

An adaptive edge finite element DtN method for Maxwell's equations in biperiodic structures

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We consider the diffraction of an electromagnetic plane wave by a biperiodic structure. This paper is concerned with a numerical solution of the diffraction grating problem for three-dimensional Maxwell's equations. Based on the Dirichlet-to-Neumann (DtN) operator, an equivalent boundary value problem is formulated in a bounded domain by using a transparent boundary condition. An *a posteriori* error estimate-based adaptive edge finite element method is developed for the variational problem with the truncated DtN operator. The estimate takes account of both the finite element approximation error and the truncation error of the DtN operator, where the former is used for local mesh refinements and the latter is shown to decay exponentially with respect to the truncation parameter. Numerical experiments are presented to demonstrate the competitive behaviour of the proposed method.

Keywords: Maxwell's equations; diffractive grating problem; biperiodic structures; adaptive finite element method; transparent boundary condition; *a posteriori* error estimate.

1. Introduction

This paper concerns the diffraction of a time-harmonic electromagnetic plane wave by a biperiodic structure in three dimensions. In optics, a biperiodic or doubly periodic structure is called a two-

dimensional or crossed grating. Scattering theory in periodic structures has played an important role in many scientific areas, particularly in micro-optics, such as the design and fabrication of optical elements including corrective lenses, antireflective interfaces, beam splitters and sensors. Since Rayleigh's time, the basic electromagnetic theory of gratings has been studied extensively. Over the past two decades, the dramatic growth of computational capability and the development of fast algorithms have transformed the methodology for scientific investigation and industrial applications of the scattering theory of gratings. We refer to the book by [Petit \(1980\)](#) for a good introduction to diffraction grating problems. Mathematical studies can be found in the paper by [Bao *et al.* \(1995\)](#) and the references cited therein on the well-posedness of grating problems. Numerical methods are available for various approaches, which include integral equation methods, finite element methods and boundary perturbation methods; see [Bruno & Reitich \(1993\)](#), [Bao \(1997\)](#), [Wu & Lu \(2009\)](#) and [Bao *et al.* \(2014\)](#). We refer to the book by [Bao *et al.* \(2001\)](#) for a comprehensive review on diffractive optics technology and its mathematical modelling as well as computational methods. One may consult monographs by [Colton & Kress \(1983\)](#) and [Monk \(2003\)](#) for extensive accounts of integral equation methods and finite element methods, respectively, for direct and inverse electromagnetic scattering problems in general structures.

Similar to many other scattering problems, the diffraction grating problem is imposed in an open domain, which needs to be truncated to a bounded domain in order to apply a numerical method such as the finite element method. Therefore, an appropriate boundary condition is indispensable for the truncated domain. To avoid artificial wave reflection, the goal of the boundary condition is to mimic the wave propagation as if the boundary did not exist. Such a boundary condition is called an absorbing boundary condition (see e.g. [Engquist & Majda, 1977](#)), a nonreflecting boundary condition (see e.g. [Hagstrom, 1999](#)) or a transparent boundary conditions (TBCs) (see e.g. [Grote & Kirsch, 2004](#)). How to design mathematically effective and computationally efficient artificial boundary conditions is a subject matter of much ongoing research. Among these boundary conditions, a good option is the perfectly matched layer (PML) technique, which was first introduced by [Bérenger \(1994\)](#) for solving the time-domain Maxwell equations. Ever since then, how to construct and analyse the PML absorbing boundary conditions for various scattering problems have been an active research topic in computational wave propagation. The basic idea of the PML technique is to add an artificial layer of medium to surround the domain of interest. The waves, coming from inside of the domain, can be attenuated, ideally at an exponential rate, in the PML layer. Hence, the amplitudes of the waves are so small that a homogeneous Dirichlet boundary condition can be imposed on the exterior boundary of the layer. In order to choose effectively the parameters of the absorbing medium and the thickness of PML layer, adaptive finite element methods were developed for the diffraction grating problems (see [Chen & Wu, 2003](#); [Bao *et al.*, 2010](#)). The adaptive finite element PML method was also used to solve the obstacle scattering problems (see [Bao & Wu, 2005](#)). The analysis of adaptive finite element methods (FEMs) with local estimators for Maxwell's equations in bounded domain may be found in [Xu \(2007\)](#), [Zhong *et al.* \(2012\)](#) and [He *et al.* \(2020\)](#).

Recently, adaptive finite element Dirichlet-to-Neumann (DtN) methods were developed to solve many scattering problems such as the two-dimensional acoustic obstacle scattering problems (see [Jiang *et al.*, 2013](#); [Jiang *et al.*, 2017](#); [Li *et al.*, 2020](#)), the two-dimensional diffraction grating problems (see [Wang *et al.*, 2015](#); [Li & Yuan, 2020](#)) and the open cavity scattering problem (see [Yuan *et al.*, 2020](#)). The DtN method is different from the PML technique. An extra artificial layer of domain is not needed to surround the domain of interest. It can significantly reduce the size of the computational domain, since the TBC is exact and the artificial boundary can be put close to the scatterers. Consequently, the method may lead to a smaller linear system and less computational effort. However, the TBC is defined by a nonlocal DtN operator and is given by an infinite Fourier series. In practice, the infinite series has to

be truncated into a sum of finitely many terms by choosing an appropriate truncation parameter N . The *a posteriori* error estimate-based finite element DtN method was developed for the obstacle scattering problem and the diffraction grating problem, respectively, in Wang *et al.* (2015) and Jiang *et al.* (2017), where the two-dimensional Helmholtz equation was considered.

In this paper, we intend to extend the finite element DtN method to solve the diffraction grating problem in bi-periodic structures. It should be pointed out that the extension is a nontrivial since the techniques differ greatly from Wang *et al.* (2015) and Jiang *et al.* (2017). Here we consider the more complicated three-dimensional Maxwell equations instead of the two-dimensional Helmholtz equation. It is also more expensive to solve the three-dimensional Maxwell equations. In this work, we derive an *a posteriori* error estimate, which includes both the finite element discretization error and the truncation error of the DtN operator. It is known that the convergence of the truncated DtN mapping could be arbitrarily slow to the original DtN mapping in the operator norm for the obstacle scattering problem; see Hsiao *et al.* (2011). The same issue arises for the diffraction grating problem. To overcome this difficulty, we make use of the Helmholtz decomposition and develop a new duality argument for the *a posteriori* error estimate between the solutions of the diffraction problem and the finite element approximation. The estimate is used to design the adaptive edge finite element algorithm to choose elements for refinement and to determine the truncation parameter N in the Fourier series. Moreover, we show that the DtN operator truncation error decays exponentially with respect to N . The convergence analysis will be useful for the study of many other electromagnetic scattering problems where the Maxwell equations are involved. For comparison, we report numerical experiments for both the PML method and the DtN method. Numerical results demonstrate that the adaptive DtN method has a comparable behaviour to the adaptive PML method, which was developed in Bao *et al.* (2010). Compared with the uniform mesh refinement, the adaptive mesh refinement shows much more competitive efficiency. This work provides a viable alternative to the adaptive finite element PML method for solving the diffraction grating problem. In addition, the adaptive finite element DtN method may be applied to solve many other scattering problems imposed in open domains.

The paper is organized as follows. In Section 2, we introduce the model problem and its weak formulation by using the TBC. The finite element discretization with the truncated DtN operator is presented in Section 3. Section 4 is devoted to the *a posteriori* error estimate by using a duality argument. In Section 5, we present some numerical experiments to demonstrate the competitive behaviour of the proposed method. The paper is concluded with some general remarks in Section 6.

2. Problem formulation

In this section, we introduce the diffraction grating problem and its variational formulation by using the TBC.

2.1 Maxwell's equations

The electromagnetic fields in the whole space are governed by the time-harmonic (time-dependence $e^{-i\omega t}$) Maxwell's equations

$$\nabla \times \mathbf{E} - i\omega\mu\mathbf{H} = 0, \quad \nabla \times \mathbf{H} + i\omega\varepsilon\mathbf{E} = 0, \quad (2.1)$$

where $\omega > 0$ is the angular frequency, \mathbf{E} and \mathbf{H} are the electric field and the magnetic field, respectively, and the dielectric permittivity $\varepsilon(\mathbf{x}) \in C(\mathbb{R}^3)$ and the magnetic permeability $\mu(\mathbf{x}) \in C(\mathbb{R}^3)$ are assumed

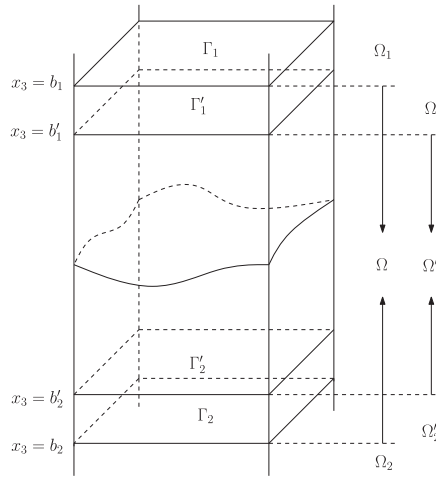


FIG. 1. Problem geometry of the diffraction grating in a biperiodic structure.

to be periodic in the x_1 and x_2 directions with periods L_1 and L_2 , respectively, i.e.,

$$\begin{aligned}\varepsilon(x_1 + n_1 L_1, x_2 + n_2 L_2, x_3) &= \varepsilon(x_1, x_2, x_3), \\ \mu(x_1 + n_1 L_1, x_2 + n_2 L_2, x_3) &= \mu(x_1, x_2, x_3).\end{aligned}$$

Here n_1, n_2 are integers. Throughout we assume that $\operatorname{Re} \varepsilon > 0$, $\operatorname{Im} \varepsilon \geq 0$ and $\mu > 0$. The problem geometry is shown in Fig. 1. Let

$$\Omega = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, b_2 < x_3 < b_1\},$$

where $b_j, j = 1, 2$ are constants. Denote by $\Omega_1 = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 > b_1\}$ and $\Omega_2 = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 < b_2\}$ the unbounded domains above and below Ω , respectively. Let $\Gamma_j = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 = b_j\}$ and $\Gamma'_j = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 = b'_j\}$, where $b'_j, j = 1, 2$ are constants satisfying $b_2 < b'_2 < b'_1 < b_1$. Let $d_j = |b_j - b'_j|, j = 1, 2$. Without loss of generality, we assume that $b'_1 - b'_2 \simeq 1$, which can be achieved by scaling the original problem. In practice, one may first choose Γ'_j as close as possible to the grating surface and then set the boundary Γ_j for $j = 1, 2$.

Define $\Omega' = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, b'_2 < x_3 < b'_1\}$. Denote by $\Omega'_1 = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 \geq b'_1\}$ and $\Omega'_2 = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, x_3 \leq b'_2\}$ the unbounded domains above and below Ω' , respectively. The medium is assumed to be homogeneous away from Ω' , i.e., there exist constants ε_j and μ_j such that

$$\varepsilon(\mathbf{x}) = \varepsilon_j, \quad \mu(\mathbf{x}) = \mu_j, \quad \mathbf{x} \in \Omega'_j, \quad j = 1, 2.$$

Moreover, we assume that $\varepsilon_1 > 0, \mu_j > 0, j = 1, 2$, but allow ε_2 to be complex for the substrate in Ω'_2 .

Let $(\mathbf{E}^{\text{inc}}, \mathbf{H}^{\text{inc}})$ be the incoming electromagnetic plane waves that are incident on the grating surface from the top, where

$$\mathbf{E}^{\text{inc}} = \mathbf{p} e^{i\mathbf{q} \cdot \mathbf{x}}, \quad \mathbf{H}^{\text{inc}} = s e^{i\mathbf{q} \cdot \mathbf{x}}, \quad s = \frac{\mathbf{q} \times \mathbf{p}}{\omega \mu_1}, \quad \mathbf{p} \cdot \mathbf{q} = 0.$$

Here $\mathbf{q} = (\alpha_1, \alpha_2, -\beta)^\top = \omega \sqrt{\varepsilon_1 \mu_1} (\sin \theta_1 \cos \theta_2, \sin \theta_1 \sin \theta_2, -\cos \theta_1)^\top$ and θ_1, θ_2 are incident angles satisfying $0 \leq \theta_1 < \pi/2, 0 \leq \theta_2 < 2\pi$.

Motivated by the uniqueness, we are interested in quasi-periodic solutions, i.e., the phase shifted electromagnetic fields $(\mathbf{E}(\mathbf{x}), \mathbf{H}(\mathbf{x})) e^{-i(\alpha_1 x_1 + \alpha_2 x_2)}$ are periodic functions in x_1 and x_2 with periods L_1 and L_2 , respectively.

Denote by $L^2(\Omega)$ the space of complex square integrable functions in Ω . Let

$$H(\text{curl}, \Omega) = \{\boldsymbol{\varphi} \in L^2(\Omega)^3 : \nabla \times \boldsymbol{\varphi} \in L^2(\Omega)^3\},$$

which is equipped with the norm

$$\|\boldsymbol{\varphi}\|_{H(\text{curl}, \Omega)} = \left(\|\boldsymbol{\varphi}\|_{L^2(\Omega)^3}^2 + \|\nabla \times \boldsymbol{\varphi}\|_{L^2(\Omega)^3}^2 \right)^{1/2}.$$

Define the periodic function space

$$\begin{aligned} H_{\text{per}}(\text{curl}, \Omega) = \{ \boldsymbol{\varphi} \in H(\text{curl}, \Omega) : (1, 0, 0)^\top \times [\boldsymbol{\varphi}(0, x_2, x_3) - \boldsymbol{\varphi}(L_1, x_2, x_3)] = 0, \\ (0, 1, 0)^\top \times [\boldsymbol{\varphi}(x_1, 0, x_3) - \boldsymbol{\varphi}(x_1, L_2, x_3)] = 0 \}. \end{aligned}$$

Let

$$H_{\text{qper}}(\text{curl}, \Omega) = \{ \boldsymbol{\varphi} : \boldsymbol{\varphi} e^{-i(\alpha_1 x_1 + \alpha_2 x_2)} \in H_{\text{per}}(\text{curl}, \Omega) \},$$

$$H_{\text{per}}^1(\Omega) = \{ \phi \in H^1(\Omega) : \phi(0, x_2, x_3) = \phi(L_1, x_2, x_3), \phi(x_1, 0, x_3) = \phi(x_1, L_2, x_3) \},$$

$$H_{\text{qper}}^1(\Omega) = \{ \phi : \phi(x_1, x_2, x_3) e^{-i(\alpha_1 x_1 + \alpha_2 x_2)} \in H_{\text{per}}^1(\Omega) \}.$$

For any smooth vector field $\boldsymbol{\psi} = (\psi_1, \psi_2, \psi_3)^\top$, denote by $\boldsymbol{\psi}_{\Gamma_j} = (\psi_1(x_1, x_2, b_j), \psi_2(x_1, x_2, b_j), 0)^\top$ the tangential component of $\boldsymbol{\psi}$ on the surface $\Gamma_j, j = 1, 2$.

