Journal of Computational Mathematics, Vol.26, No.3, 2008, 261–283.

# COUPLING OF FINITE ELEMENT AND BOUNDARY ELEMENT METHODS FOR THE SCATTERING BY PERIODIC CHIRAL STRUCTURES*

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**Dedicated to Professor Junzhi Cui on the occasion of his 70th birthday**

**Abstract**

Consider a time-harmonic electromagnetic plane wave incident on a biperiodic structure in $\mathbf{R}^3$. The periodic structure separates two homogeneous regions. The medium inside the structure is *chiral* and *nonhomogeneous.* In this paper, variational formulations coupling finite element methods in the chiral medium with a method of integral equations on the periodic interfaces are studied. The well-posedness of the continuous and discretized problems is established. Uniform convergence for the coupling variational approximations of the model problem is obtained.

*Mathematics subject classification:* 65N30, 78A45, 35J20.
*Key words:* Chiral media, Periodic structures, Finite element method, Boundary element method, Convergence.

## 1. Introduction

Consider a time-harmonic electromagnetic plane wave incident on a biperiodic structure in $\mathbf{R}^3$. By biperiodic structure or doubly periodic structure, we mean that the structure is periodic in two orthogonal directions. The periodic structure separates two homogeneous regions. The medium inside the structure is chiral and nonhomogeneous. The diffraction problem is to study the propagation of the reflected and transmitted waves away from the structure. Recently, there has been a considerable interest in the study of scattering and diffraction by chiral media. Such media are isotropic, reciprocal, and more importantly circularly birefringent, with potential applications in antennas, microwave devices, waveguides, and many other fields. In general, electromagnetic wave propagation in a chiral medium is governed by Maxwell's 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 coupling is responsible for the chirality of the medium. It is measured by the magnitude of the chirality admittance $\beta$, which along with the dielectric coefficient $\varepsilon$ and the magnetic permeability constant $\mu$ characterize completely the electromagnetic properties of the medium. On the other hand, periodic (gratings) structures

* Received December 12, 2007 / Revised version received March 18, 2008 / Accepted March 20, 2008 /

have received increasing attentions through the years because of important applications in integrated optics, optical lenses, anti-reflective structures, holography, lasers, communication, and computing. Chiral gratings provide an exciting combination of the medium and structure. The combination gives rise to new features and applications. For instance, chiral gratings are capable of converting a linearly polarized incident field into two nearly circularly polarized diffracted modes in different directions. For an interesting explanation and references of these equations and various physical and computational aspects of the electromagnetic wave propagation inside chiral media, we refer to Lakhtakia [39] and Lakhtakia, Varadan, and Varadan [40] (non-periodic chiral structures), and to Jaggar, *et al.* [38], Lakhtakia, Varadan, and Varadan [41], and Yueh and Kong [55] (periodic chiral structures). Results and additional references on closely related periodic achiral structures may be found in Petit [42] and Bao, Dobson, and Cox [16], Dobson and Friedman [33], Abboud [1], Bao [13], Bao and Dobson [15], Bao and Zhou [18], Chen and Wu [26], Bao, Chen, and Wu [14], Arens, Chandler-Wilde, and DeSanto [12], and Rathsfeld, Schmidt, and Kleeman [51]. Other related recent results for Maxwell's equations in general media may be found in [17, 27, 35, 36].

This paper is devoted to a new approach for solving the diffraction problem, which couples a finite element method (FEM) in the nonhomogeneous chiral medium with a method of integral equations or boundary element method (BEM) on the periodic interfaces. More precisely, the approach consists of two processes: First, a finite element method is used for solving the diffraction problem in the complicated structure of a nonhomogeneous and possibly chiral material. Second, a method of integral equations is developed to derive the exact boundary conditions. The fact that these exact boundary conditions are formulated on the surface of the structure implies that no mesh of the surrounding medium would be needed. In this work, the well-posedness of the continuous and discretized formulations is established. Uniform convergence for the coupling variational approximations of the model problem is obtained. We point out that the variational coupling formulations introduced here are extremely general in terms of material, grating geometry, as well as the incident angle. The material functions $\varepsilon$, $\mu$, and $\beta$ are only assumed to be bounded measurable. Also, a recent result of Torres [52] indicates that the boundary on which the integral equations are derived needs only be Lipschitz.

