{\partial n} - T^{(1,*)}\psi = 0, \qquad \text{on } \Gamma_1, \tag{4.4}$$

$$\frac{\partial\varphi}{\partial n} - T^{(2,*)}\varphi = 0, \ \frac{\partial\psi}{\partial n} - T^{(2,*)}\psi = 0, \qquad \text{on } \Gamma_2, \tag{4.5}$$

where the dual operators take the following form:

$$T^{(j,*)}s = -\sum_{n\in Z} i\,\overline{\beta_j^n}s^{(n)}e^{i(\alpha_n+\alpha)x_1}, \qquad j = 1, 2.$$

Just as discussed for the dual problem in [9], the existence of solutions for (4.2)-(4.5) can be obtained from the Fredholm theory and the related proof of [7]. Here we assume this problem has a unique (weak) solution. Then it can be shown that w satisfies

$$\|w\|_1 \le C_0 \|\xi\|_0 . \tag{4.6}$$

Note that, unlike the duality argument for a priori error estimates, the assumption of the H^2 regularity of w can be removed.

4.1. Error Representation Formulae

In this subsection, we describe several relations on the error ξ, which is the beginning for the a posteriori error analysis.

Lemma 4.1. *Let u, u_h^N, and w be the solutions to the problems* (2.15), (3.3) *and* (4.1), *respectively. Then*

$$\begin{aligned}\|\xi\|_1^2 \le C\Big(&\mathrm{Re}\Big(A(\xi,\xi) + \sum_{j=1}^{2}\big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)} - T^{(j,N_j)})\xi_E\overline{\xi_E} \\ &+ \frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)} - T^{(j,N_j)})\xi_H\overline{\xi_H}\big)\Big) + \|\xi\|_0^2\Big),\end{aligned} \tag{4.7}$$

$$\|\xi\|_0^2 = A(\xi, w) + \sum_{j=1}^{2}\left(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)} - T^{(j,N_j)})\xi_E\overline{\varphi} + \frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)} - T^{(j,N_j)})\xi_H\overline{\psi}\right)$$

$$-\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{\varphi}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{\psi}\Big), \tag{4.8}$$

$$\begin{aligned}A(\xi,v)&+\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{p}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{q}\Big)\\&=\langle f_I,v-v_h\rangle-A^N(u_h^N,v-v_h)+\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})E\overline{p}\\&\quad+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})H\overline{q}\Big).\end{aligned} \tag{4.9}$$

Proof. By the definition of the sesquilinear form A, we have

$$\begin{aligned}A(\xi,\xi)&+\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{\xi_E}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{\xi_H}\Big)\\&+\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}T^{(j,N_j)}\xi_E\overline{\xi_E}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}T^{(j,N_j)}\xi_H\overline{\xi_H}\Big)\\=&\int_\Omega\Big(\frac{1}{\mu}|\nabla\xi_E|^2+\frac{1}{\varepsilon}|\nabla\xi_H|^2\Big)-\int_\Omega\Big(\frac{\gamma^2}{\mu}|\xi_E|^2+\frac{\gamma^2}{\varepsilon}|\xi_H|^2\Big)\\&+i\omega\int_\Omega\beta\big(\nabla\xi_E\cdot\nabla\overline{\xi_H}-\nabla\xi_H\cdot\nabla\overline{\xi_E}\big)+i\omega\int_\Omega\gamma^2\beta\big(\xi_E\overline{\xi_H}-\xi_H\overline{\xi_E}\big).\end{aligned} \tag{4.10}$$

Further, from the definitions of $T^{(j,N_j)}$ and β_j^n, we can obtain

$$\begin{aligned}&\mathrm{Re}\Big(\sum_{j=1}^{2}\big(\frac{1}{\mu_j}\int_{\Gamma_j}T^{(j,N_j)}\xi_E\overline{\xi_E}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}T^{(j,N_j)}\xi_H\overline{\xi_H}\big)\Big)\\&=-L\sum_{j=1}^{2}\sum_{|n+n_\alpha|\le N_j}\mathrm{Im}(\beta_j^n)\big(\frac{1}{\mu_j}|\xi_E^{(n)}|^2+\frac{1}{\varepsilon_j}|\xi_H^{(n)}|^2\big)\le 0.\end{aligned} \tag{4.11}$$

Using the young inequality, we have

$$\begin{aligned}&\mathrm{Re}\Big(i\omega\int_\Omega\beta\big(\nabla\xi_E\cdot\nabla\overline{\xi_H}-\nabla\xi_H\cdot\nabla\overline{\xi_E}\big)\Big)=2\omega\int_\Omega\mathrm{Im}(\beta\nabla\xi_H\cdot\nabla\overline{\xi_E})\\&\ge-\int_\Omega\frac{2k\beta}{\sqrt{\varepsilon}\sqrt{\mu}}|\nabla\xi_E|\cdot|\nabla\xi_H|\ge-\int_\Omega\big(\frac{k\beta}{\mu}|\nabla\xi_E|^2+\frac{k\beta}{\varepsilon}|\nabla\xi_H|^2\big).\end{aligned} \tag{4.12}$$