To describe the DtN operators and the TBC for the boundary value problem, we introduce some trace function spaces. Denote by $H_{\text{qper}}^{1/2}(\Gamma_j)$ the function space consisting of the restriction on Γ_j of functions in $H_{\text{qper}}^1(\Omega)$, and by $H_{\text{qper}}^{-1/2}(\Gamma_j)$ the dual space of $H_{\text{qper}}^{1/2}(\Gamma_j)$. Let $\mathbf{n} = (n_1, n_2)^\top \in \mathbb{Z}^2$ and

$\alpha_{jn} = \alpha_j + 2\pi n_j/L_j, j = 1, 2$. For any $\phi \in H_{\text{qper}}^{-1/2}(\Gamma_j)$, it has the following Fourier series expansion:

$$\phi(x_1, x_2, b_j) = \sum_{n \in \mathbb{Z}^2} \phi_n(b_j) e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}.$$

The norm can be characterized by

$$\|\phi\|_{H_{\text{qper}}^{-1/2}(\Gamma_j)}^2 = L_1 L_2 \sum_{n \in \mathbb{Z}^2} (1 + |\alpha_n|^2)^{-1/2} |\phi_n(b_j)|^2,$$

where $\alpha_n = (\alpha_{1n}, \alpha_{2n})^\top$.

For any vector field $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \varphi_3)^\top$ and scalar field ψ , denote by

$$\begin{aligned} \text{curl}_{\Gamma_j} \boldsymbol{\varphi} &= \partial_{x_1} \varphi_2 - \partial_{x_2} \varphi_1, \\ \nabla_{\Gamma_j} \psi &= (\partial_{x_1} \psi, \partial_{x_2} \psi, 0)^\top, \\ \text{div}_{\Gamma_j} \boldsymbol{\varphi} &= \partial_{x_1} \varphi_1 + \partial_{x_2} \varphi_2 \end{aligned}$$

the surface scalar curl, the surface gradient and the surface divergence on $\Gamma_j, j = 1, 2$, respectively. Introduce the following tangential function spaces:

$$\begin{aligned} TL^2(\Gamma_j) &= \{\boldsymbol{\varphi} \in L^2(\Gamma_j)^3, \varphi_3 = 0\}, \\ TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j) &= \{\boldsymbol{\varphi} \in H_{\text{qper}}^{-1/2}(\Gamma_j)^3 : \text{curl}_{\Gamma_j} \boldsymbol{\varphi} \in H^{-1/2}(\Gamma_j), \varphi_3 = 0\}. \end{aligned}$$

For any quasi-periodic tangential vector field $\boldsymbol{\varphi}$, it has the Fourier series expansion

$$\boldsymbol{\varphi} = \sum_{n \in \mathbb{Z}^2} (\varphi_{1n}, \varphi_{2n}, 0)^\top e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}.$$

The $TL^2(\Gamma_j)$ norm of $\boldsymbol{\varphi}$ may be represented as

$$\|\boldsymbol{\varphi}\|_{TL^2(\Gamma_j)}^2 = L_1 L_2 \sum_{n \in \mathbb{Z}^2} (|\varphi_{1n}|^2 + |\varphi_{2n}|^2).$$

The norm on $TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j)$ can be characterized by

$$\begin{aligned} \|\boldsymbol{\varphi}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j)}^2 &= L_1 L_2 \sum_{n \in \mathbb{Z}^2} (1 + |\alpha_n|^2)^{-1/2} [|\varphi_{1n}(b_j)|^2 + |\varphi_{2n}(b_j)|^2 \\ &\quad + |\alpha_{1n}\varphi_{2n}(b_j) - \alpha_{2n}\varphi_{1n}(b_j)|^2]. \end{aligned} \quad (2.2)$$

2.2 Variational formulation

In this section, we introduce the TBC and the variational formulation of the diffraction grating problem. The details on the derivation of the TBC can be found; see [Bao et al. \(2010\)](#).

By Rayleigh's expansions of (\mathbf{E}, \mathbf{H}) in Ω_j , the following TBCs hold:

$$\begin{aligned} (\mathbf{H} - \mathbf{H}^{\text{inc}}) \times \mathbf{v}_1 &= \mathcal{T}_1(\mathbf{E} - \mathbf{E}^{\text{inc}})_{\Gamma_1} \quad \text{on } \Gamma_1, \\ \mathbf{H} \times \mathbf{v}_2 &= \mathcal{T}_2 \mathbf{E}_{\Gamma_2} \quad \text{on } \Gamma_2, \end{aligned}$$

where \mathbf{v}_j is the unit outward normal vector on Γ_j , i.e., $\mathbf{v}_j = (0, 0, (-1)^{j-1})^\top$, and the DtN operator \mathcal{T}_j is defined as follows: for any tangential vector field $\boldsymbol{\varphi} \in TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j)$, which has Fourier series expansion

$$\boldsymbol{\varphi} = \sum_{n \in \mathbb{Z}^2} (\varphi_{1n}^{(j)}, \varphi_{2n}^{(j)}, 0)^\top e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)},$$

define

$$\mathcal{T}_j \boldsymbol{\varphi} = \sum_{n \in \mathbb{Z}^2} (r_{1n}^{(j)}, r_{2n}^{(j)}, 0)^\top e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}, \quad (2.3)$$

where

$$\begin{aligned} r_{1n}^{(j)} &= \frac{1}{\omega \mu_j \beta_{jn}} [(\kappa_j^2 - \alpha_{2n}^2) \varphi_{1n}^{(j)} + \alpha_{1n} \alpha_{2n} \varphi_{2n}^{(j)}], \\ r_{2n}^{(j)} &= \frac{1}{\omega \mu_j \beta_{jn}} [(\kappa_j^2 - \alpha_{1n}^2) \varphi_{2n}^{(j)} + \alpha_{1n} \alpha_{2n} \varphi_{1n}^{(j)}]. \end{aligned}$$

Here

$$\beta_{jn} = (\kappa_j^2 - |\alpha_n|^2)^{1/2}, \quad \text{Im} \beta_{jn} \geq 0, \quad \kappa_j^2 = \omega^2 \varepsilon_j \mu_j. \quad (2.4)$$

We exclude possible resonances by assuming that $\kappa_j^2 \neq |\alpha_n|^2, n \in \mathbb{Z}^2, j = 1, 2$.

Now we present the variational formulation of the Maxwell system (2.1) in the space $H_{\text{qper}}(\text{curl}, \Omega)$. Eliminating the magnetic field \mathbf{H} from (2.1), we obtain

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} = 0 \quad \text{in } \Omega. \quad (2.5)$$

Multiplying the complex conjugate of a test function $\boldsymbol{\psi}$ in $H_{\text{qper}}(\text{curl}, \Omega)$, integrating over Ω and using the integration by parts, we arrive at the variational form for the scattering problem: find $\mathbf{E} \in H_{\text{qper}}(\text{curl}, \Omega)$ such that

$$a(\mathbf{E}, \boldsymbol{\psi}) = \langle \mathbf{f}, \boldsymbol{\psi} \rangle_{\Gamma_1} \quad \forall \boldsymbol{\psi} \in H_{\text{qper}}(\text{curl}, \Omega), \quad (2.6)$$

where the sesquilinear form

$$a(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \int_{\Omega} \mu^{-1} \nabla \times \boldsymbol{\varphi} \cdot \nabla \times \bar{\boldsymbol{\psi}} - \omega^2 \int_{\Omega} \varepsilon \boldsymbol{\varphi} \cdot \bar{\boldsymbol{\psi}} - i\omega \sum_{j=1}^2 \int_{\Gamma_j} \mathcal{T}_j \boldsymbol{\varphi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j}, \quad (2.7)$$

and the linear functional

$$\langle \boldsymbol{f}, \boldsymbol{\psi} \rangle_{\Gamma_1} = i\omega \int_{\Gamma_1} (\boldsymbol{H}^{\text{inc}} \times \boldsymbol{v}_1 - \mathcal{T}_1 \boldsymbol{E}_{\Gamma_1}^{\text{inc}}) \cdot \bar{\boldsymbol{\psi}}_{\Gamma_1} = -2i\omega \int_{\Gamma_1} \mathcal{T}_1 \boldsymbol{E}_{\Gamma_1}^{\text{inc}} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_1}.$$

Here we have used the identity

$$\boldsymbol{H}^{\text{inc}} \times \boldsymbol{v}_1 = -\mathcal{T}_1 \boldsymbol{E}_{\Gamma_1}^{\text{inc}} \quad \text{on } \Gamma_1.$$

The well-posedness of the variational problem (2.6) was established in Dobson (1994) and Bao (1997). It was shown that the variational problem (2.6) admits a unique solution for all but possibly a discrete set of frequencies. Here we simply assume that the variational problem (2.6) admits a unique weak solution in $H_{\text{qper}}(\text{curl}, \Omega)$. Then it follows from the general theory in Babuška & Aziz (1972) that there exists a constant $\gamma_1 > 0$ such that the following inf-sup condition holds:

$$\sup_{0 \neq \boldsymbol{\psi} \in H_{\text{qper}}(\text{curl}, \Omega)} \frac{|a(\boldsymbol{\varphi}, \boldsymbol{\psi})|}{\|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)}} \geq \gamma_1 \|\boldsymbol{\varphi}\|_{H(\text{curl}, \Omega)} \quad \forall \boldsymbol{\varphi} \in H_{\text{qper}}(\text{curl}, \Omega). \quad (2.8)$$

3. Finite element approximation

In this section, we introduce the finite element approximation and present the *a posteriori* error estimate, which plays an important role for the adaptive finite element method.

3.1 The discrete problem

Let \mathcal{M}_h be a regular tetrahedral mesh of the domain Ω . To deal with the quasi-periodic boundary conditions, we assume further that the mesh is periodic in both x_1 and x_2 directions, i.e., the surface mesh of Ω perpendicular to the x_1 -axis or the x_2 -axis coincides with the mesh on the opposite face.

Denote by \mathcal{F}_h the set of all faces of tetrahedrons in \mathcal{M}_h . Let $V_h \subset H_{\text{qper}}(\text{curl}, \Omega)$ denote the space of the lowest order Nédélec edge elements, i.e.,

$$V_h = \{\boldsymbol{v}_h \in H_{\text{qper}}(\text{curl}, \Omega) : \boldsymbol{v}_h|_T = \boldsymbol{a}_T + \boldsymbol{b}_T \times \boldsymbol{x}, \boldsymbol{a}_T, \boldsymbol{b}_T \in \mathbb{C}^3, \forall T \in \mathcal{M}_h\}. \quad (3.1)$$

The finite element approximation to the problem (2.6) reads as follows: find $\boldsymbol{E}_h \in V_h$ such that

$$a(\boldsymbol{E}_h, \boldsymbol{\psi}_h) = \langle \boldsymbol{f}, \boldsymbol{\psi}_h \rangle_{\Gamma_1} \quad \forall \boldsymbol{\psi}_h \in V_h. \quad (3.2)$$

In the above formulation, the DtN operator \mathcal{T}_j given by (2.3) is defined by an infinite series. It is necessary to truncate the series by taking finitely many terms in order to apply any feasible algorithm.

We truncate the DtN operator \mathcal{T}_j as follows:

$$\mathcal{T}_j^{N_j} \boldsymbol{\varphi} = \sum_{n \in U_{N_j}} (r_{1n}^{(j)}, r_{2n}^{(j)}, 0)^\top e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}, \quad (3.3)$$

where the index set U_{N_j} is defined as

$$U_{N_j} = \left\{ n = (n_1, n_2)^\top \in \mathbb{Z}^2 : |\alpha_n| \leq 2\pi N_j / \sqrt{L_1 L_2} \right\}, \quad j = 1, 2. \quad (3.4)$$

Roughly speaking, the points in U_{N_j} occupy an area of πN_j^2 .

Now we are ready to define the truncated finite element formulation, which leads to the discrete approximation to (2.6): find $\mathbf{E}_h^N \in V_h$ such that

$$a_N(\mathbf{E}_h^N, \boldsymbol{\psi}_h) = \langle \mathbf{f}^{N_1}, \boldsymbol{\psi}_h \rangle_{\Gamma_1} \quad \forall \boldsymbol{\psi}_h \in V_h, \quad (3.5)$$

where the sesquilinear form $a_N: V_h \times V_h \rightarrow \mathbb{C}$ is defined as follows:

$$a_N(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \int_{\Omega} \mu^{-1} \nabla \times \boldsymbol{\varphi} \cdot \nabla \times \bar{\boldsymbol{\psi}} - \omega^2 \int_{\Omega} \varepsilon \boldsymbol{\varphi} \cdot \bar{\boldsymbol{\psi}} - i\omega \sum_{j=1}^2 \int_{\Gamma_j} \mathcal{T}_j^{N_j} \boldsymbol{\varphi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j}, \quad (3.6)$$

and

$$\langle \mathbf{f}^{N_1}, \boldsymbol{\psi}_h \rangle_{\Gamma_1} = -2i\omega \int_{\Gamma_1} \mathcal{T}_1^{N_1} \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot (\bar{\boldsymbol{\psi}}_h)_{\Gamma_1}.$$

REMARK 3.1 In this work, we do not plan to discuss the existence and uniqueness of the discrete problems (3.2) and (3.5) since the focus is on the *a posteriori* and convergence analysis for the adaptive finite element with the truncated DtN operator. Generally speaking, it is required that $\kappa^3 h^2$ should be sufficiently small to ensure the well-posedness of the discrete problem. We refer to [Feng & Wu \(2014\)](#) and [Lu et al. \(2019\)](#) for the interior penalty discontinuous Galerkin method, and the continuous interior penalty finite element method for solving Maxwell's equations in a bounded domain. There is no rigorous analysis for Maxwell's equations in biperiodic structures. In general, we require a sufficiently fine initial mesh, especially for high wave number problems.