Our present coupling approach is related to several other works in the literature. Levillain [43] implemented computationally several versions of a coupling procedure for Maxwell's equations in a three dimensional medium surrounding a bounded perfectly conducting body. de La Bourdonnaye [20] analyzed some coupling formulations for the Helmholtz equation as well as Maxwell's equations. Mathematical analysis of the coupling formulations in [43] has been carried out by Ammari and Nédélec [7, 8]. The results of [7] and [8] are further extended in [9] to study coupling FEM/BEM formulations for Maxwell's equations with a Leontovich boundary condition. We also refer to Wendland [53] and Gatica and Wendland [34] for a survey of asymptotic error estimates for symmetric and nonsymmetric coupling of finite and boundary element methods and to Nédélec [49] for a recent survey of the integral equation methods for computational electromagnetics.

Recently, in [2, 3], the authors have studied mathematical aspects of the diffraction problem by a periodic chiral structure. It is shown that for all but possibly a discrete set of parameters, the diffraction problem attains a unique quasi-periodic weak solution. Our proof is based on a Hodge decomposition lemma along with a new compact imbedding result. An important step of our approach is to reduce the diffraction problem into a bounded domain by using a pair of transparent boundary conditions. The approach in the present paper is different from the previous one in the following aspects: Here, the transparent boundary operators are not used and the exact radiation conditions are derived on the boundary of the chiral medium. No computation in the region surrounding the chiral medium is required. The well-posedness of the discretized problems excluding possibly a discrete set of singular frequencies is established and uniform convergence for the coupling FEM/BEM variational formulations is obtained. To the best of our knowledge, this paper presents the first coupling FEM/BEM variational approach for solving the diffraction problem. The approach has the potential for developing computationally attractive algorithms. It also gives a new proof of existence and uniqueness for solutions of the diffraction problem.

The paper is outlined as follows. In Section 2, the Maxwell equations and the constitutive equations, the Drude-Born-Fedorov equations, are presented. Section 3 is devoted to both symmetric and nonsymmetric variational formulations of the diffraction problem, which couple BEM with FEM. The well-posedness of the coupling formulations is established. Results on existence and uniqueness of the weak quasi-periodic solutions are proved. In Section 4, uniform convergence for the coupling FEM/BEM variational approximations is obtained. The paper is concluded in Section 5 by some general remarks.

## 2. The Diffraction Problem

Electromagnetic wave propagation in chiral media is governed by the time harmonic Maxwell equations and a set of constitutive equations, known as the Drude-Born-Fedorov equations, in which the electric and magnetic fields are coupled. The time harmonic Maxwell equations are (time dependence $e^{-i\omega t}$):

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

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

where $E$, $H$, $D$, and $B$ denote the electric field, the magnetic field, the electric, and magnetic displacement vectors in $\mathbf{R}^3$, respectively. The following Drude-Born-Fedorov equations hold:

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

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

where $\varepsilon$ is the electric permittivity, $\mu$ is the magnetic permeability, and $\beta$ is the chirality admittance. The parameters $\beta, \varepsilon$, and $\mu$ characterize completely the electromagnetic properties of the medium.

It is easily seen that the following equations are equivalent to the constitutive equations (2.3)-(2.4):

$$\Big(1 - (k(x)\beta(x))^2\Big)\, D = \varepsilon(x)E + \frac{i\beta(x)}{\omega}(k(x))^2\, H \,, \tag{2.5}$$

$$\Big(1 - (k(x)\beta(x))^2\Big)\, B = \mu(x)H - \frac{i\beta(x)}{\omega}(k(x))^2\, E \,, \tag{2.6}$$

where $k(x) = \omega\sqrt{\varepsilon(x)\,\mu(x)}$.

Similarly, the Maxwell equations may be rewritten as

$$\nabla \times E = (\gamma(x))^2 \, \beta(x) E + i\omega\mu(x) (\frac{\gamma(x)}{k(x)})^2 \, H \, , \tag{2.7}$$

$$\nabla \times H = (\gamma(x))^2 \, \beta(x) \, H - i\omega\varepsilon(x) (\frac{\gamma(x)}{k(x)})^2 \, E \, . \tag{2.8}$$

In these equations, the parameter $\gamma(x)$ is defined as :

$$(\gamma(x))^2 \; = \; \frac{(k(x))^2}{1 - (\, k(x) \, \beta(x) \,)^2} \; .$$

Throughout, we always assume that $(\, k(x) \, \beta(x) \,)^2 \neq 1, x \in \mathbb{R}^3$.