Similar to the deduction of the above inequality, we can find that

$$\begin{aligned}&\mathrm{Re}\Big(i\omega\int_\Omega\gamma^2\beta\big(\xi_E\overline{\xi_H}-\xi_H\overline{\xi_E}\big)\Big)\\&=2\omega\int_\Omega\gamma^2\beta\,\mathrm{Im}(\xi_H\overline{\xi_E})\ge-\int_\Omega\omega\gamma^2\beta(|\xi_E|^2+|\xi_H|^2).\end{aligned} \tag{4.13}$$

Clearly by taking the real parts in the identity of (4.10), together with (4.11)-(4.13), we arrive at

$$\begin{aligned}&\mathrm{Re}\Big(A(\xi,\xi)+\sum_{j=1}^{2}\big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{\xi_E}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{\xi_H}\big)\Big)\\&\ge\int_\Omega\Big(\frac{1-k\beta}{\mu}|\nabla\xi_E|^2+\frac{1-k\beta}{\varepsilon}|\nabla\xi_H|^2\Big)-\int_\Omega\gamma^2\Big((\frac{1}{\mu}+\omega\beta)|\xi_E|^2+(\frac{1}{\varepsilon}+\omega\beta)|\xi_H|^2\Big)\end{aligned}$$

This implies the desired estimate (4.7) upon using the restriction of $\varepsilon(x)$ and $\mu(x)$ and the fact that $1-k\beta \geq d_0(>0)$. Moreover, it is easy to see that (4.8) follows by taking $v=\xi$ in (4.1).

It remains to prove (4.9). By a similar argument as for (4.7) in Ref. [46], we have

$$\begin{aligned}
&A(\xi,v)=A(u-u_h^N,v-v_h)+A(u-u_h^N,v_h)=\langle f_I,v-v_h\rangle - A^N(u_h^N,v-v_h)\\
&\quad+\big(A^N(u_h^N,v-v_h)-A(u_h^N,v-v_h)\big)+\big(A^N(u_h^N,v_h)-A(u_h^N,v_h)\big)\\
=&\langle f_I,v-v_h\rangle - A^N(u_h^N,v-v_h)+\big(A^N(u_h^N,v)-A(u_h^N,v)\big)\\
=&\langle f_I,v-v_h\rangle - A^N(u_h^N,v-v_h)\\
&-\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{p}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{q}\Big)\\
&+\sum_{j=1}^{2}\Big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})E\overline{p}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})H\overline{q}\Big),
\end{aligned}$$

which yields (4.9). This completes the proof of the lemma. □

4.2. Proof of Theorem 3.1

In this subsection, we shall derive the a posteriori error estimation. This will be done by employing two important lemmas proved in the next two subsections.

Lemma 4.2. *There exist integers N_{j1} independent of h and satisfying $(2\pi N_{j1}/L)^2>k_j^2$, $j=1,2$, such that for any $N_j\geq N_{j1}$ and $v\in X(\Omega)\times X(\Omega)$ we have*

$$\begin{aligned}
&\Big|A(\xi,v)+\sum_{j=1}^{2}\big(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{p}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{q}\big)\Big|\\
\leq& C_1\bigg(\Big(\sum_{T\in\mathcal{M}_h}\eta_T^2\Big)^{1/2}+\sum_{j=1}^{2}e^{-|b_j-b_j'|\sqrt{(2\pi N_j/L)^2-k_j^2}}\bigg)\|v\|_1,
\end{aligned}$$

where C_1 is a constant independent of h and N_j.

Lemma 4.3. *For the solution w of (4.1), there exist integers N_{j2} independent of h and satisfying $(2\pi N_{j2}/L)^2>k_j^2$, $j=1,2$, such that for $N_j\geq N_{j2}$, we have the following estimate:*

$$\Big|\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{\varphi}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{\psi}\Big|\leq C_2N_j^{-2}\|\xi\|_1^2,$$

where C_2 is a constant independent of h and N_j.

Now we are in the position to prove Theorem 3.1. By (4.7) and Lemma 4.2, the following estimate can be obtained

$$\|\xi\|_1^2\leq C_1\bigg(\Big(\sum_{T\in\mathcal{M}_h}\eta_T^2\Big)^{1/2}+\sum_{j=1}^{2}e^{-|b_j-b_j'|\sqrt{(2\pi N_j/L)^2-k_j^2}}\bigg)\|\xi\|_1+C_3\|\xi\|_0^2.$$

It remains to estimate $\|\xi\|_0$. By (4.8), (4.6), Lemma 4.2 and Lemma 4.3, we know that

$$\|\xi\|_0^2\leq C_1\bigg(\Big(\sum_{T\in\mathcal{M}_h}\eta_T^2\Big)^{1/2}+\sum_{j=1}^{2}e^{-|b_j-b_j'|\sqrt{(2\pi N_j/L)^2-k_j^2}}\bigg)C_0\|\xi\|_0+C_2(N_1^{-2}+N_2^{-2})\|\xi\|_1^2,$$

Then it follows from the above two estimates that

$$\begin{aligned}\|\xi\|_1^2 \leq & C_1(1+C_0C_3)\bigg(\Big(\sum_{T\in\mathcal{M}_h}\eta_T^2\Big)^{1/2}+\sum_{j=1}^{2}e^{-|b_j-b_j'|\sqrt{(2\pi N_j/L)^2-k_j^2}}\bigg)\|\xi\|_1 \\ & + C_2C_3(N_1^{-2}+N_2^{-2})\|\xi\|_1^2.\end{aligned}$$

Choose integer N_{j3} such that

$$C_2C_3N_{j3}^{-2}\leq\frac{1}{4},\qquad j=1,2.$$

By taking

$$N_{j0}=\max(N_{j1},N_{j2},N_{j3}),\quad \widetilde{C}=2C_1(1+C_0C_3), \tag{4.14}$$

the proof of Theorem 3.1 is complete. □

4.3. Proof of Lemma 4.2

We need the following lemma used in deriving the truncation error (cf. [9]).