3.2 The *a posteriori* error estimate

In this section, we give the *a posteriori* error estimate and present the main result of the paper. For any $T \in \mathcal{M}_h$, we define the residuals

$$\mathbf{R}_T^{(1)} := \omega^2 \varepsilon \mathbf{E}_h^N|_T - \nabla \times (\mu^{-1} \nabla \times \mathbf{E}_h^N|_T), \quad \mathbf{R}_T^{(2)} := -\omega^2 \nabla \cdot (\varepsilon \mathbf{E}_h^N|_T).$$

Given an interior face $F \in \mathcal{F}_h$, which is the common face of T_1 and T_2 , we define the jump residuals across F as

$$\mathbf{J}_F^{(1)} := \mu^{-1}(\nabla \times \mathbf{E}_h^N|_{T_1} - \nabla \times \mathbf{E}_h^N|_{T_2}) \times \mathbf{v}_F, \quad \mathbf{J}_F^{(2)} := \omega^2(\varepsilon \mathbf{E}_h^N|_{T_2} - \varepsilon \mathbf{E}_h^N|_{T_1}) \cdot \mathbf{v}_F,$$

where the unit normal vector \mathbf{v}_F on F points from T_2 to T_1 . Given a face $F \in \mathcal{F}_h \cap \Gamma_1$, we define the residuals as

$$\begin{aligned} \mathbf{J}_F^{(1)} &= 2[-(\mu^{-1} \nabla \times \mathbf{E}_h^N) \times \mathbf{v}_1 + i\omega \mathcal{T}_1^{N_1}(\mathbf{E}_h^N)_{\Gamma_1} - 2i\omega \mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}}] \\ \mathbf{J}_F^{(2)} &= 2[\omega^2 \varepsilon \mathbf{E}_h^N \cdot \mathbf{v}_1 - i\omega \text{div}_{\Gamma_1}(\mathcal{T}_1^{N_1}(\mathbf{E}_h^N)_{\Gamma_1}) + 2i\omega \text{div}_{\Gamma_1}(\mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}})]. \end{aligned}$$

Given a face $F \in \mathcal{F}_h \cap \Gamma_2$, we define the residuals as

$$\begin{aligned} \mathbf{J}_F^{(1)} &= 2[-(\mu^{-1} \nabla \times \mathbf{E}_h^N) \times \mathbf{v}_2 + i\omega \mathcal{T}_2^{N_2}(\mathbf{E}_h^N)_{\Gamma_2}] \\ \mathbf{J}_F^{(2)} &= 2[\omega^2 \varepsilon \mathbf{E}_h^N \cdot \mathbf{v}_2 - i\omega \text{div}_{\Gamma_2}(\mathcal{T}_2^{N_2}(\mathbf{E}_h^N)_{\Gamma_2})]. \end{aligned}$$

For $j = 0, 1$, define

$$\begin{aligned} \Gamma_{1j} &= \{\mathbf{x} \in \mathbb{R}^3 : x_1 = jL_1, 0 < x_2 < L_2, b_2 < x_3 < b_1\}, \\ \Gamma_{2j} &= \{\mathbf{x} \in \mathbb{R}^3 : x_2 = jL_2, 0 < x_1 < L_1, b_2 < x_3 < b_1\}. \end{aligned}$$

For any face $F \in \mathcal{F}_h \cap \Gamma_{l0}$, let $F' \in \mathcal{F}_h$ be the corresponding face on Γ_{l1} ($l = 1, 2$), and let $T, T' \in \mathcal{M}_h$ be the two elements such that $T \supset F$ and $T' \supset F'$. We define the jump residuals across F and F' as

$$\begin{aligned} \mathbf{J}_F^{(1)} &:= \mu^{-1}(e^{-i\alpha_j L_j} \nabla \times \mathbf{E}_h^N|_{T'} - \nabla \times \mathbf{E}_h^N|_T) \times \mathbf{v}_F, \\ \mathbf{J}_{F'}^{(1)} &:= \mu^{-1}(\nabla \times \mathbf{E}_h^N|_{T'} - e^{i\alpha_j L_j} \nabla \times \mathbf{E}_h^N|_T) \times \mathbf{v}_F, \\ \mathbf{J}_F^{(2)} &:= \omega^2(\varepsilon \mathbf{E}_h^N|_T - e^{-i\alpha_j L_j} \varepsilon \mathbf{E}_h^N|_{T'}) \cdot \mathbf{v}_F, \\ \mathbf{J}_{F'}^{(2)} &:= \omega^2(e^{i\alpha_j L_j} \varepsilon \mathbf{E}_h^N|_T - \varepsilon \mathbf{E}_h^N|_{T'}) \cdot \mathbf{v}_F, \end{aligned}$$

where \mathbf{v}_F is the unit outward normal vector to F .

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

$$\eta_T^2 = h_T^2 \left(\|\mathbf{R}_T^{(1)}\|_{L^2(T)^3}^2 + \|\mathbf{R}_T^{(2)}\|_{L^2(T)}^2 \right) + h_T \sum_{F \subset \partial T} \left(\|\mathbf{J}_F^{(1)}\|_{L^2(F)^3}^2 + \|\mathbf{J}_F^{(2)}\|_{L^2(F)}^2 \right).$$

We now state the main result of this paper.

THEOREM 3.2 Let \mathbf{E} and \mathbf{E}_h^N be the solutions of (2.6) and (3.5), respectively. Then there exist two integers M_j , $j = 1, 2$ independent of h and satisfying $\left(\frac{2\pi M_j}{\sqrt{L_1 L_2}}\right)^2 > \text{Re} \kappa_j^2$ such that for $N_j \geq M_j$ the

following *a posteriori* error estimate holds:

$$\|\mathbf{E} - \mathbf{E}_h^N\|_{H(\text{curl}, \Omega)} \leq C(\epsilon_h + \epsilon_N),$$

where $\epsilon_h = (\sum_{T \in \mathcal{M}_h} \eta_T^2)^{1/2}$, $\epsilon_N = \sum_{j=1}^2 e^{-d_j \sigma_j} \|\mathbf{E}^{\text{inc}}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)}$. Here $\sigma_j = ((\frac{2\pi N_j}{\sqrt{L_1 L_2}})^2 - \text{Re} \kappa_j^2)^{1/2}$ and the constant C is independent of h and M_j .

4. Proof of the main theorem

The section is devoted to the proof of Theorem 3.2. The difficulty is to estimate the truncation error of the DtN operator. We introduce a dual problem to overcome it.

4.1 The dual problem

Denote the error by $\boldsymbol{\xi} = \mathbf{E} - \mathbf{E}_h^N$. Consider the Helmholtz decomposition

$$\varepsilon \boldsymbol{\xi} = \varepsilon \nabla q + \boldsymbol{\zeta}, \quad q \in H_0^1(\Omega), \quad \text{div} \boldsymbol{\zeta} = 0. \quad (4.1)$$

Obviously one has

$$\|\nabla q\|_{L^2(\Omega)} \lesssim \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}, \quad \|\boldsymbol{\zeta}\|_{L^2(\Omega)^3} \lesssim \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}. \quad (4.2)$$

Hereafter, $A \lesssim B$ means $A \leq CB$ where C is a positive constant C independent of N , N_j and d_j .

Introduce the following dual problem to the original scattering problem: find $\mathbf{W} \in H_{\text{qper}}(\text{curl}, \Omega)$ such that it satisfies the variational problem

$$a(\mathbf{v}, \mathbf{W}) = (\mathbf{v}, \boldsymbol{\zeta}) \quad \forall \mathbf{v} \in H_{\text{qper}}(\text{curl}, \Omega). \quad (4.3)$$

It is easy to verify that \mathbf{W} is the weak solution of the boundary value problem:

$$\begin{cases} \nabla \times ((\bar{\mu})^{-1} \nabla \times \mathbf{W}) - \omega^2 \bar{\varepsilon} \mathbf{W} = \boldsymbol{\zeta} & \text{in } \Omega, \\ ((\bar{\mu})^{-1} \nabla \times \mathbf{W}) \times \mathbf{v}_j = -i\omega \mathcal{T}_j^* \mathbf{W}_{\Gamma_j} & \text{on } \Gamma_j, \end{cases}$$

where the adjoint operator \mathcal{T}_j^* takes the following form:

$$\mathcal{T}_j^* \boldsymbol{\varphi} = \sum_{n \in \mathbb{Z}^2} (\rho_{1n}^{(j)}, \rho_{2n}^{(j)}, 0)^\top e^{i(\alpha_{1n} x_1 + \alpha_{2n} x_2)}, \quad j = 1, 2. \quad (4.4)$$

Here

$$\begin{aligned} \rho_{1n}^{(j)} &= \frac{1}{\omega \mu_j \bar{\beta}_{jn}} [(\bar{\kappa}_j^2 - \alpha_{2n}^2) \varphi_{1n}^{(j)} + \alpha_{1n} \alpha_{2n} \varphi_{2n}^{(j)}], \\ \rho_{2n}^{(j)} &= \frac{1}{\omega \mu_j \bar{\beta}_{jn}} [(\bar{\kappa}_j^2 - \alpha_{1n}^2) \varphi_{2n}^{(j)} + \alpha_{1n} \alpha_{2n} \varphi_{1n}^{(j)}]. \end{aligned}$$

The well-posedness of the dual problem can be similarly proved as that for the variational problem (2.6). The proof is skipped for brevity. Assuming that the dual problem has a unique weak solution, we have the stability estimate

$$\|\mathbf{W}\|_{H(\text{curl}, \Omega)} \leq C_0 \|\boldsymbol{\zeta}\|_{L^2(\Omega)^3}, \quad (4.5)$$

where C_0 is a positive constant.

Denote by $U_h \subset H_{\text{qper}}^1(\Omega)$ the standard continuous piecewise linear finite element space. Clearly, we have

$$\nabla U_h \subseteq V_h,$$

where V_h is the lowest order Nédélec edge element space defined in (3.1).

4.2 An estimate of $\boldsymbol{\xi}$

The following lemma gives some relations on the error $\boldsymbol{\xi}$, which is the starting point for the *a posteriori* error analysis.

LEMMA 4.1 Let $\mathbf{E}, \mathbf{E}_h^N$ and \mathbf{W} be the solutions to the problems (2.6), (3.5) and (4.3), respectively. Then we have

$$\begin{aligned} \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}^2 &\lesssim \text{Re} \left[a(\boldsymbol{\xi}, \boldsymbol{\xi}) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\boldsymbol{\xi}}_{\Gamma_j} \right] \\ &\quad - \omega \sum_{j=1}^2 \text{Im} \int_{\Gamma_j} \mathcal{T}_j^{N_j} \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\boldsymbol{\xi}}_{\Gamma_j} + \text{Re} \int_{\Omega} (\omega^2 \varepsilon + \mathbf{D}) \boldsymbol{\xi} \cdot \bar{\boldsymbol{\xi}}, \end{aligned} \quad (4.6)$$

$$\begin{aligned} (\varepsilon \boldsymbol{\xi}, \boldsymbol{\xi}) &= \left[a(\boldsymbol{\xi}, \mathbf{W}) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\mathbf{W}}_{\Gamma_j} \right] \\ &\quad + (\varepsilon \boldsymbol{\xi}, \nabla q) - i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\mathbf{W}}_{\Gamma_j}. \end{aligned} \quad (4.7)$$

For any $\boldsymbol{\psi}_h \in V_h$, $\boldsymbol{\psi} \in H_{\text{qper}}(\text{curl}, \Omega)$, $q_h \in U_h \cap H_0^1(\Omega)$, there hold

$$\begin{aligned} &a(\boldsymbol{\xi}, \boldsymbol{\psi}) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \\ &= \langle \mathbf{f}, \boldsymbol{\psi} - \boldsymbol{\psi}_h \rangle_{\Gamma_1} - a_N(\mathbf{E}_h^N, \boldsymbol{\psi} - \boldsymbol{\psi}_h) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \mathbf{E}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \\ &\quad - 2i\omega \int_{\Gamma_1} (\mathcal{T}_1 - \mathcal{T}_1^{N_1}) \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot (\bar{\boldsymbol{\psi}}_h)_{\Gamma_1}, \end{aligned} \quad (4.8)$$

$$(\varepsilon \xi, \nabla q) = -(\varepsilon E_h^N, \nabla(q - q_h)). \quad (4.9)$$

Proof. The inequality (4.6) follows from the definition of the sesquilinear form a in (2.7). The identity (4.7) follows by taking $\mathbf{v} = \xi$ in (4.3) and using (4.1). It remains to prove (4.8) and (4.9). Using (2.6) and (3.5), we obtain

$$\begin{aligned} a(\xi, \psi) &= a(E, \psi - \psi_h) - a(E_h^N, \psi - \psi_h) + a(E - E_h^N, \psi_h) \\ &= \langle f, \psi - \psi_h \rangle_{\Gamma_1} - a_N(E_h^N, \psi - \psi_h) \\ &\quad + a_N(E_h^N, \psi - \psi_h) - a(E_h^N, \psi - \psi_h) + \langle f, \psi_h \rangle_{\Gamma_1} - a(E_h^N, \psi_h) \\ &= \langle f, \psi - \psi_h \rangle_{\Gamma_1} - a_N(E_h^N, \psi - \psi_h) \\ &\quad + a_N(E_h^N, \psi) - a(E_h^N, \psi) + \langle f - f^{N_1}, \psi_h \rangle_{\Gamma_1} \\ &= \langle f, \psi - \psi_h \rangle_{\Gamma_1} - a_N(E_h^N, \psi - \psi_h) \\ &\quad - \sum_{j=1}^2 i\omega \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \xi_{\Gamma_j} \cdot \bar{\psi}_{\Gamma_j} + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) E_{\Gamma_j} \cdot \bar{\psi}_{\Gamma_j} \\ &\quad - 2i\omega \int_{\Gamma_1} (\mathcal{T}_1 - \mathcal{T}_1^{N_1}) E_{\Gamma_1}^{\text{inc}} \cdot (\bar{\psi}_h)_{\Gamma_1}, \end{aligned}$$

which implies (4.8). By taking $\psi = \psi_h = \nabla q_h, \forall q_h \in U_h \cap H_0^1(\Omega)$ in the above identity and using (2.7), we conclude that

$$(\varepsilon \xi, \nabla q_h) = 0.$$

Then (4.9) follows by noting that $\text{div}(\varepsilon E) = 0$. This completes the proof of the lemma. \square

4.3 Several trace results

The following lemmas are trace regularity results for $H_{\text{qper}}(\text{curl}, \Omega)$. The proof can be found in [Bao et al. \(2010\)](#) and [Li et al. \(2011\)](#), respectively.

LEMMA 4.2 Let $\gamma_0 = \max\{\sqrt{1 + (b_1 - b_2)^{-1}}, \sqrt{2}\}$. Then the following estimate holds:

$$\|\psi_{\Gamma_j}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j)} \leq \gamma_0 \|\psi\|_{H(\text{curl}, \Omega)} \quad \forall \psi \in H_{\text{qper}}(\text{curl}, \Omega).$$

LEMMA 4.3 For any $\delta > 0$, there exists a constant C depending only on δ, b_1 and b_2 such that the following estimate holds:

$$\|\psi_{\Gamma_j}\|_{H_{\text{qper}}^{-1/2}(\Gamma_j)^3}^2 \leq \delta \|\nabla \times \psi\|_{L^2(\Omega)^3}^2 + C(\delta) \|\psi\|_{L^2(\Omega)^3}^2 \quad \forall \psi \in H_{\text{qper}}(\text{curl}, \Omega).$$

The following lemma gives an estimate for quasi-periodic divergence-free functions.

LEMMA 4.4 Let $\mathbf{v} = (v_{1n}(x_3), v_{2n}(x_3), v_{3n}(x_3))^T e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)} \in H(\text{curl}, \Omega_j)$. Suppose $\text{div } \mathbf{v} = 0$. Then for any $\delta > 0$, the following estimate holds:

$$\left| \int_{\Gamma_j} v'_{3n} \bar{v}_{3n} \right| \leq |\alpha_n|^2 (1 + \delta) \|\mathbf{v}\|_{L^2(\tilde{\Omega}_j)^3}^2 + C\delta^{-1} d_j^{-2} \|\mathbf{v}\|_{H(\text{curl}, \tilde{\Omega}_j)}^2, \quad j = 1, 2,$$

where $\tilde{\Omega}_j = \Omega'_j \setminus \Omega_j$ and $d_j = |b_j - b'_j|$.

Proof. We only prove the case of $j = 1$ since the proof for $j = 2$ is similar. Clearly, $v'_{3n} = -i\alpha_{1n}v_{1n} - i\alpha_{2n}v_{2n}$ and

$$\begin{aligned} \|\nabla \times \mathbf{v}\|_{L^2(\tilde{\Omega}_1)^3}^2 &= L_1 L_2 \sum_{n \in \mathbb{Z}^2} \left(\|v'_{1n} - i\alpha_{1n}v_{3n}\|_{L^2(B_1)}^2 + \|v'_{2n} - i\alpha_{2n}v_{3n}\|_{L^2(B_1)}^2 \right. \\ &\quad \left. + \|\alpha_{1n}v_{2n} - \alpha_{2n}v_{1n}\|_{L^2(B_1)}^2 \right), \end{aligned}$$

where $B_1 = [b'_1, b_1]$. Let $\chi \in C^2(B_1)$ be a function satisfying

$$\chi(x_3) \begin{cases} = 1, & x_3 \in [b'_1 + \frac{2}{3}d_1, b_1], \\ = 0, & x_3 \in [b'_1, b'_1 + \frac{1}{3}d_1], \\ \in [0, 1], & x_3 \in (b'_1 + \frac{1}{3}d_1, b'_1 + \frac{2}{3}d_1), \end{cases} \quad |\chi'| \lesssim d_1^{-1}, \text{ and } |\chi''| \lesssim d_1^{-2}. \quad (4.10)$$

Letting $\mathbf{w} = \chi \mathbf{v}$, we conclude that

$$\begin{aligned} |v'_{3n}(b_1) \bar{v}_{3n}(b_1)| &= |w'_{3n}(b_1) \bar{w}_{3n}(b_1)| = \left| \int_{b'_1}^{b_1} (w''_{3n} \bar{w}_{3n} + |w'_{3n}|^2) \right| \\ &= \left| \int_{b'_1}^{b_1} \left(\chi^2 (i\alpha_{1n}(i\alpha_{1n}v_{3n} - v'_{1n}) + i\alpha_{2n}(i\alpha_{2n}v_{3n} - v'_{2n})) \bar{v}_{3n} + \chi^2 |\alpha_n|^2 |v_{3n}|^2 \right. \right. \\ &\quad \left. \left. + \chi^2 |v'_{3n}|^2 + \chi' \chi (3v'_{3n} \bar{v}_{3n} + v_{3n} \bar{v}'_{3n}) + (\chi'' \chi + |\chi'|^2) |v_{3n}|^2 \right) \right| \\ &\leq (1 + \delta) (|\alpha_n|^2 \|v_{3n}\|_{L^2(B_1)}^2 + \|v'_{3n}\|_{L^2(B_1)}^2) \\ &\quad + C\delta^{-1} (\|i\alpha_{1n}v_{3n} - v'_{1n}\|_{L^2(B_1)}^2 + \|i\alpha_{2n}v_{3n} - v'_{2n}\|_{L^2(B_1)}^2 + d_1^{-2} \|v_{3n}\|_{L^2(B_1)}^2). \end{aligned}$$

Using the above inequality and $\|v'_{3n}\|_{L^2(B_1)}^2 \leq |\alpha_n|^2 (\|v_{1n}\|_{L^2(B_1)}^2 + \|v_{2n}\|_{L^2(B_1)}^2)$ gives

$$\begin{aligned} \left| \int_{\Gamma_1} v'_{3n} \bar{v}_{3n} \right| &= L_1 L_2 |v'_{3n}(b_1) \bar{v}_{3n}(b_1)| \\ &\leq |\alpha_n|^2 (1 + \delta) \|\mathbf{v}\|_{L^2(\tilde{\Omega}_1)^3}^2 + C\delta^{-1} d_1^{-2} \|\mathbf{v}\|_{H(\text{curl}, \tilde{\Omega}_1)}^2, \end{aligned}$$

which completes the proof. \square

4.4 Estimates of (4.8) and (4.9)

We first discuss the exponentially decaying property of the evanescent modes.

Let $\mathbf{E} = (E_1, E_2, E_3)^\top$ be the solution to the variational problem (2.6). Since $E_l(\mathbf{x})$ is a quasi-periodic function with respect to x_1 and x_2 , it has the following Fourier expansion:

$$E_l(\mathbf{x}) = \sum_{n \in \mathbb{Z}^2} E_{ln}(x_3) e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}, \quad l = 1, 2, 3. \quad (4.11)$$

The following lemma is crucial to derive the truncation error.

LEMMA 4.5 Let $\mathbf{E} = (E_1, E_2, E_3)^\top$ be the solution to (2.6) and E_{ln} are the Fourier coefficients given in (4.11). If $\text{Re}\kappa_j^2 \leq |\alpha_n|^2$, then the following estimates hold:

$$\begin{aligned} |E_{ln}(b_j)| &\leq |E_{ln}(b'_j)| e^{-d_j(|\alpha_n|^2 - \text{Re}\kappa_j^2)^{1/2}}, \quad l = 1, 2, \\ |E_{3n}(b_j)| &\leq \frac{1}{|\beta_{jn}|} |\alpha_{1n}E_{1n}(b'_j) + \alpha_{2n}E_{2n}(b'_j)| e^{-d_j(|\alpha_n|^2 - \text{Re}\kappa_j^2)^{1/2}}, \\ |\alpha_{1n}E_{2n}(b_j) - \alpha_{2n}E_{1n}(b_j)| &\leq |\alpha_{1n}E_{2n}(b'_j) - \alpha_{2n}E_{1n}(b'_j)| e^{-d_j(|\alpha_n|^2 - \text{Re}\kappa_j^2)^{1/2}}. \end{aligned}$$

Proof. Since μ and ε are constants in Ω'_1 and Ω'_2 , the Maxwell equation (2.5) reduces to the Helmholtz equations:

$$\Delta E_l + \kappa_j^2 E_l = 0 \quad \text{in } \Omega'_j, \quad l = 1, 2, 3. \quad (4.12)$$

Plugging (4.11) into (4.12), we derive the second-order ordinary differential equation for the Fourier coefficients E_{ln} :

$$E_{ln}''(x_3) + (\kappa_j^2 - |\alpha_n|^2)E_{ln}(x_3) = 0, \quad x_3 \notin (b'_2, b'_1). \quad (4.13)$$

The general solution of (4.13) is

$$E_{ln}(x_3) = A_{ln} e^{i\beta_{jn}x_3} + B_{ln} e^{-i\beta_{jn}x_3}.$$

Noting (2.4) and using the radiation condition, we obtain

$$E_{ln}(x_3) = \begin{cases} E_{ln}(b'_1) e^{i\beta_{1n}(x_3 - b'_1)}, & x_3 > b'_1, \\ E_{ln}(b'_2) e^{-i\beta_{2n}(x_3 - b'_2)}, & x_3 < b'_2, \end{cases} \quad (4.14)$$

which gives that

$$\begin{aligned} |E_{ln}(b_j)| &= |E_{ln}(b'_j)| e^{-d_j \text{Im}\beta_{jn}}, \quad l = 1, 2, \\ |\alpha_{1n}E_{2n}(b_j) - \alpha_{2n}E_{1n}(b_j)| &= |\alpha_{1n}E_{2n}(b'_j) - \alpha_{2n}E_{1n}(b'_j)| e^{-d_j \text{Im}\beta_{jn}}. \end{aligned}$$

On the other hand, it follows from the divergence free condition that

$$\partial_{x_1} E_1 + \partial_{x_2} E_2 + \partial_{x_3} E_3 = 0 \quad \text{in } \Omega'_j,$$

which yields

$$E'_{3n}(b'_j) + i\alpha_{1n}E_{1n}(b'_j) + i\alpha_{2n}E_{2n}(b'_j) = 0. \quad (4.15)$$

It follows from (4.14) that

$$E'_{3n}(x_3) = i\beta_{1n}E_{3n}(b'_1)e^{i\beta_{1n}(x_3-b'_1)}, \quad x_3 > b'_1.$$

Evaluating the above equation at $x_3 = b'_1$ and using the divergence free condition (4.15), we have

$$E_{3n}(b'_1) = -\frac{\alpha_{1n}}{\beta_{1n}}E_{1n}(b'_1) - \frac{\alpha_{2n}}{\beta_{1n}}E_{2n}(b'_1),$$

which implies

$$E_{3n}(x_3) = \frac{-1}{\beta_{1n}}(\alpha_{1n}E_{1n}(b'_1) + \alpha_{2n}E_{2n}(b'_1))e^{i\beta_{1n}(x_3-b'_1)}.$$

Taking $x_3 = b_1$ in the above equation yields

$$|E_{3n}(b_1)| = \frac{1}{|\beta_{1n}|} |\alpha_{1n}E_{1n}(b'_1) + \alpha_{2n}E_{2n}(b'_1)| e^{-d_1 \text{Im}\beta_{1n}}.$$

Similarly, we can obtain

$$|E_{3n}(b_2)| = \frac{1}{|\beta_{2n}|} |\alpha_{1n}E_{1n}(b'_2) + \alpha_{2n}E_{2n}(b'_2)| e^{-d_2 \text{Im}\beta_{2n}}.$$

Using (2.4) again, we have

$$\text{Im}\beta_{jn}^2 = \text{Im}(\kappa_j^2 - |\alpha_n|^2) = \text{Im}\kappa_j^2 = \omega^2\mu_j\text{Im}\varepsilon_j \geq 0$$

and

$$\begin{aligned} \text{Im}\beta_{jn} &= \frac{1}{\sqrt{2}} \left[\left((\text{Im}\beta_{jn}^2)^2 + (\text{Re}\beta_{jn}^2)^2 \right)^{1/2} - \text{Re}\beta_{jn}^2 \right]^{1/2} \\ &\geq (-\text{Re}\beta_{jn}^2)^{1/2} = (\alpha_n^2 - \text{Re}\kappa_j^2)^{1/2}, \end{aligned}$$

which completes the proof. \square

Noting that Ω is a cuboid, we have the following Hodge decomposition: for any $\boldsymbol{\psi} \in H_{\text{qper}}(\text{curl}, \Omega)$, there exist $\boldsymbol{\psi}^{(1)} \in H_{\text{qper}}^1(\Omega)^3$ and $\psi^{(2)} \in H_{\text{qper}}^1(\Omega)$ such that

$$\boldsymbol{\psi} = \boldsymbol{\psi}^{(1)} + \nabla \psi^{(2)}, \quad \nabla \cdot \boldsymbol{\psi}^{(1)} = 0.$$

In fact, $\psi^{(2)}$ can be obtained in the quotient space $H_{\text{qper}}^1(\Omega)/\{\text{constant}\}$ by solving $\nabla \cdot \boldsymbol{\psi} = \nabla \cdot \nabla \psi^{(2)}$ with the periodic boundary condition on $\partial\Omega \setminus \{\Gamma_1, \Gamma_2\}$ and the Neumann boundary condition on Γ_1 and Γ_2 . Then one has $\boldsymbol{\psi}^{(1)} = \boldsymbol{\psi} - \nabla \psi^{(2)}$. We refer to Monk (2003) for details on the general Hodge decomposition.

Let $P_h : H_{\text{qper}}^1(\Omega) \rightarrow U_h$ and $\mathbf{P}_h : H_{\text{qper}}^1(\Omega)^3 \rightarrow U_h^3$ be the scalar and vector Scott–Zhang interpolation operators, respectively. For any element $T \in \mathcal{M}_h$ with the size of h_T and any face $F \in \mathcal{F}_h$ with the size of h_F , one has (see Scott & Zhang, 1990)

$$\begin{aligned} \|\mathbf{P}_h \boldsymbol{\psi}^{(1)}\|_{L^2(T)^3} &\leq C(\|\boldsymbol{\psi}^{(1)}\|_{L^2(\tilde{T})^3} + h_T |\boldsymbol{\psi}^{(1)}|_{H^1(\tilde{T})^3}), \\ \|\boldsymbol{\psi}^{(1)} - \mathbf{P}_h \boldsymbol{\psi}^{(1)}\|_{L^2(T)^3} &\leq Ch_T \|\boldsymbol{\psi}^{(1)}\|_{H^1(\tilde{T})^3}, \\ \|\boldsymbol{\psi}^{(1)} - \mathbf{P}_h \boldsymbol{\psi}^{(1)}\|_{L^2(F)^3} &\leq Ch_F^{1/2} \|\boldsymbol{\psi}^{(1)}\|_{H^1(\tilde{F})^3}. \end{aligned}$$

Here \tilde{T} and \tilde{F} are the union of all the elements in \mathcal{M}_h , which have nonempty intersection with the element T and the face F , respectively.