Lemma 4.4. *Let $u=(E,H)^T$ be the solution to (2.15) and $u^{(n)}=(E^{(n)},H^{(n)})^T$ be defined in (2.9). Suppose that $(\alpha_n+\alpha)^2\geq k_j^2$. Then*

$$|\, f^{(n)}(b_j)\,|\leq|\, f^{(n)}(b_j')\,|\, e^{-|b_j-b_j'|\sqrt{(\alpha_n+\alpha)^2-k_j^2}},\quad \text{for}\ \ j=1,2,$$

where f denotes E or H.

we recall the following trace property(cf. [20]).

Lemma 4.5. *For any $p\in X(\Omega)$, we have*

$$\|p\|_{H^{1/2}(\Gamma_j)}\leq\widehat{C}\|p\|_{H^1(\Omega)},$$

with $\widehat{C}=\sqrt{1+(b_1-b_2)^{-1}}$ and $j=1,2$. Here if $p(x_1,b_j)=\sum_{n\in Z}p^{(n)}(b_j)e^{i(\alpha_n+\alpha)x_1}$ on Γ_j,

$$\|p\|_{H^{1/2}(\Gamma_j)}=\Big(L\sum_{n\in Z}\big(1+|\alpha_n+\alpha|^2\big)^{1/2}|p^{(n)}(b_j)|^2\Big)^{1/2}.$$

Next we turn to the estimate of Lemma 4.2. Denote by

$$\begin{aligned}&\mathbb{J}^1:=\langle f_{\mathrm{I}},v-v_h\rangle-A^N(u_h^N,v-v_h),\\ &\mathbb{J}^2:=\sum_{j=1}^{2}\bigg(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})E\overline{p}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})H\overline{q}\bigg).\end{aligned}$$

Then from (4.9), we have

$$\begin{aligned}&A(\xi,\xi)+\sum_{j=1}^{2}\bigg(\frac{1}{\mu_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_E\overline{\xi_E}+\frac{1}{\varepsilon_j}\int_{\Gamma_j}(T^{(j)}-T^{(j,N_j)})\xi_H\overline{\xi_H}\bigg)\\ =&:\mathbb{J}^1+\mathbb{J}^2.\end{aligned}$$

From the definition of the sesquilinear form (3.4), $\mathbb{J}^1$ is rewritten as

$$\begin{aligned}\mathbb{J}^1 = &-\sum_{T\in\mathcal{M}_h}\Big(\int_T\big(\frac{1}{\mu}\nabla E_h^N\cdot\nabla(\overline{p-p_h})-\frac{\gamma^2}{\mu}E_h^N(\overline{p-p_h})-i\omega\beta\nabla H_h^N\cdot\nabla(\overline{p-p_h})\\&-i\omega\gamma^2\beta H_h^N(\overline{p-p_h})\big)-\sum_{j=1}^{2}\sum_{F\subset\partial T\bigcap\Gamma_j}\frac{1}{\mu_j}\int_F T^{(j,N_j)}E_h^N(\overline{p-p_h})\Big)\\&-\sum_{T\in\mathcal{M}_h}\Big(\int_T\big(\frac{1}{\varepsilon}\nabla H_h^N\cdot\nabla(\overline{q-q_h})-\frac{\gamma^2}{\varepsilon}H_h^N(\overline{q-q_h})+i\omega\beta\nabla E_h^N\cdot\nabla(\overline{q-q_h})\\&+i\omega\gamma^2\beta E_h^N(\overline{q-q_h})\big)-\sum_{j=1}^{2}\sum_{F\subset\partial T\bigcap\Gamma_j}\frac{1}{\varepsilon_j}\int_F T^{(j,N_j)}H_h^N(\overline{q-q_h})\Big)\\&-\sum_{T\in\mathcal{M}_h}\sum_{F\subset\partial T\bigcap\Gamma_1}\Big(\frac{1}{\mu_1}\int_F 2i\beta_1 E_I(\overline{p-p_h})+\frac{1}{\varepsilon_1}\int_F 2i\beta_1 H_I(\overline{q-q_h})\Big).\end{aligned}$$

Integration by parts yields

$$\begin{aligned}\mathbb{J}^1 = &-\sum_{T\in\mathcal{M}_h}\Big(\int_T\big(-\nabla\cdot(\frac{1}{\mu}\nabla E_h^N)+i\omega\nabla\cdot(\beta\nabla H_h^N)-i\omega\gamma^2\beta H_h^N-\frac{\gamma^2}{\mu}E_h^N\big)\\&\times(\overline{p-p_h})+\sum_{F\subset\partial T}\Big(\int_F\frac{1}{\mu}\nabla E_h^N\cdot n(\overline{p-p_h})-i\omega\int_F\beta\nabla H_h^N\cdot n(\overline{p-p_h})\Big)\Big)\\&-\sum_{T\in\mathcal{M}_h}\Big(\int_T\big(-\nabla\cdot(\frac{1}{\varepsilon}\nabla H_h^N)-i\omega\nabla\cdot(\beta\nabla E_h^N)+i\omega\gamma^2\beta E_h^N-\frac{\gamma^2}{\varepsilon}H_h^N\big)\\&\times(\overline{q-q_h})+\sum_{F\subset\partial T}\Big(\int_F\frac{1}{\varepsilon}\nabla H_h^N\cdot n(\overline{q-q_h})+i\omega\int_F\beta\nabla E_h^N\cdot n(\overline{q-q_h})\Big)\Big)\\&+\sum_{T\in\mathcal{M}_h}\Big(\sum_{F\subset\partial T\bigcap\Gamma_1}\Big(\frac{1}{\mu_1}\int_F(T^{(1,N_1)}E_h^N-2i\beta_1E_I)(\overline{p-p_h})\\&+\frac{1}{\varepsilon_1}\int_F(T^{(1,N_1)}H_h^N-2i\beta_1H_I)(\overline{q-q_h})\Big)\\&+\sum_{F\subset\partial T\bigcap\Gamma_2}\Big(\frac{1}{\mu_2}\int_F T^{(2,N_2)}E_h^N(\overline{p-p_h})+\frac{1}{\varepsilon_2}\int_F T^{(2,N_2)}H_h^N(\overline{q-q_h})\Big)\Big).\end{aligned}$$

Now we take $p_h=\Pi_h p\in V_h$ and $q_h=\Pi_h q\in V_h$. Here Π_h is the Scott-Zhang interpolation operator in [38] which satisfies the following interpolation estimates:

$$\|s-\Pi_h s\|_{L^2(T)}\le Ch_T\|\nabla s\|_{L^2(\widetilde{T})},\quad \|s-\Pi_h s\|_{L^2(e)}\le Ch_e^{1/2}\|\nabla s\|_{L^2(\widetilde{e})},$$

where $\widetilde{T}$ and $\widetilde{e}$ are the union of all the elements in $\mathcal{M}_h$ having nonempty intersection with the element T and the edge e, respectively. By using the interpolation estimates and standard argument in the a posteriori error analysis, we obtain

$$
\begin{aligned}
|\mathbb{J}^1| \leq & C \sum_{T\in\mathcal{M}_h} \Big(h_T \big(\|R_T^{(1)}\|_{L^2(T)} |p|_{H^1(\widetilde{T})} + \|R_T^{(2)}\|_{L^2(T)} |q|_{H^1(\widetilde{T})} \big) + \sum_{F\subset\partial T} h_F^{1/2} \big(\|J_F^{(1)}\|_{L^2(F)} |p|_{H^1(\widetilde{F})} \\
& + \|J_F^{(2)}\|_{L^2(F)} |q|_{H^1(\widetilde{F})} + \|K_F^{(1)}\|_{L^2(F)} |p|_{H^1(\widetilde{F})} + \|K_F^{(2)}\|_{L^2(F)} |q|_{H^1(\widetilde{F})} \big) \Big) \\
\leq & C \Big(\sum_{T\in\mathcal{M}_h} \eta_T^2 \Big)^{1/2} \big(|p|_{H^1(\Omega)}^2 + |q|_{H^1(\Omega)}^2 \big)^{1/2} \leq C \Big(\sum_{T\in\mathcal{M}_h} \eta_T^2 \Big)^{1/2} \|v\|_1. \qquad (4.15)
\end{aligned}
$$

It remains to estimate $\mathbb{J}^2$. Using an analogous analysis to that presented in [46], here we omit their derivation and just give their final result. For $N_j \geq N_{j1}$ we have

$$
\begin{aligned}
&\sum_{j=1}^{2} \frac{1}{\mu_j} \int_{\Gamma_j} (T^{(j)} - T^{(j,N_j)}) E\overline{p} \leq C \sum_{j=1}^{2} e^{-|b_j - b_j'|\sqrt{(2\pi N_j/L)^2 - k_j^2}} \|E\|_{H^1(\Omega)} \cdot \|p\|_{H^1(\Omega)}, \\
&\sum_{j=1}^{2} \frac{1}{\varepsilon_j} \int_{\Gamma_j} (T^{(j)} - T^{(j,N_j)}) H\overline{q} \leq C \sum_{j=1}^{2} e^{-|b_j - b_j'|\sqrt{(2\pi N_j/L)^2 - k_j^2}} \|H\|_{H^1(\Omega)} \cdot \|q\|_{H^1(\Omega)}.
\end{aligned}
$$

Further, it follows from the above two estimates, (2.16) and (2.17) that

$$
|\mathbb{J}^2| \leq C \sum_{j=1}^{2} e^{-|b_j - b_j'|\sqrt{(2\pi N_j/L)^2 - k_j^2}} \Big(\|E_{\mathrm{I}}\|_{L^2(\Omega)} + \|H_{\mathrm{I}}\|_{L^2(\Omega)} \Big) \cdot \|v\|_1. \qquad (4.16)
$$

Thus, this proof is completed by combing (4.15) and (4.16). □

4.4. Proof of Lemma 4.3

Here we mention that Lemma 4.3 may be viewed as generalization of our relevant result in [46]. However, there are also some differences in results and techniques because the model of this article is somewhat more complicated. In the following subsection, we prove only in the case when $j = 1$, because the proof of the case when $j = 2$ is almost the same.