Define $\boldsymbol{\psi}_h^{(1)} = \mathbf{P}_h \boldsymbol{\psi}^{(1)}$, $\psi_h^{(2)} = P_h \psi^{(2)}$, $\boldsymbol{\psi}_h = \boldsymbol{\psi}_h^{(1)} + \nabla \psi_h^{(2)}$. Then we have

$$\|\boldsymbol{\psi}_h\|_{H(\text{curl}, \Omega)} \lesssim \|\boldsymbol{\psi}^{(1)}\|_{H^1(\Omega)} + \|\psi^{(2)}\|_{H^1(\Omega)} \lesssim \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)}. \quad (4.16)$$

LEMMA 4.6 There exist positive integers N_{j1} independent of h and satisfying $\left(\frac{2\pi N_{j1}}{\sqrt{L_1 L_2}}\right)^2 > \text{Re} \kappa_j^2$, $j = 1, 2$ such that for any $N_j \geq N_{j1}$ and $\boldsymbol{\psi} \in H_{\text{qper}}(\text{curl}, \Omega)$ the following estimate holds:

$$\left| a(\boldsymbol{\xi}, \boldsymbol{\psi}) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \right| \leq C_1 (\epsilon_h + \epsilon_N) \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)},$$

where $C_1 > 0$ is a constant independent of h and N_{j1} . Moreover,

$$|(\epsilon \boldsymbol{\xi}, \nabla q)| \lesssim \epsilon_h \|\nabla q\|_{L^2(\Omega)^3}.$$

Proof. The second estimate is a direct consequence of (4.9) with $q_h = P_h q$. It remains to prove the first estimate. A simple calculation yields that

$$a(\boldsymbol{\xi}, \boldsymbol{\psi}) + i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} := J_1 + J_2 + J_3,$$

where

$$\begin{aligned}
 J_1 &= \langle \mathbf{f}, \boldsymbol{\psi} - \boldsymbol{\psi}_h \rangle_{\Gamma_1} - a_N(\mathbf{E}_h^N, \boldsymbol{\psi} - \boldsymbol{\psi}_h) \\
 &= - \int_{\Omega} \mu^{-1} (\nabla \times \mathbf{E}_h^N) \cdot \nabla \times (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h) + \omega^2 \int_{\Omega} \varepsilon \mathbf{E}_h^N \cdot (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h) \\
 &\quad + i\omega \sum_{j=1}^2 \int_{\Gamma_j} \mathcal{T}_j^{N_j}(\mathbf{E}_h^N)_{\Gamma_j} \cdot (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h)_{\Gamma_j} + \langle \mathbf{f}, \boldsymbol{\psi} - \boldsymbol{\psi}_h \rangle_{\Gamma_1} \\
 &= J_1^1 + J_1^2 + J_1^3 + J_1^4,
 \end{aligned}$$

and

$$J_2 = i\omega \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \mathbf{E}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j}, \quad J_3 = -2i\omega \int_{\Gamma_1} (\mathcal{T}_1 - \mathcal{T}_1^{N_1}) \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot (\bar{\boldsymbol{\psi}}_h)_{\Gamma_1}.$$

Using the fact $\nabla \times \nabla(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) = 0$ and Green's theorem yields

$$\begin{aligned}
 J_1^1 &= - \int_{\Omega} \mu^{-1} (\nabla \times \mathbf{E}_h^N) \cdot \nabla \times (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h) \\
 &= - \sum_{T \in \mathcal{M}_h} \int_T \mu^{-1} (\nabla \times \mathbf{E}_h^N) \cdot \nabla \times (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) \\
 &= - \sum_{T \in \mathcal{M}_h} \left[\int_T \nabla \times (\mu^{-1} \nabla \times \mathbf{E}_h^N) \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) \right. \\
 &\quad \left. + \int_{\partial T} (\mu^{-1} \nabla \times \mathbf{E}_h^N) \times \mathbf{v} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) \right]
 \end{aligned}$$

and

$$\begin{aligned}
 J_1^2 &= \omega^2 \int_{\Omega} \varepsilon \mathbf{E}_h^N \cdot (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h) = \sum_{T \in \mathcal{M}_h} \omega^2 \int_T \varepsilon \mathbf{E}_h^N \cdot (\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h) \\
 &= \sum_{T \in \mathcal{M}_h} \left[\omega^2 \int_T \varepsilon \mathbf{E}_h^N \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) - \omega^2 \int_T \nabla \cdot (\varepsilon \mathbf{E}_h^N) (\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \right. \\
 &\quad \left. + \omega^2 \int_{\partial T} (\varepsilon \mathbf{E}_h^N \cdot \mathbf{v}) (\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \right].
 \end{aligned}$$

Since ε, μ are bi-periodic functions and $\mathbf{E}_h^N, \bar{\boldsymbol{\psi}}^{(1)} - \boldsymbol{\psi}_h^{(1)}, \bar{\boldsymbol{\psi}}^{(2)} - \boldsymbol{\psi}_h^{(2)}$ are quasi-periodic functions, it is easy to verify that

$$\sum_{j=1}^2 \sum_{T \in \mathcal{M}_h} \left[\int_{\partial T \cap \Gamma_{j0}} (\varepsilon \mathbf{E}_h^N \cdot \boldsymbol{\nu})(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) + \int_{\partial T' \cap \Gamma_{j1}} (\varepsilon \mathbf{E}_h^N \cdot \boldsymbol{\nu})(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \right] = 0,$$

where T' is the tetrahedron having one of its faces on Γ_{j1} corresponding to T . Again using Green's formula, we have

$$\begin{aligned} J_1^3 &= i\omega \sum_{j=1}^2 \int_{\Gamma_j} \mathcal{T}_j^{Nj}(\mathbf{E}_h^N)_{\Gamma_j} \cdot \left[(\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_j} + \nabla_{\Gamma_j}(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \right] \\ &= \sum_{T \in \mathcal{M}_h} \sum_{j=1}^2 \sum_{F \subset \partial T \cap \Gamma_j} i\omega \int_F (\mathcal{T}_j^{Nj}(\mathbf{E}_h^N)_{\Gamma_j}) \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_j} \\ &\quad - \sum_{T \in \mathcal{M}_h} \sum_{j=1}^2 \sum_{F \subset \partial T \cap \Gamma_j} i\omega \int_F \operatorname{div}_{\Gamma_j}(\mathcal{T}_j^{Nj}(\mathbf{E}_h^N)_{\Gamma_j})(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \end{aligned}$$

and

$$\begin{aligned} J_1^4 &= \langle \mathbf{f}, \boldsymbol{\psi} - \boldsymbol{\psi}_h \rangle_{\Gamma_1} = -2i\omega \int_{\Gamma_1} \mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot \left[(\bar{\boldsymbol{\psi}} - \bar{\boldsymbol{\psi}}_h)_{\Gamma_1} + \nabla_{\Gamma_1}(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \right] \\ &= -2i\omega \int_{\Gamma_1} \mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_1} + 2i\omega \int_{\Gamma_1} \operatorname{div}_{\Gamma_1}(\mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}})(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}) \\ &= \sum_{T \in \mathcal{M}_h} \sum_{F \subset \partial T \cap \Gamma_1} -2i\omega \int_F \mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_1} \\ &\quad + \sum_{T \in \mathcal{M}_h} \sum_{F \subset \partial T \cap \Gamma_1} 2i\omega \int_F \operatorname{div}_{\Gamma_1}(\mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}})(\bar{\boldsymbol{\psi}}^{(2)} - \bar{\boldsymbol{\psi}}_h^{(2)}). \end{aligned}$$

Let $\mathring{\mathcal{F}}_h := \{F \in \mathcal{F}_h : F \cap (\Gamma_1 \cup \Gamma_2) = \emptyset\}$. Using the above identities and the residuals, we have

$$\begin{aligned}
 J_1 &= \sum_{T \in \mathcal{M}_h} \left\{ \int_T \mathbf{R}_T^{(1)} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) + \int_T \mathbf{R}_T^{(2)} (\bar{\psi}^{(2)} - \bar{\psi}_h^{(2)}) \right. \\
 &\quad + \sum_{F \in \mathring{\mathcal{F}}_h: F \subset \partial T} \left[\int_F \frac{1}{2} \mathbf{J}_F^{(1)} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) + \int_F \frac{1}{2} \mathbf{J}_F^{(2)} (\bar{\psi}^{(2)} - \bar{\psi}_h^{(2)}) \right] \\
 &\quad \left. + \sum_{j=1}^2 \sum_{F \subset \partial T \cap \Gamma_j} \left[\int_F \frac{1}{2} \mathbf{J}_F^{(1)} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_j} + \int_F \frac{1}{2} \mathbf{J}_F^{(2)} (\bar{\psi}^{(2)} - \bar{\psi}_h^{(2)}) \right] \right\} \\
 &= \sum_{T \in \mathcal{M}_h} \left\{ \int_T \mathbf{R}_T^{(1)} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)}) + \int_T \mathbf{R}_T^{(2)} (\bar{\psi}^{(2)} - \bar{\psi}_h^{(2)}) \right. \\
 &\quad \left. + \sum_{F \subset \partial T} \left[\int_F \frac{1}{2} \mathbf{J}_F^{(1)} \cdot (\bar{\boldsymbol{\psi}}^{(1)} - \bar{\boldsymbol{\psi}}_h^{(1)})_{\Gamma_j} + \int_F \frac{1}{2} \mathbf{J}_F^{(2)} (\bar{\psi}^{(2)} - \bar{\psi}_h^{(2)}) \right] \right\}.
 \end{aligned}$$

Recalling $\boldsymbol{\psi}_h^{(1)} = \mathbf{P}_h \boldsymbol{\psi}^{(1)}$ and $\psi_h^{(2)} = P_h \psi^{(2)}$, we obtain

$$\begin{aligned}
 |J_1| &\leq C \sum_{T \in \mathcal{M}_h} \left\{ \left[h_T \|\mathbf{R}_T^{(1)}\|_{L^2(T)^3} |\boldsymbol{\psi}^{(1)}|_{H^1(\tilde{T})^3} + h_T \|\mathbf{R}_T^{(2)}\|_{L^2(T)} |\psi^{(2)}|_{H^1(\tilde{T})} \right] \right. \\
 &\quad \left. + \sum_{F \in \partial T} \left[h_F^{1/2} \|\mathbf{J}_F^{(1)}\|_{L^2(F)^3} |\boldsymbol{\psi}^{(1)}|_{H^1(\tilde{F})^3} + h_F^{1/2} \|\mathbf{J}_F^{(2)}\|_{L^2(F)} |\psi^{(2)}|_{H^1(\tilde{F})} \right] \right\} \\
 &\leq C \epsilon_h \left(|\psi^{(1)}|_{H^1(\Omega)^3}^2 + |\psi^{(2)}|_{H^1(\Omega)}^2 \right)^{1/2} \leq C \epsilon_h \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)}. \tag{4.17}
 \end{aligned}$$

For J_2 , a straightforward calculation yields

$$\begin{aligned}
 |J_2| &= \omega \left| \sum_{j=1}^2 \int_{\Gamma_j} (\mathcal{J}_j - \mathcal{J}_j^{N_j}) \mathbf{E}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \right| = \omega L_1 L_2 \left| \sum_{j=1}^2 \sum_{n \notin U_{N_j}} (r_{1n}^{(j)} \bar{\psi}_{1n}^{(j)} + r_{2n}^{(j)} \bar{\psi}_{2n}^{(j)}) \right| \\
 &= L_1 L_2 \left| \sum_{j=1}^2 \sum_{n \notin U_{N_j}} \frac{1}{\mu_j \beta_{jn}} \left[\omega^2 \varepsilon_j \mu_j (E_{1n}(b_j) \bar{\psi}_{1n}^{(j)} + E_{2n}(b_j) \bar{\psi}_{2n}^{(j)}) \right. \right. \\
 &\quad \left. \left. - (\alpha_{1n} E_{2n}(b_j) - \alpha_{2n} E_{1n}(b_j)) (\alpha_{1n} \bar{\psi}_{2n}^{(j)} - \alpha_{2n} \bar{\psi}_{1n}^{(j)}) \right] \right|.
 \end{aligned}$$

Let N_{j1} be a sufficiently large integer such that

$$\left(\frac{2\pi N_{j1}}{\sqrt{L_1 L_2}}\right)^2 > \operatorname{Re} \kappa_j^2, \quad |\mu_j \beta_{jn}| \gtrsim (|\alpha_n|^2 + 1)^{1/2}, \quad \forall n \geq N_{j1}.$$

Suppose $N_j \geq N_{j1}$. It follows from Lemma 4.5 that

$$\begin{aligned} |J_2| &\leq L_1 L_2 \sum_{j=1}^2 \sum_{n \notin U_{N_j}} \frac{e^{-d_j(|\alpha_n|^2 - \operatorname{Re} \kappa_j^2)^{1/2}}}{|\mu_j \beta_{jn}|} \left[|\omega^2 \varepsilon_j \mu_j| (|E_{1n}(b'_j)| |\psi_{1n}(b_j)| \right. \\ &\quad \left. + |E_{2n}(b'_j)| |\psi_{2n}(b_j)|) + |\alpha_{1n} E_{2n}(b'_j) - \alpha_{2n} E_{1n}(b'_j)| |\alpha_{1n} \psi_{2n}(b_j) - \alpha_{2n} \psi_{1n}(b_j)| \right] \\ &\lesssim L_1 L_2 \sum_{j=1}^2 e^{-d_j \left(\left(\frac{2\pi N_j}{\sqrt{L_1 L_2}} \right)^2 - \operatorname{Re} \kappa_j^2 \right)^{1/2}} \\ &\quad \times \left\{ \sum_{n \notin U_{N_j}} (|\alpha_n|^2 + 1)^{-\frac{1}{2}} \left[|E_{1n}(b'_j)|^2 + |E_{2n}(b'_j)|^2 + |\alpha_{1n} E_{2n}(b'_j) - \alpha_{2n} E_{1n}(b'_j)|^2 \right] \right\}^{\frac{1}{2}} \\ &\quad \times \left\{ \sum_{n \notin U_{N_j}} (|\alpha_n|^2 + 1)^{-\frac{1}{2}} \left[|\psi_{1n}(b_j)|^2 + |\psi_{2n}(b_j)|^2 + |\alpha_{1n} \psi_{2n}(b_j) - \alpha_{2n} \psi_{1n}(b_j)|^2 \right] \right\}^{\frac{1}{2}} \\ &\lesssim \sum_{j=1}^2 e^{-d_j \left(\left(\frac{2\pi N_j}{\sqrt{L_1 L_2}} \right)^2 - \operatorname{Re} \kappa_j^2 \right)^{1/2}} \|E\|_{TH_{\text{qper}}^{-1/2}(\operatorname{curl}, \Gamma'_j)} \|\psi\|_{TH_{\text{qper}}^{-1/2}(\operatorname{curl}, \Gamma_j)} \\ &\lesssim \sum_{j=1}^2 e^{-d_j \left(\left(\frac{2\pi N_j}{\sqrt{L_1 L_2}} \right)^2 - \operatorname{Re} \kappa_j^2 \right)^{1/2}} \|E\|_{H(\operatorname{curl}, \Omega)} \|\psi\|_{H(\operatorname{curl}, \Omega)}. \end{aligned}$$

In the last inequality, we have used the trace estimate (4.2) in $\Omega \setminus \Omega'_j$ and Ω to get

$$\|E\|_{TH_{\text{qper}}^{-1/2}(\operatorname{curl}, \Gamma'_j)} \leq \gamma'_j \|E\|_{H(\operatorname{curl}, \Omega \setminus \Omega'_j)} \lesssim \|E\|_{H(\operatorname{curl}, \Omega)}$$

and

$$\|\psi\|_{TH_{\text{qper}}^{-1/2}(\operatorname{curl}, \Gamma'_j)} \lesssim \|\psi\|_{H(\operatorname{curl}, \Omega)},$$

respectively, where $\gamma'_j = \max\{\sqrt{1 + |b'_j - b_{j+1}|^{-1}}, \sqrt{2}\}$ with $b_3 = b_1$. Using the inf-sup condition (2.8) yields

$$\|E\|_{H(\operatorname{curl}, \Omega)} \leq \frac{1}{\gamma_1} \sup_{0 \neq \psi \in H_{\text{qper}}(\operatorname{curl}, \Omega)} \frac{|a(E, \psi)|}{\|\psi\|_{H(\operatorname{curl}, \Omega)}}.$$

It follows from (2.6) and (4.2) that

$$\begin{aligned} |a(\mathbf{E}, \boldsymbol{\psi})| &= |2\omega \int_{\Gamma_1} \mathcal{T}_1 \mathbf{E}_{\Gamma_1}^{\text{inc}} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_1}| \\ &\leq C \|\mathbf{E}^{\text{inc}}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)} \|\boldsymbol{\psi}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)} \\ &\lesssim \|\mathbf{E}^{\text{inc}}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)} \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)}. \end{aligned}$$

Combining the above estimates and using Lemma 4.2 give

$$|J_2| \lesssim \sum_{j=1}^2 e^{-d_j \left(\left(\frac{2\pi N_j}{\sqrt{L_1 L_2}} \right)^2 - \text{Re} \kappa_j^2 \right)^{1/2}} \|\mathbf{E}^{\text{inc}}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)} \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)}. \quad (4.18)$$

Similar to the estimate of J_2 , one can get from Lemma 4.2 and (4.16) that

$$|J_3| \lesssim e^{-d_1 \left(\left(\frac{2\pi N_1}{\sqrt{L_1 L_2}} \right)^2 - \text{Re} \kappa_1^2 \right)^{1/2}} \|\mathbf{E}^{\text{inc}}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_1)} \|\boldsymbol{\psi}\|_{H(\text{curl}, \Omega)},$$

which, together with (4.17) and (4.18), completes the proof. \square

4.5 Estimates of the DtN operator

The following lemma gives an estimate of the second term in the right-hand side of (4.6).

LEMMA 4.7 There exists a positive constant C such that

$$\text{Im} \int_{\Gamma_j} \mathcal{T}_j^{N_j} \boldsymbol{\psi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \geq -C \|\boldsymbol{\psi}\|_{H_{\text{qper}}^{-1/2}(\Gamma_j)^3}^2, \quad \forall \boldsymbol{\psi} \in TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma_j) \subset H_{\text{qper}}^{-1/2}(\Gamma_j)^3.$$

Proof. Define

$$\kappa_j^2 = \omega^2 \varepsilon_j \mu_j = u_j + iv_j,$$

It follows from $\mu_j > 0$, $\text{Re}(\varepsilon_j) > 0$ and $\text{Im}(\varepsilon_j) \geq 0$ that $u_j > 0$ and $v_j \geq 0$. Recall

$$\beta_{jn}^2 = \kappa_j^2 - |\alpha_n|^2 = w_{jn} + iv_j.$$

where

$$w_{jn} = \text{Re}(\omega^2 \varepsilon_j \mu_j) - |\alpha_n|^2 = u_j - |\alpha_n|^2.$$

It is clear to note that $u_j \geq w_{jn}$. Noting that $\mu_j > 0$, $\text{Re}(\varepsilon_j) > 0$ and $\text{Im}(\varepsilon_j) \geq 0$, we get

$$\beta_{jn} = \gamma_{jn} + i\lambda_{jn},$$

where

$$\begin{aligned}\gamma_{jn} &= \operatorname{Re}(\beta_{jn}) = \frac{1}{\sqrt{2}} \left(\sqrt{w_{jn}^2 + v_j^2} + w_{jn} \right)^{1/2}, \\ \lambda_{jn} &= \operatorname{Im}(\beta_{jn}) = \frac{1}{\sqrt{2}} \left(\sqrt{w_{jn}^2 + v_j^2} - w_{jn} \right)^{1/2}.\end{aligned}$$

As a quasi-periodic function, ψ_{Γ_j} has the expansion

$$\psi_{\Gamma_j}(x_1, x_2, b_j) = \sum_{n \in \mathbb{Z}^2} (\psi_{1n}(b_j), \psi_{2n}(b_j), 0)^\top e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}.$$

We have from the definition of the capacity operator \mathcal{T}_j that

$$\int_{\Gamma_j} \mathcal{T}_j^{N_j} \psi_{\Gamma_j} \cdot \bar{\psi}_{\Gamma_j} = \frac{L_1 L_2}{\omega \mu_j} \sum_{n \in U_{N_j}} \left[\frac{\kappa_j^2}{\beta_{jn}} (|\psi_{1n}|^2 + |\psi_{2n}|^2) - \frac{1}{\beta_{jn}} |\alpha_{1n} \psi_{2n} - \alpha_{2n} \psi_{1n}|^2 \right].$$

Taking the imaginary part gives

$$\begin{aligned}\operatorname{Im}(\mathcal{T}_j^{N_j} \psi, \psi)_{\Gamma_j} &= \frac{L_1 L_2}{\omega \mu_j} \sum_{n \in U_{N_j}} \left[\frac{\lambda_{jn}}{\gamma_{jn}^2 + \lambda_{jn}^2} |\alpha_{1n} \psi_{2n} - \alpha_{2n} \psi_{1n}|^2 \right. \\ &\quad \left. + \frac{v_j \gamma_{jn} - u_j \lambda_{jn}}{\gamma_{jn}^2 + \lambda_{jn}^2} (|\psi_{1n}|^2 + |\psi_{2n}|^2) \right] \\ &\geq \frac{L_1 L_2}{\omega \mu_j} \sum_{n \in U_{N_j}} \frac{v_j \gamma_{jn} - u_j \lambda_{jn}}{\gamma_{jn}^2 + \lambda_{jn}^2} (|\psi_{1n}|^2 + |\psi_{2n}|^2).\end{aligned}$$

To prove the lemma, it is required to estimate

$$\begin{aligned}& \frac{1}{\omega \mu_j} \left| \frac{v_j \gamma_{jn} - u_j \lambda_{jn}}{\gamma_{jn}^2 + \lambda_{jn}^2} (1 + |\alpha_n|^2)^{1/2} \right| \\ &= \frac{1}{\omega \mu_j} \left[\frac{1 + u_j - w_{jn}}{w_{jn}^2 + v_j^2} \left(v_j^2 \frac{\sqrt{w_{jn}^2 + v_j^2} + w_{jn}}{2} + u_j^2 \frac{\sqrt{w_{jn}^2 + v_j^2} - w_{jn}}{2} - u_j v_j^2 \right) \right]^{1/2}.\end{aligned}$$

Let

$$G_j(t) = \frac{1 + u_j - t}{t^2 + v_j^2} \left(v_j^2 \frac{\sqrt{t^2 + v_j^2} + t}{2} + u_j^2 \frac{\sqrt{t^2 + v_j^2} - t}{2} - u_j v_j^2 \right).$$

Since the assumption $\kappa_j^2 \neq |\alpha_n|$ for $n \in \mathbb{Z}^2$ and $j = 1, 2$, implies that $v_j \neq 0$ or $v_j = 0$, but $w_{jn} \neq 0$, it can be seen that $G_j(t)$ is a continuous and positive function for $t \leq u_j$ and $G_j(t) \rightarrow u_j^2$ as $t \rightarrow -\infty$. Thus, the function $G_j(t)$ reaches its maximum at some t^* . Therefore, we have

$$\frac{1}{\omega\mu_j} \left| \frac{v_j \gamma_{jn} - u_j \lambda_{jn}}{\gamma_{jn}^2 + \lambda_{jn}^2} (1 + \alpha_n^2)^{1/2} \right| \leq \frac{\sqrt{G_j(t^*)}}{\omega\mu_j} := C.$$

A simple calculation yields that

$$\begin{aligned} & \operatorname{Im} \int_{\Gamma_j} \mathcal{T}_j^{N_j} \boldsymbol{\psi}_{\Gamma_j} \cdot \bar{\boldsymbol{\psi}}_{\Gamma_j} \\ & \geq -CL_1 L_2 \sum_{n \in U_{N_j}} (1 + |\alpha_n|^2)^{-1/2} (|\psi_{1n}|^2 + |\psi_{2n}|^2) \\ & \geq -CL_1 L_2 \sum_{n \in \mathbb{Z}^2} (1 + |\alpha_n|^2)^{-1/2} (|\psi_{1n}|^2 + |\psi_{2n}|^2) \\ & = -C \|\boldsymbol{\psi}\|_{H_{\text{qper}}^{-1/2}(\Gamma_j)^3}^2, \end{aligned}$$

which completes the proof. \square

The following lemma gives an estimate of the last term in (4.7).

LEMMA 4.8 Let \mathbf{W} be the solution of the dual problem (4.3). Then there exist integers N_{j2} independent of h and satisfying $(\frac{2\pi N_{j2}}{\sqrt{L_1 L_2}})^2 > \operatorname{Re}(\kappa_j^2)$, $j = 1, 2$ such that for $N_j \geq N_{j2}$, the following estimate holds:

$$\sum_{j=1}^2 \left| \omega \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\mathbf{W}}_{\Gamma_j} \right| \leq \frac{2}{3} |(\varepsilon \boldsymbol{\xi}, \boldsymbol{\xi})| + C \sum_{j=1}^2 N_j^{-2} (1 + d_j^{-4}) \|\boldsymbol{\xi}\|_{H(\operatorname{curl}, \Omega)}^2,$$

where C is a constant independent of h and N_j .

Proof. We only show the details of the proof for $j = 1$ since the proof is similar for $j = 2$. It follows from the definitions of \mathcal{T}_1 and $\mathcal{T}_1^{N_1}$ and (4.1) that

$$\begin{aligned} & \left| \omega \int_{\Gamma_1} (\mathcal{T}_1 - \mathcal{T}_1^{N_1}) \boldsymbol{\xi}_{\Gamma_1} \cdot \bar{\mathbf{W}}_{\Gamma_1} \right| = \left| \frac{\omega}{\varepsilon_1} \int_{\Gamma_1} (\mathcal{T}_1 - \mathcal{T}_1^{N_1}) \boldsymbol{\xi}_{\Gamma_1} \cdot \bar{\mathbf{W}}_{\Gamma_1} \right| \\ & = \frac{L_1 L_2}{\varepsilon_1 \mu_1} \sum_{n \notin U_{N_1}} \left| \frac{1}{\beta_{1n}} \left[\kappa_1^2 (\zeta_{1n}(b_1) \bar{W}_{1n}(b_1) + \zeta_{2n}(b_1) \bar{W}_{2n}(b_1)) - \tau_n(b_1) \bar{V}_n(b_1) \right] \right|, \end{aligned} \quad (4.19)$$

where

$$\tau_n(x_3) = \alpha_{1n} \zeta_{2n}(x_3) - \alpha_{2n} \zeta_{1n}(x_3), \quad (4.20)$$

$$V_n(x_3) = \alpha_{1n} W_{2n}(x_3) - \alpha_{2n} W_{1n}(x_3). \quad (4.21)$$

Let $\tilde{\Omega}_1 = \Omega'_1 \setminus \Omega_1 = \{\mathbf{x} \in \mathbb{R}^3 : 0 < x_1 < L_1, 0 < x_2 < L_2, b'_1 < x_3 < b_1\}$. Next we consider the dual problem in $\tilde{\Omega}_1$ in order to express $W_{1n}(b_1)$ and $W_{2n}(b_1)$ in $\boldsymbol{\zeta}$. Since ε and μ are real constants in $\tilde{\Omega}_1$, the dual problem (4.3) can be rewritten as

$$\nabla \times (\nabla \times \mathbf{W}) - \omega^2 \varepsilon_1 \mu_1 \mathbf{W} = \mu_1 \boldsymbol{\zeta} \quad \text{in } \tilde{\Omega}_1.$$

Using the divergence free condition $\nabla \cdot \mathbf{W} = 0$ in $\tilde{\Omega}_1$, we may reduce the above equation into the Helmholtz equation

$$\Delta \mathbf{W} + \kappa_1^2 \mathbf{W} = -\mu_1 \boldsymbol{\zeta}.$$

Let $\mathbf{W} = (W_1, W_2, W_3)^\top$. Componentwisely, we have

$$\Delta W_j + \kappa_1^2 W_j = -\mu_1 \zeta_j, \quad j = 1, 2, 3.$$

Since W_j and ζ_j are quasi-periodic functions, they have the following Fourier series expansions:

$$W_j = \sum_{n \in \mathbb{Z}^2} W_{jn} e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}, \quad \zeta_j = \sum_{n \in \mathbb{Z}^2} \zeta_{jn} e^{i(\alpha_{1n}x_1 + \alpha_{2n}x_2)}.$$

A direction calculation yields that the Fourier coefficients W_{jn} with $n \notin U_{N_1}$ and $j = 1, 2$ satisfy the following two-point boundary value problem of the ordinary differential equations on the interval (b'_1, b_1) :

$$\begin{cases} W''_{jn}(x_3) - |\beta_{1n}|^2 W_{jn}(x_3) = -\mu_1 \zeta_{jn}(x_3), \\ W_{jn}(b'_1) = W_{jn}(b_1), \\ W'_{jn}(b_1) + |\beta_{1n}| W_{jn}(b_1) = -i\kappa_1^{-2} \mu_1 \alpha_{jn} \zeta_{3n}(b_1). \end{cases} \quad (4.22)$$

Here we have used $W'_{3n} = -i\alpha_{1n} W_{1n} - i\alpha_{2n} W_{2n}$ due to $\nabla \cdot \mathbf{W} = 0$ and $W''_{3n} - |\beta_{1n}|^2 W_{3n} = -\mu_1 \zeta_{3n}$ to derive the boundary conditions; see Appendix A. It is easy to verify that the solutions to (4.22) can be expressed as

$$\begin{aligned} W_{jn}(x_3) = & \frac{\mu_1}{2|\beta_{1n}|} \left(- \int_{b_1}^{x_3} e^{|\beta_{1n}|(x_3-s)} \zeta_{jn}(s) \, ds + \int_{b'_1}^{x_3} e^{|\beta_{1n}|(s-x_3)} \zeta_{jn}(s) \, ds \right. \\ & \left. - \int_{b'_1}^{b_1} e^{|\beta_{1n}|(2b'_1-x_3-s)} \zeta_{jn}(s) \, ds \right) + e^{|\beta_{1n}|(b'_1-x_3)} W_{jn}(b'_1) \\ & - \frac{i\mu_1 \alpha_{jn} \zeta_{3n}(b_1)}{2\kappa_1^2 |\beta_{1n}|} \left(e^{|\beta_{1n}|(x_3-b_1)} - e^{|\beta_{1n}|(2b'_1-b_1-x_3)} \right), \end{aligned}$$

which leads to

$$W_{jn}(b_1) = \omega_{jn}^I + \omega_{jn}^{II},$$

where

$$\omega_{jn}^I = \frac{\mu_1}{2|\beta_{1n}|} \left(\int_{b'_1}^{b_1} e^{|\beta_{1n}|(s-b_1)} \zeta_{jn}(s) \, ds - \int_{b'_1}^{b_1} e^{|\beta_{1n}|(2b'_1-b_1-s)} \zeta_{jn}(s) \, ds \right) \quad (4.23)$$

$$\begin{aligned} &+ e^{-d_1|\beta_{1n}|} W_{jn}(b'_1) \\ \omega_{jn}^{II} &= - \frac{i\mu_1 \alpha_{jn} \zeta_{3n}(b_1)}{2\kappa_1^2 |\beta_{1n}|} (1 - e^{-2d_1|\beta_{1n}|}). \end{aligned} \quad (4.24)$$

Denote $B_1 = [b'_1, b_1]$. Clearly,

$$|\omega_{jn}^I| \leq \frac{\mu_1}{2|\beta_{1n}|^2} \|\zeta_{jn}\|_{L^\infty(B_1)} + e^{-d_1|\beta_{1n}|} |W_{jn}(b'_1)|. \quad (4.25)$$