Based on Lemma 4.5 and Cauchy-Schwarz inequality, we easily obtain that

$$
\begin{aligned}
& \left| \frac{1}{\mu_1} \int_{\Gamma_1} (T^{(1)} - T^{(1,N_1)}) \xi_E \overline{\varphi} + \frac{1}{\varepsilon_1} \int_{\Gamma_1} (T^{(1)} - T^{(1,N_1)}) \xi_H \overline{\psi} \right| \\
\leq & C \max_{|n+n_\alpha|>N_1} (|\alpha_n + \alpha| |\beta_1^n|^3)^{-1/2} \Big(\big(L \sum_{|n+n_\alpha|>N_1} |\alpha_n + \alpha| |\xi_E^{(n)}(b_1)|^2 \big)^{1/2} \\
& \times \big(L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 |\varphi^{(n)}(b_1)|^2 \big)^{1/2} + \big(L \sum_{|n+n_\alpha|>N_1} |\alpha_n + \alpha| |\xi_H^{(n)}(b_1)|^2 \big)^{1/2} \\
& \times \big(L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 |\psi^{(n)}(b_1)|^2 \big)^{1/2} \Big) \\
\leq & C N_1^{-2} \Big(\|\xi_E\|_{H^1(\Omega)} \big(L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 |\varphi^{(n)}(b_1)|^2 \big)^{1/2} \\
& + \|\xi_H\|_{H^1(\Omega)} \big(L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 |\psi^{(n)}(b_1)|^2 \big)^{1/2} \Big) \\
\leq & C N_1^{-2} \|\xi\|_{H^1(\Omega)} \Big(L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 \big(|\varphi^{(n)}(b_1)|^2 + |\psi^{(n)}(b_1)|^2 \big) \Big)^{1/2}. \qquad (4.17)
\end{aligned}
$$

Next, to estimate the term with $\varphi^{(n)}(b_1)$ and $\psi^{(n)}(b_1)$ in (4.17) we consider the dual problem (4.2)–(4.5) in the following domain near Γ_1:

$$\widetilde{\Omega}^1 = \Big\{(x_1, x_3) : 0 < x_1 < L,\ b_1' < x_3 < b_1\Big\}.$$

By plugging the series expansion of φ and ψ into (4.2)-(4.5), the following boundary value problem can be obtained:

$$\begin{cases} (\varphi^{(n)})''(x_3) - |\beta_1^n|^2\varphi^{(n)}(x_3) = -\xi_E^{(n)}(x_3) \ \text{ in } \ (b_1', b_1), \\ (\varphi^{(n)})'(b_1) + |\beta_1^n|\varphi^{(n)}(b_1) = 0, \\ \varphi^{(n)}(b_1') = \varphi^{(n)}(b_1'), \end{cases} \tag{4.18}$$

and

$$\begin{cases} (\psi^{(n)})''(x_3) - |\beta_1^n|^2\psi^{(n)}(x_3) = -\xi_H^{(n)}(x_3) \ \text{ in } \ (b_1', b_1), \\ (\psi^{(n)})'(b_1) + |\beta_1^n|\psi^{(n)}(b_1) = 0, \\ \psi^{(n)}(b_1') = \psi^{(n)}(b_1'), \end{cases} \tag{4.19}$$

where n is required to satisfy the inequality that $|n + n_\alpha| > N_1$.

It follows from the general theory of ordinary differential equation and similar argument as in [46] that

$$\begin{aligned} |\varphi^{(n)}(b_1)| \le & \frac{1}{2|\beta_1^n|}\bigg(\int_{b_1'}^{b_1} \big(e^{|\beta_1^n|(s-b_1)} - e^{|\beta_1^n|(2b_1'-s-b_1)}\big) \cdot |\xi_E^{(n)}(s)|ds\bigg) \\ & + e^{-d|\beta_1^n|}|\varphi^{(n)}(b_1')| \\ \le & \frac{(1-e^{-d|\beta_1^n|})^2}{2|\beta_1^n|^2}\|\xi_E^{(n)}\|_{L^\infty([b_1',b_1])} + e^{-d|\beta_1^n|}|\varphi^{(n)}(b_1')| \\ \le & \frac{1}{2|\beta_1^n|^2}\|\xi_E^{(n)}\|_{L^\infty([b_1',b_1])} + e^{-d|\beta_1^n|}|\varphi^{(n)}(b_1')|, \end{aligned}$$

where $d := b_1 - b_1'$. For any $s \in (b_1', b_1)$, It is easily deduced that

$$\begin{aligned} |\xi_E^{(n)}(s)|^2 = & \frac{1}{b_1 - s}\int_{b_1}^{s} \big((b_1 - t)|\xi_E^{(n)}(t)|^2\big)' dt \\ \le & \frac{1}{b_1 - s}\int_{b_1'}^{b_1} |\xi_E^{(n)}(t)|^2 dt + 2\int_{b_1'}^{b_1} |\xi_E^{(n)}(t)||(\xi_E^{(n)}(t))'|dt \end{aligned}$$

Further, we get

$$\|\xi_E^{(n)}\|^2_{L^\infty([b_1',b_1])} \le \frac{2}{d}\|\xi_E^{(n)}\|^2_{L^2([b_1',b_1])} + 2\|\xi_E^{(n)}\|_{L^2([b_1',b_1])}\|(\xi_E^{(n)})'\|_{L^2([b_1',b_1])}. \tag{4.20}$$

By a similar argument as for (4.20), we have

$$\|\xi_H^{(n)}\|^2_{L^\infty([b_1',b_1])} \le \frac{2}{d}\|\xi_H^{(n)}\|^2_{L^2([b_1',b_1])} + 2\|\xi_H^{(n)}\|_{L^2([b_1',b_1])}\|(\xi_H^{(n)})'\|_{L^2([b_1',b_1])}.$$

By virtue of the Young inequality, we have

$$
\begin{aligned}
&L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 \big(|\varphi^{(n)}(b_1)|^2 + |\psi^{(n)}(b_1)|^2\big) \\
\le & CL \sum_{|n+n_\alpha|>N_1} \Big(|\beta_1^n| \big(\|\xi_E^{(n)}\|^2_{L^\infty([b_1',b_1])} + \|\xi_H^{(n)}\|^2_{L^\infty([b_1',b_1])}\big) \\
&\quad + |\beta_1^n|^5 e^{-2d|\beta_1^n|} \big(|\varphi^{(n)}(b_1')|^2 + |\psi^{(n)}(b_1')|^2\big)\Big) \\
\le & CL \sum_{|n+n_\alpha|>N_1} \Big(\big((d|\beta_1^n|)^{-1} + 1\big)|\beta_1^n|^2 \big(\|\xi_E^{(n)}\|^2_{L^2([b_1',b_1])} + \|\xi_H^{(n)}\|^2_{L^2([b_1',b_1])}\big) \\
&\quad + \|(\xi_E^{(n)})'\|^2_{L^2([b_1',b_1])} + \|(\xi_H^{(n)})'\|^2_{L^2([b_1',b_1])}\Big) \\
&\quad + CL \max_{|n+n_\alpha|>N_1} \big(|\beta_1^n|^4 e^{-2d|\beta_1^n|}\big) \sum_{|n+n_\alpha|>N_1} |\beta_1^n| \big(|\varphi^{(n)}(b_1')|^2 + |\psi^{(n)}(b_1')|^2\big) \\
:= & T_1 + T_2.
\end{aligned}
$$

Note that

$$
|\beta_1^n| \le |\alpha_n + \alpha| \le (1 + |\alpha_n + \alpha|^2)^{1/2}, \quad N_1 \le C|\beta_1^n|, \quad \text{for } |n+n_\alpha| > N_1
$$

and from the definition of $\|.\|_{H^1(\Omega)}$, we get

$$
T_1 \le C\big((N_1 d)^{-1} + 1\big)\|\xi\|_1^2.
$$

On the other hand, it follows from similar techniques used in the same reference [46] that

$$
\begin{aligned}
T_2 \le & Cd^{-4} L \max_{|n+n_\alpha|>N_1} \Big(|2d\beta_1^n|^4 e^{-2d|\beta_1^n|}\Big)\Big(\|\varphi\|^2_{H^{1/2}(\Gamma_1')} + \|\psi\|^2_{H^{1/2}(\Gamma_1')}\Big) \\
\le & Cd^{-4} \|w\|_1^2 \le Cd^{-4} \|\xi\|_0^2 .
\end{aligned}
$$

Therefore,

$$
L \sum_{|n+n_\alpha|>N_1} |\beta_1^n|^5 \Big(|\varphi^{(n)}(b_1)|^2 + |\psi^{(n)}(b_1)|^2\Big) \le C\Big(1 + (N_1 d)^{-1} + d^{-4}\Big)\|\xi\|_1^2. \tag{4.21}
$$

By inserting (4.21) into (4.17) and setting

$$
C_2 = C\big(1 + (N_1 d)^{-1/2} + d^{-2}\big), \tag{4.22}
$$

we complete the proof of Lemma 4.3. □

5. Implementation and Numerical Examples

Based on the a posteriori error estimate from Theorem 3.1, we use the PDF toolbox of MATLAB to implement the adaptive DtN finite element method given in Ref. [46]. In the following, two examples are from [43] and presented to demonstrate the competitiveness of our algorithm.

Example 5.1. Consider the chiral grating whose surface has corners, as shown in Fig. 5.1(a). Assume that plane waves

$$
E_I = e^{i\alpha x_1 - i\beta_1 x_3}, \quad H_I = 0
$$

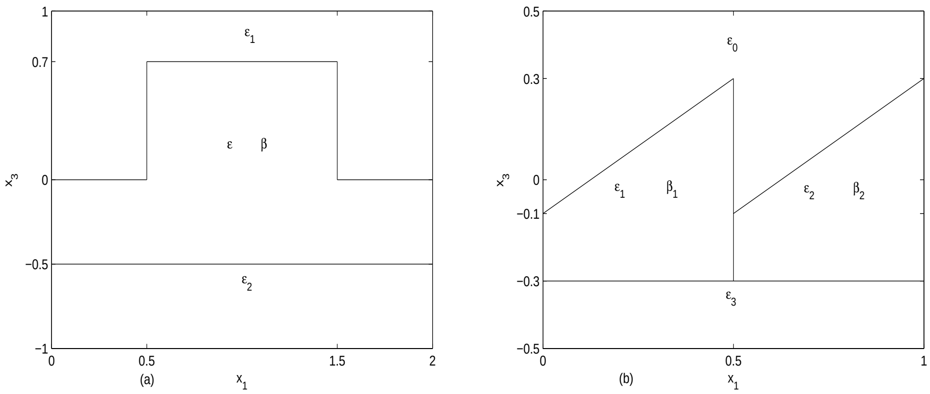

Fig. 5.1. (a): Geometry of the domain in Example 5.1; (b): Geometry of the domain in Example 5.2.