Next we turn to estimate the terms in (4.19). First, we have from (4.25) that

$$\begin{aligned} |\zeta_{jn}(b_1) \bar{\omega}_{jn}^I| &\lesssim \|\zeta_{jn}\|_{L^\infty(B_1)} \left(|\beta_{1n}|^{-2} \|\zeta_{jn}\|_{L^\infty(B_1)} + e^{-d_1|\beta_{1n}|} |W_{jn}(b'_1)| \right) \\ &\lesssim |\beta_{1n}|^{-2} \|\zeta_{jn}\|_{L^\infty(B_1)}^2 + |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} |W_{jn}(b'_1)|^2. \end{aligned}$$

It is easy to show that (cf. Wang *et al.*, 2015, Lemma 4.5)

$$\|\zeta_{jn}\|_{L^\infty(B_1)}^2 \leq \frac{2}{d_1} \|\zeta_{jn}\|_{L^2(B_1)}^2 + 2 \|\zeta_{jn}\|_{L^2(B_1)} \|\zeta'_{jn}\|_{L^2(B_1)}. \quad (4.26)$$

Therefore,

$$\begin{aligned} |\zeta_{jn}(b_1) \bar{\omega}_{jn}^I| &\lesssim |\beta_{1n}|^{-3} \left(|\beta_{1n}| (|\beta_{1n}| + d_1^{-1}) \|\zeta_{jn}\|_{L^2(B_1)}^2 + \|\zeta'_{jn}\|_{L^2(B_1)}^2 \right) \\ &\quad + |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} |W_{jn}(b'_1)|^2. \end{aligned} \quad (4.27)$$

We may choose N_{12} such that for $N_1 > N_{12}$

$$|\alpha_n| \geq |\beta_{1n}| \geq (1 + \delta)^{-1} |\alpha_n| \gtrsim \max \{\kappa_1, N_1\} \quad \text{for } n \notin U_{N_1}, \quad (4.28)$$

where δ is a positive constant which will be given later. Following from (4.27) to (4.28), (2.2), Lemma 4.2 and (4.5), we conclude that

$$\begin{aligned}
& L_1 L_2 \left| \sum_{n \notin U_{N_1}} \frac{\kappa_1^2}{\varepsilon_1 \mu_1 \beta_{1n}} (\zeta_{1n}(b_1) \bar{\omega}_{1n}^I + \zeta_{2n}(b_1) \bar{\omega}_{2n}^I) \right| \\
& \lesssim \sum_{n \notin U_{N_1}} \sum_{j=1}^2 \left[|\beta_{1n}|^{-4} \left(|\beta_{1n}| (|\beta_{1n}| + d_1^{-1}) \|\zeta_{jn}\|_{L^2(B_1)}^2 + \|\zeta'_{jn}\|_{L^2(B_1)}^2 \right) \right. \\
& \quad \left. + |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} (1 + |\alpha_n|^2)^{-1/2} |W_{jn}(b'_1)|^2 \right] \\
& \lesssim \sum_{n \notin U_{N_1}} \sum_{j=1}^2 \left[|\alpha_n|^{-4} \left(|\alpha_n| (|\alpha_n| + d_1^{-1}) \|\zeta_{jn}\|_{L^2(B_1)}^2 + \|\zeta'_{jn} - i\alpha_{jn}\zeta_{3n}\|_{L^2(B_1)}^2 \right) \right. \\
& \quad \left. + |\alpha_{jn}|^2 \|\zeta_{3n}\|_{L^2(B_1)}^2 \right] + \max_{n \notin U_{N_1}} \left\{ |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} \right\} \|\mathbf{W}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma'_1)}^2 \\
& \lesssim N_1^{-2} \left((1 + (N_1 d_1)^{-1}) \|\zeta\|_{H(\text{curl}, \tilde{\Omega})}^2 + \max_{n \notin U_{N_1}} \left\{ |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} \right\} \|\mathbf{W}\|_{H(\text{curl}, \omega)}^2 \right) \\
& \lesssim N_1^{-2} (1 + d_1^{-4}) \|\zeta\|_{H(\text{curl}, \Omega)}^2, \tag{4.29}
\end{aligned}$$

where we have used $\max_{s \geq 0} (s^4 e^{-2d_1 s}) \lesssim d_1^{-4}$ to derive the last inequality.

By (4.24), $\text{div} \zeta = 0$ and (4.28), we obtain

$$\begin{aligned}
& L_1 L_2 \left| \sum_{n \notin U_{N_1}} \frac{\kappa_1^2}{\varepsilon_1 \mu_1 \beta_{1n}} (\zeta_{1n}(b_1) \bar{\omega}_{1n}^{II} + \zeta_{2n}(b_1) \bar{\omega}_{2n}^{II}) \right| \\
& = L_1 L_2 \left| \sum_{n \notin U_{N_1}} (-i\alpha_{1n}\zeta_{1n}(b_1) - i\alpha_{2n}\zeta_{2n}(b_1)) \bar{\zeta}_{3n}(b_1) \frac{1 - e^{-2d_1|\beta_{1n}|}}{2\varepsilon_1|\beta_{1n}|^2} \right| \\
& = L_1 L_2 \left| \sum_{n \notin U_{N_1}} \zeta'_{3n}(b_1) \bar{\zeta}_{3n}(b_1) \frac{1 - e^{-2d_1|\beta_{1n}|}}{2\varepsilon_1|\beta_{1n}|^2} \right| \\
& = \left| \sum_{n \notin U_{N_1}} \frac{1 - e^{-2d_1|\beta_{1n}|}}{2|\beta_{1n}|^2} \varepsilon_1^{-1} \int_{\Gamma_1} \zeta'_{3n} \bar{\zeta}_{3n} \right| \leq \frac{(1 + \delta)^2}{2} \sum_{n \notin U_{N_1}} |\alpha_n|^{-2} \left| \varepsilon_1^{-1} \int_{\Gamma_1} \zeta'_{3n} \bar{\zeta}_{3n} \right|.
\end{aligned}$$

It follows from (4.20) to (4.22) that

$$\begin{cases} V_n''(x_3) - |\beta_{1n}|^2 V_n(x_3) = -\mu_1 \tau_n(x_3), \\ V_n(b'_1) = V_n(b'_1), \\ V_n'(b_1) + |\beta_{1n}| V_n(b_1) = 0. \end{cases} \tag{4.30}$$

Similarly, we may obtain the solution of (4.30)

$$|V_n(b_1)| \leq \frac{\mu_1}{2|\beta_{1n}|^2} \|\tau_n\|_{L^\infty(B_1)} + e^{-d_1|\beta_{1n}|} |V_n(b'_1)|,$$

which implies by combining with (4.28), (4.26), (2.2), Lemma 4.2 and (4.5) that

$$\begin{aligned} & L_1 L_2 \left| \sum_{n \notin U_{N_1}} \frac{1}{\varepsilon_1 \mu_1 \beta_{1n}} \tau_n(b_1) \cdot \bar{V}_n(b_1) \right| \\ & \lesssim \sum_{n \notin U_{N_1}} \left(|\beta_{1n}|^{-3} \|\tau_n\|_{L^\infty(B_1)}^2 + |\beta_{1n}| e^{-2d_1|\beta_{1n}|} |V_n(b'_1)|^2 \right) \\ & \lesssim \sum_{n \notin U_{N_1}} \left[|\beta_{1n}|^{-4} \left(|\beta_{1n}| (|\beta_{1n}| + d_1^{-1}) \|\tau_n\|_{L^2(B_1)}^2 + \|\tau'_n\|_{L^2(B_1)}^2 \right) \right. \\ & \quad \left. + |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} (1 + |\alpha_n|^2)^{-1/2} |V_n(b'_1)|^2 \right] \\ & \lesssim \sum_{n \notin U_{N_1}} \left[|\alpha_n|^{-4} \left(|\alpha_n| (|\alpha_n| + d_1^{-1}) \|\tau_n\|_{L^2(B_1)}^2 \right. \right. \\ & \quad \left. \left. + \|\alpha_{1n}(\zeta'_{2n} - i\alpha_{2n}\zeta_{3n}) - \alpha_{2n}(\zeta'_{1n} - i\alpha_{1n}\zeta_{3n})\|_{L^2(B_1)}^2 \right) \right] \\ & \quad + \max_{n \notin U_{N_1}} |\beta_{1n}|^2 e^{-2d_1|\beta_{1n}|} \|\mathbf{W}\|_{TH_{\text{qper}}^{-1/2}(\text{curl}, \Gamma'_1)}^2 \\ & \lesssim N_1^{-2} \left((1 + (N_1 d_1)^{-1}) \|\zeta\|_{H(\text{curl}, \tilde{\Omega}_1)}^2 + \max_{n \notin U_{N_1}} |\beta_{1n}|^4 e^{-2d_1|\beta_{1n}|} \|\mathbf{W}\|_{H(\text{curl}, \Omega)}^2 \right) \\ & v \lesssim N_1^{-2} (1 + d_1^{-4}) \|\zeta\|_{H(\text{curl}, \Omega)}^2. \end{aligned} \tag{4.31}$$

Plugging (4.29) and (4.31) into (4.19) and using Lemma 4.4, we get

$$\begin{aligned} & \left| \sum_{j=1}^2 \left(i\omega \int_{\Gamma_j} (\mathcal{T}_j - \mathcal{T}_j^{N_j}) \boldsymbol{\xi}_{\Gamma_j} \cdot \bar{\mathbf{W}}_{\Gamma_j} \right) \right| \\ & \leq \frac{(1+\delta)^3}{2} \sum_{j=1}^2 \left(|\varepsilon_j|^{-1} \|\boldsymbol{\xi}\|_{L^2(\tilde{\Omega}_j)}^2 + C N_j^{-2} (\delta^{-1} d_j^{-2} + 1 + d_j^{-4}) \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}^2 \right) \\ & \leq \frac{(1+\delta)^3}{2} |(\varepsilon \boldsymbol{\xi}, \boldsymbol{\xi})| + C \sum_{j=1}^2 N_j^{-2} (\delta^{-2} + 1 + d_j^{-4}) \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}^2, \end{aligned}$$

where we have used $|(\varepsilon^{-1} \boldsymbol{\zeta}, \boldsymbol{\zeta})| \leq |(\varepsilon \boldsymbol{\xi}, \boldsymbol{\xi})|$ and $\|\boldsymbol{\zeta}\|_{H(\text{curl}, \Omega)} \lesssim \|\boldsymbol{\xi}\|_{H(\text{curl}, \Omega)}$ to derive the last inequality. Then the proof is completed by taking $\delta = \left(\frac{4}{3}\right)^{1/3} - 1$. \square

4.6 Proof of Theorem 3.2

Let $N_j \geq \max(N_{j1}, N_{j2})$, $j = 1, 2$. First, it follows from the error estimate (4.6), Lemmas 4.6, 4.7 and 4.3 that

$$\begin{aligned} \|\xi\|_{H(\text{curl}, \Omega)}^2 &\leq C(\epsilon_h + \epsilon_N) \|\xi\|_{H(\text{curl}, \Omega)} + \delta \|\nabla \times \xi\|_{L^2(\Omega)^3}^2 \\ &\quad + C(\delta) \|\xi\|_{L^2(\Omega)^3}^2 + C \|\xi\|_{L^2(\Omega)^3}^2. \end{aligned}$$

Taking $\delta = 1/2$ and using the Young's inequality in the above estimate yield immediately

$$\|\xi\|_{H(\text{curl}, \Omega)}^2 \lesssim (\epsilon_h + \epsilon_N)^2 + \|\xi\|_{L^2(\Omega)^3}^2. \quad (4.32)$$

Using (4.7), Lemmas 4.6 and 4.8 we obtain

$$\begin{aligned} |(\varepsilon \xi, \xi)| &\leq C(\epsilon_h + \epsilon_N) \|\mathbf{W}\|_{H(\text{curl}, \Omega)} + \epsilon_h \|\nabla q\|_{L^2(\Omega)^3} \\ &\quad + \frac{2}{3} |(\varepsilon \xi, \xi)| + C \sum_{j=1}^2 N_j^{-2} (1 + d_j^{-4}) \|\xi\|_{H(\text{curl}, \Omega)}^2. \end{aligned}$$

It follows from (4.5), (4.2) and the Young's inequality that

$$\|\xi\|_{L^2(\Omega)^3}^2 \lesssim (\epsilon_h + \epsilon_N)^2 + \tilde{\delta} \|\xi\|_{H(\text{curl}, \Omega)}^2 + \sum_{j=1}^2 N_j^{-2} (1 + d_j^{-4}) \|\xi\|_{H(\text{curl}, \Omega)}^2,$$

where $\tilde{\delta}$ is a sufficiently small positive constant. The proof is completed by combining the above estimate and (4.32).

REMARK 4.9 In the proof of Theorem 3.2, the factor $N_j^{-2} d_j^{-4}$ implies that a larger N_j is required for the case of smaller d_j . In fact, the original problem can be re-scaled such that the amplitude of the biperiodic material is of $O(1)$, and then one may choose proper b'_j and b_j to satisfy $d_j \simeq 1$. Thus the truncation parameter N_j does not have to be large in practical computations.

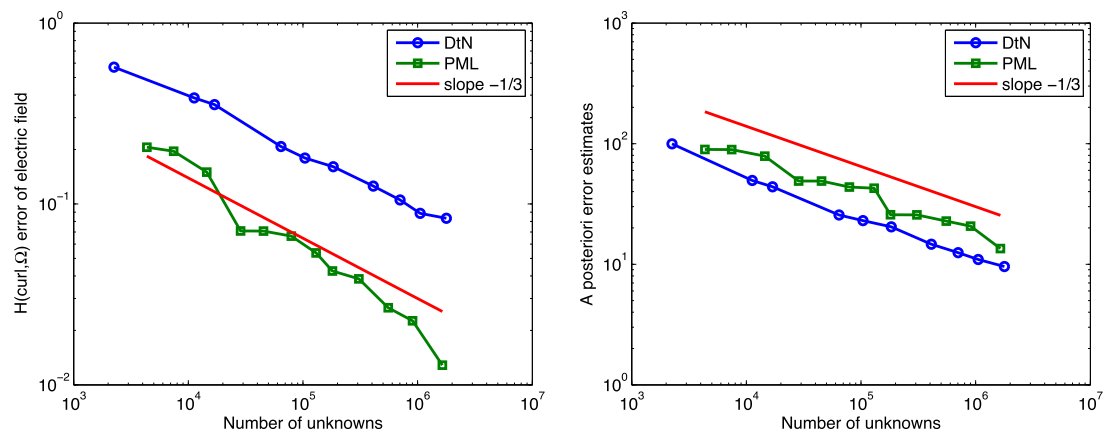
5. Numerical experiments

In this section, we report two examples to demonstrate the competitive performance of the proposed method. The implementation of the adaptive algorithm is based on parallel hierarchical grid (see PHG, 2021), which is a toolbox for developing parallel adaptive finite element programs on unstructured tetrahedral meshes. The first-order Nédélec's edge element is used in the numerical tests. The linear system resulted from finite element discretization is solved by the MUMPS direct solver, which is a general purpose library for the direct solution of large, sparse systems of linear equations. The adaptive FEM algorithm is summarized in Table 1.

In the experiments, let λ , θ_1 , θ_2 and $p = (p_1, p_2, p_3)^\top$ denote the wavelength, the incident angles and the polarization of the incident wave, respectively, and let n denote the refractive index. The examples are computed by using both the adaptive DtN algorithm and the adaptive PML method in Bao *et al.*

TABLE 1 The adaptive FEM-DtN algorithm

1	Given a tolerance $\epsilon > 0$ and mesh refinement threshold $\tau \in (0, 1)$;
2	Choose d_j and σ_j defined in Theorem 3.2 such that $e^{-d_j\sigma_j} < 10^{-8}$;
3	Construct an initial partition \mathcal{M}_h over Ω and compute error estimators;
4	While $\epsilon_h > \epsilon$ do;
5	choose $\hat{\mathcal{M}}_h \subset \mathcal{M}_h$ according to the strategy $\eta_{\hat{\mathcal{M}}_h} > \tau \eta_{\mathcal{M}_h}$;
6	refine the elements in $\hat{\mathcal{M}}_h$ and obtain a new mesh denoted still by \mathcal{M}_h ;
7	solve the discrete problem (3.5) on the new mesh \mathcal{M}_h ;
8	compute the corresponding error estimators;
9	End while.

Fig. 2. Optimal reduction rates of the *a priori* errors (left) and the *a posteriori* error estimates (right) for Example 5.1.

(2010). The complex coordinate stretching of the PML method is defined by

$$\tilde{x}_3 = \begin{cases} x_3 + i\sigma_0 \int_{b_1}^{x_3} \left(\frac{|t| - |b_1|}{d_{\text{PML}}} \right)^2 dt & \text{if } x_3 > b_1, \\ x_3 + i\sigma_0 \int_{b_2}^{x_3} \left(\frac{|t| - |b_2|}{d_{\text{PML}}} \right)^2 dt & \text{if } x_3 < b_2, \end{cases}$$

where σ_0 is the PML medium parameter and d_{PML} is the thickness of the PML layer. We choose σ_0 and d_{PML} such that the PML error is negligible compared with the finite element discretization error.

EXAMPLE 5.1 We consider the simplest bi-periodic structure, a flat plane, where the exact solution is available. We assume that a plane wave $\mathbf{E}^{\text{inc}} = \mathbf{q}e^{i(\alpha_1 x_1 + \alpha_2 x_2 - \beta x_3)}$ is incident on the flat plane $\{x_3 = 0\}$, which separates two homogeneous media: $n_1 = 1$ and $n_2 = 1.5$. In this example, the parameters are chosen as $\lambda = 1 \mu\text{m}$, $\theta_1 = \pi/6$, $\theta_2 = \pi/6$, $p = (-\alpha_2, \alpha_1, 0)^T$. Then $\alpha_1 = \frac{2\pi}{\lambda} \sin \theta_1 \cos \theta_2 = \sqrt{3}\pi/2$, $\alpha_2 = \frac{2\pi}{\lambda} \sin \theta_1 \sin \theta_2 = \pi/2$, $\beta = \frac{2\pi}{\lambda} \cos \theta_1 = \sqrt{3}\pi$. The computational domain $\Omega = (0, 0.5) \times (0, 0.5) \times (-0.3, 0.3)$. The exact solution is as follows:

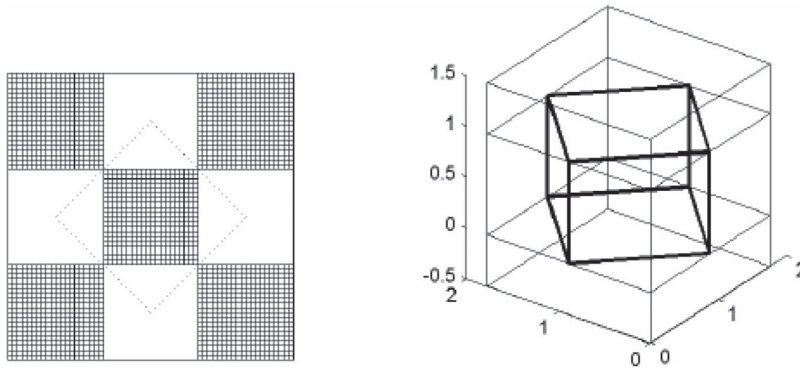


FIG. 3. A top view of the grating along with the unit cell (left) and the computational domain (right) for Example 5.2.

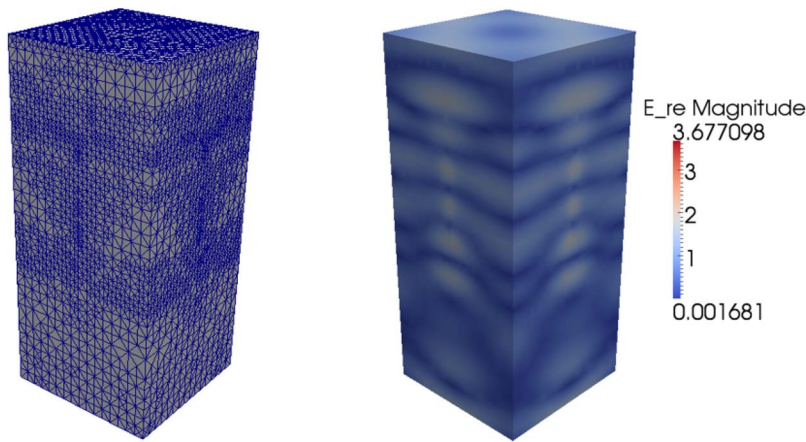


FIG. 4. The mesh plot and the surface plot of the amplitude of the field E_h after 11 adaptive iterations for Example 5.2.

$$E = \begin{cases} pe^{i(\alpha_1 x_1 + \alpha_2 x_2 - \beta_1 x_3)} + rpe^{i(\alpha_1 x_1 + \alpha_2 x_2 + \beta_1 x_3)} & \text{if } x_3 \geq 0, \\ tpe^{i(\alpha_1 x_1 + \alpha_2 x_2 - \beta_2 x_3)} & \text{if } x_3 < 0, \end{cases}$$

where $r = (\beta_1 - \beta_2)/(\beta_1 + \beta_2)$, $t = 2\beta_1/(\beta_1 + \beta_2)$. Here $\beta_j := \beta_{j0} = (\kappa_j^2 - \alpha_1^2 - \alpha_2^2)^{1/2}$, which gives $\beta_1 = \sqrt{3}\pi$, $\beta_2 = 2\sqrt{2}\pi$. For the adaptive PML method, the thickness of the PML is set to be $d_{\text{PML}} = 0.3$.

Figure 2 shows the curves of $\log N_k$ versus $\log \|E - E_h^N\|_{H(\text{curl}, \Omega)}$, and the *a posteriori* error estimates η_h , where N_k is the total number of degree of freedoms (DoFs) of the mesh. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\|E - E_h^N\|_{H(\text{curl}, \Omega)} = O(N_k^{-1/3})$ are valid asymptotically.

EXAMPLE 5.2 This example concerns the scattering of the time-harmonic plane wave E^{inc} on the checkerboard grating Li (1997), as seen in Fig. 3. The parameters are chosen as $\lambda = 1\mu\text{m}$, $\theta_1 = \theta_2 = 0$,

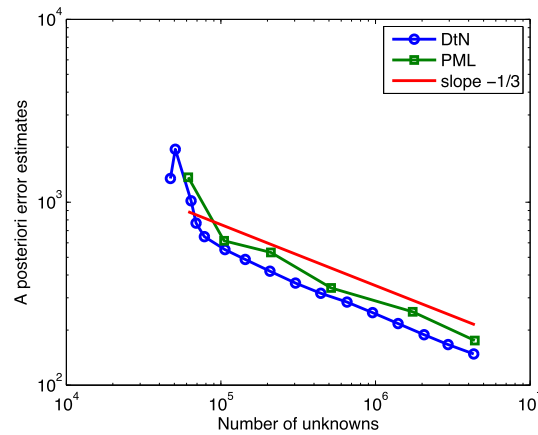


FIG. 5. Optimal reduction rates of the *a posteriori* error estimates for Example 5.2.

$p = (1, 1, (\alpha_1 + \alpha_2)/\beta)^\top$. The computational domain is $\Omega = (0, 1.25\sqrt{2}) \times (0, 1.25\sqrt{2}) \times (-2, 2)$. For the adaptive PML method, the thickness of the PML is set to be $d_{\text{PML}} = 2$.

Figure 4 shows the mesh and the amplitude of the associated solution for the total field E_h^N when the mesh has 1002488 DoFs. Figure 5 shows the curves of $\log N_k$ versus the *a posteriori* error estimates η_h . It can be seen that $\eta_h = O(N_k^{-1/3})$ is valid asymptotically.

6. Concluding remarks

In this paper, we have presented an adaptive edge finite element DtN method for the diffraction grating problem in biperiodic structures. A new duality argument is developed to derive the *a posteriori* error estimate, which takes account of both the finite element discretization error and the DtN truncation error. Moreover, the estimate is used to design the adaptive method to determine the DtN truncation parameter and choose elements for refinements. Numerical results show that the proposed method is effective and is a viable alternative to the adaptive finite element PML method for solving the diffraction grating problem. Indeed, the proposed method enriches the range of choices available for solving many other scattering problems imposed in open domains.

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Conflict of interest

The named authors have no conflict of interest, financial or otherwise.

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A. Derivation of the boundary condition in (4.22)

For $j = 1$, using (4.4), we get

$$\begin{aligned} \frac{1}{\mu}(\nabla \times W) \times \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} &= -i\omega \mathcal{T}_1^* W_{\Gamma_1}, \\ \frac{1}{\mu_1}(W'_{jn} - i\alpha_{jn}W_{3n}) &= -i\omega \frac{1}{\omega\mu_1\bar{\beta}_{1n}} \left((\bar{\beta}_{1n}^2 + \alpha_{jn}^2)W_{jn} + \alpha_{1n}\alpha_{2n}W_{(3-j)n} \right), \quad j = 1, 2, \\ W'_{jn} &= i\alpha_{jn}W_{3n} - i \left(\bar{\beta}_{1n}W_{jn} + \frac{\alpha_{jn}^2}{\bar{\beta}_{1n}}W_{jn} + \frac{\alpha_{1n}\alpha_{2n}}{\bar{\beta}_{1n}}W_{(3-j)n} \right), \quad j = 1, 2. \end{aligned}$$

Since $\beta_{1n} = i\sqrt{|\alpha_n|^2 - \kappa_1^2}$ has real part zero, we obtain $|\beta_{1n}| = i\bar{\beta}_{1n}$ and

$$W'_{jn} + |\beta_{1n}|W_{jn} = \frac{\alpha_{jn}^2}{|\beta_{1n}|}W_{jn} + i\alpha_{jn}W_{3n} - i\frac{\alpha_{1n}\alpha_{2n}}{\bar{\beta}_{1n}}W_{(3-j)n}, \quad j = 1, 2.$$

Of course, this is valid at $x_3 = b_1$ only. Now we apply the two formulas $W'_{3n} = -i\alpha_{1n}W_{1n}$ and $W''_{3n} - |\beta_{1n}|^2W_{3n} = -\mu_1\zeta_{3n}$. Hence, we substitute $W_{3n} = \frac{W'_{3n} + \mu_1\zeta_{3n}}{|\beta_{1n}|^2}$ to get

$$W'_{jn} + |\beta_{1n}|W_{jn} = \frac{\alpha_{jn}^2}{|\beta_{1n}|}W_{jn} + \frac{i\alpha_{jn}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} + i\alpha_{jn}\frac{W'_{3n}}{|\beta_{1n}|^2} - i\frac{\alpha_{1n}\alpha_{2n}}{\bar{\beta}_{1n}}W_{(3-j)n}, \quad j = 1, 2.$$

Substituting $W''_{3n} = -i\alpha_{jn}W'_{jn} - i\alpha_{(3-j)n}W'_{(3-j)n}$, we arrive at

$$\begin{aligned} W'_{jn} + |\beta_{1n}|W_{jn} &= \frac{i\alpha_{jn}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} + \alpha_{jn} \frac{\alpha_{jn}(W'_{jn} + |\beta_{1n}|W_{jn}) + \alpha_{(3-j)n}(W'_{(3-j)n} + |\beta_{1n}|W_{(3-j)n})}{|\beta_{1n}|^2} \\ &\quad - \alpha_{jn} \frac{\alpha_{jn}W_{jn} + \alpha_{(3-j)n}W_{(3-j)n}}{|\beta_{1n}|} - i \frac{\alpha_{1n}\alpha_{2n}}{\bar{\beta}_{1n}} W_{(3-j)} + \frac{\alpha_{jn}^2}{|\beta_{1n}|} W_{jn} \\ &= \frac{i\alpha_{jn}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} + \alpha_{jn} \frac{\alpha_{jn}(W'_{jn} + |\beta_{1n}|W_{jn}) + \alpha_{(3-j)n}(W'_{(3-j)n})}{|\beta_{1n}|^2}, \quad j = 1, 2. \end{aligned}$$

We get

$$\begin{pmatrix} \left(1 - \frac{\alpha_{1n}^2}{|\beta_{1n}|^2}\right) & -\frac{\alpha_{1n}\alpha_{2n}}{|\beta_{1n}|^2} \\ -\frac{\alpha_{1n}\alpha_{2n}}{|\beta_{1n}|^2} & \left(1 - \frac{\alpha_{2n}^2}{|\beta_{1n}|^2}\right) \end{pmatrix} \begin{pmatrix} W'_{1n} + |\beta_{1n}|W_{1n} \\ W'_{2n} + |\beta_{1n}|W_{2n} \end{pmatrix} = \begin{pmatrix} \frac{i\alpha_{1n}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} \\ \frac{i\alpha_{2n}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} \end{pmatrix},$$

which yields

$$\begin{pmatrix} W'_{1n} + |\beta_{1n}|W_{1n} \\ W'_{2n} + |\beta_{1n}|W_{2n} \end{pmatrix} = -\frac{|\beta_{1n}|^2}{\kappa_1^2} \begin{pmatrix} \left(1 - \frac{\alpha_{2n}^2}{|\beta_{1n}|^2}\right) & \frac{\alpha_{1n}\alpha_{2n}}{|\beta_{1n}|^2} \\ \frac{\alpha_{1n}\alpha_{2n}}{|\beta_{1n}|^2} & \left(1 - \frac{\alpha_{1n}^2}{|\beta_{1n}|^2}\right) \end{pmatrix} \begin{pmatrix} \frac{i\alpha_{1n}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} \\ \frac{i\alpha_{2n}\mu_1\zeta_{3n}}{|\beta_{1n}|^2} \end{pmatrix} = -\frac{i\mu_1\zeta_{3n}}{\kappa_1^2} \begin{pmatrix} \alpha_{1n} \\ \alpha_{2n} \end{pmatrix}.$$