is incidence on the structure with $L = 2$ and $\theta = \pi/4$. The parameters are taken as follows: $\omega = \pi$, $\beta = 0.1$, $\varepsilon_1 = 1$, $\varepsilon_2 = 1$, $\varepsilon = 2.25$, $b_1 = 1$, $b_2 = -1$, $b_1' = 0.7$, $b_2' = -0.5$, N_1=20 and $N_2 = 12$. The mesh plot and the amplitude of the electric field and magnetic field after 9 adaptive iterations are shown in Fig. 5.2(a) and Fig. 5.3 when the grating efficiency is stabilized. It is observed that our algorithm has the ability to capture the singularities of the problem. And it is easy to reach the conclusion that although there is a big difference in the meshes, the surface plots of the amplitude of the numerical solution is almost the same for our adaptive DtN finite element method and the PML finite element method(cf., [43]). Fig. 5.4(a) shows the curve of $\log\mathrm{DoF}_h$ versus $\log\epsilon_h$, where DoF_h is the number of nodal points of the mesh $\mathcal{M}_h$. It implies that decay of the a posteriori error estimate for the adaptive mesh refinements is $\mathcal{O}(\mathrm{DoF}_h^{-1/2})$. It also shows the advantage of using adaptive mesh refinements. Fig. 5.4(b)

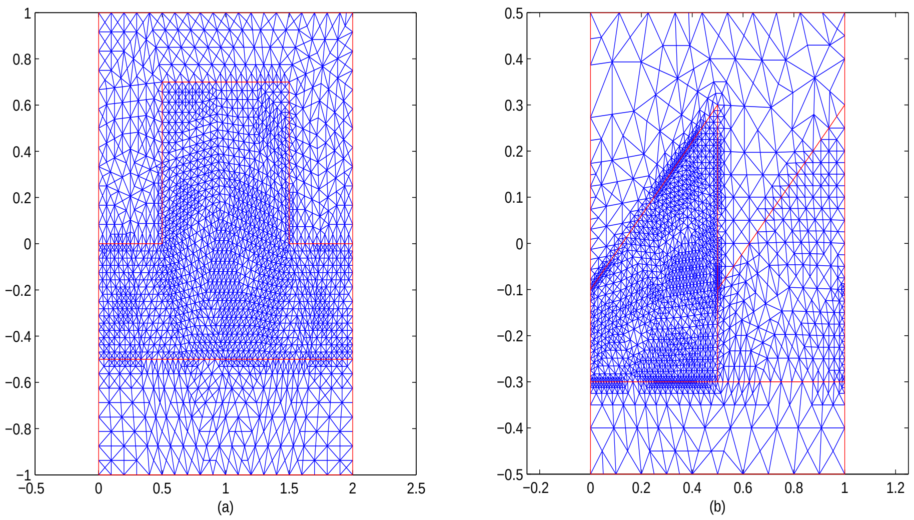

Fig. 5.2. (a): An adaptively refined mesh with 5329 elements for Example 5.1; (b): An adaptively refined mesh with 4470 elements for Example 5.2.

shows the grating efficiency of the reflected and transmitted waves as well as the total grating efficiency as a function of the number of nodal points, it is observed that the efficiencies are convergence for our adaptive algorithm.

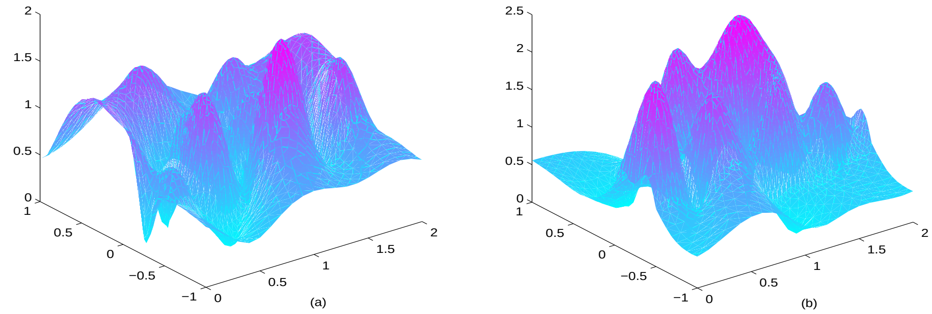

Fig. 5.3. The surface plot of the amplitude of the associated numerical solution on the mesh in Fig. 5.2(a) for Example 5.1. (a): the electric field; (b): the magnetic field.

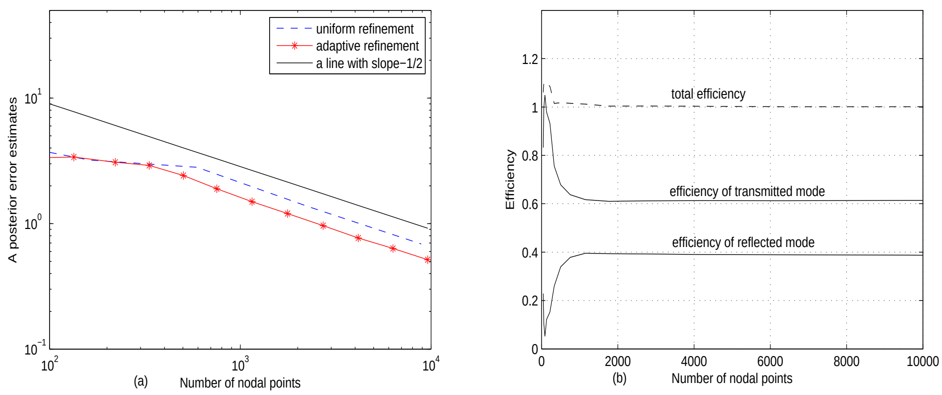

Fig. 5.4. Quasi-optimality of the adaptive mesh refinements (a) and grating efficiency versus the number of nodal points (b) in Example 5.1.

Example 5.2. This example concerns a chiral grating with two sharp angles, indicated in Fig. 5.1(b). The incident plane waves are

$$E_I = 4/5e^{i\alpha x_1 - i\beta_1 x_3}, \quad H_I = 3/5e^{i\alpha x_1 - i\beta_1 x_3}$$

with $\theta = \pi/6$. The parameters are chosen as $\omega = 2.5$, $\beta_1 = 0.2$, $\beta_2 = 0.1$, $\varepsilon_0 = 1$, $\varepsilon_1 = 2.56$, $\varepsilon_2 = 4.84$, $\varepsilon_3 = 1$, $b_1 = 0.5$, $b_2 = -0.5$, $b_1' = 0.3$, $b_2' = -0.3$, N_1=15 and $N_2 = 15$. Fig. 5.2(b) and Fig. 5.5 show the adaptively refined meshes and amplitude of the electric field and magnetic field after 11 adaptive iterations when the grating efficiency is stabilized. Just the same as Example 5.1, similar conclusions can be obtained: our example shows the ability of our algorithm to capture the singularities of the problem by using the local grid refinement. Fig. 5.6(a) shows the curve of $\log\mathrm{DoF}_h$ versus $\log\epsilon_h$. It indicates that the meshes and the

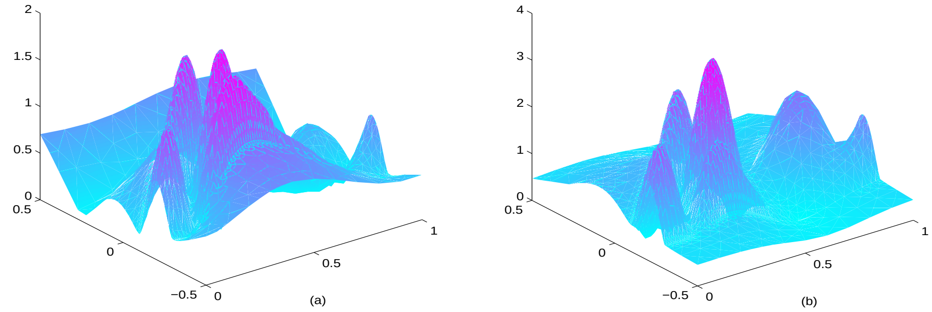

Fig. 5.5. The surface plot of the amplitude of the associated numerical solution on the mesh in Fig. 5.2(b) for Example 5.2. (a): the electric field; (b): the magnetic field.

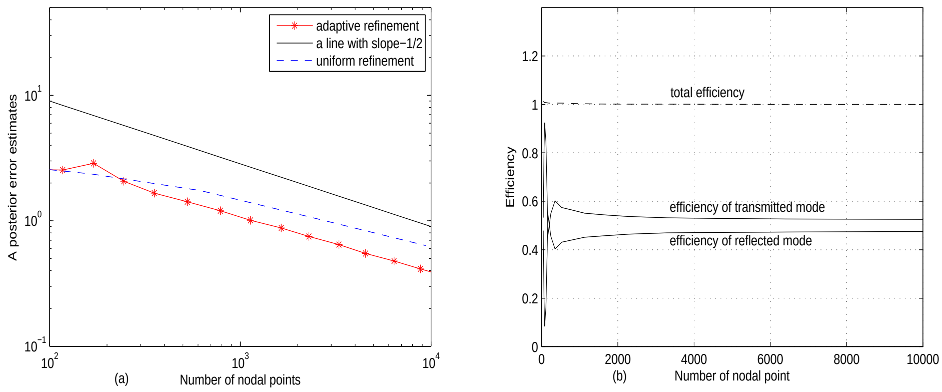

Fig. 5.6. Quasi-optimality of the adaptive mesh refinements (a) and grating efficiency versus the number of nodal points (b) in Example 5.2.

associated numerical complexity are quasi-optimal: $\epsilon_h = \mathcal{O}(\mathrm{DoF}_h^{-1/2})$ is valid asymptotically for our adaptive algorithm, but invalid for uniform refinement. The grating efficiency of the reflected and transmitted waves as well as the total grating efficiency are displayed in Fig. 5.6(b).

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