Moreover, the above system may be shown to be equivalent in a weak sense to

$$\nabla \times \Big( \frac{1 - \omega^2 \beta^2 \varepsilon\mu}{\mu} \Big) \nabla \times E - \omega^2 \nabla \times (\varepsilon\beta E) - \omega^2 \varepsilon\beta \nabla \times E - \omega^2 \varepsilon E = 0 \, , \tag{2.9}$$

$$\nabla \times E = (\gamma(x))^2 \, \beta(x) E + i\omega\mu(x) (\frac{\gamma(x)}{k(x)})^2 \, H \, . \tag{2.10}$$

Standard jump conditions may be deduced from the above system. In fact, the tangential parts of the electric and magnetic fields are continuous across an interface. Let $\nu$ denote the unit normal to the interface. We then have

$$\begin{aligned} &[\nu \times E] = 0 \, , \\ &[\nu \times \frac{1 - \beta^2 k^2}{i\omega\mu} \nabla \times E - \frac{\gamma^2 \beta (1 - k^2 \beta^2)}{i\omega\mu} \nu \times E] = 0 \, . \end{aligned}$$

We next specify the geometry of the problem. Let $\Lambda_1$ and $\Lambda_2$ be two positive constants, such that the material functions $\varepsilon$, $\mu$, and $\beta$ satisfy, for any $n_1$, $n_2 \in Z = \{0, \pm 1, \pm 2, \cdots\}$,

$$\begin{aligned} \varepsilon(x_1 + n_1 \Lambda_1, x_2 + n_2 \Lambda_2, x_3) &= \varepsilon(x_1, x_2, x_3) \, , \\ \mu(x_1 + n_1 \Lambda_1, x_2 + n_2 \Lambda_2, x_3) &= \mu(x_1, x_2, x_3) \, , \\ \beta(x_1 + n_1 \Lambda_1, x_2 + n_2 \Lambda_2, x_3) &= \beta(x_1, x_2, x_3) \, . \end{aligned}$$

In addition, it is assumed that, for some fixed positive constant $b$,

$$\begin{aligned} &\varepsilon(x) = \varepsilon_1 \, , \;\; \mu(x) = \mu_1 \, , \;\; \beta(x) = 0 \text{ for } x_3 > b \, , \\ &\varepsilon(x) = \varepsilon_2 \, , \;\; \mu(x) = \mu_2 \, , \;\; \beta(x) = 0 \text{ for } x_3 < -b \, , \end{aligned}$$

where $\varepsilon_1$, $\varepsilon_2$, $\mu_1$, and $\mu_2$ are positive constants.

We make the following general assumptions:

- $\varepsilon(x)$, $\mu(x)$, and $\beta(x)$ are all real valued $L^\infty$ functions, $\varepsilon(x) \geq \varepsilon_0$, $\mu(x) \geq \mu_0$, and $\beta \geq 0$, where $\varepsilon_0$ and $\mu_0$ are positive constants;
- $d(x) = (1 - \omega^2 \beta^2 \varepsilon\mu)/\mu \geq d_0 > 0$, for some positive constant $d_0$.

Note that the second assumption is essential. Fortunately it appears to be common in the literature and justifiable since $\beta$ is generally small. The first assumption is a technical one. Analogous results may be possible for materials that absorb energy.

Let $\Omega$ be the domain where the material parameters $\varepsilon, \mu$, and $\beta$ are variable functions, $\Omega_1$ be the domain above $\Omega$, and $\Omega_2$ be the domain below $\Omega$. Denote $\Gamma_j = \partial\Omega_j, j = 1, 2$.

Consider a plane wave in $\Omega_1$

$$E^{in} = se^{iq\cdot x} \ , \quad H^{in} = pe^{iq\cdot x} \ , \tag{2.11}$$

incident on $\Omega$. Here

$$q = (\alpha_1, \alpha_2, -\beta_1^{(0)}) = \omega\sqrt{\varepsilon_1\mu_1}(\cos\theta_1\cos\theta_2, \cos\theta_1\sin\theta_2, -\sin\theta_1)$$

is the incident wave vector whose direction is specified by $\theta_1$ and $\theta_2$, with $0 < \theta_1 < \pi$ and $0 < \theta_2 \leq 2\pi$. The vectors $s$ and $p$ satisfy

$$s = \frac{1}{\omega\varepsilon_1}(p \times q) \ , \quad q \cdot q = \omega^2\varepsilon_1\mu_1 \ , \quad p \cdot q = 0 \ . \tag{2.12}$$

We are interested in quasi-periodic solutions, *i.e.*, solutions $E$ and $H$ such that the fields $E_\alpha$, $H_\alpha$ defined by, for $\alpha = (\alpha_1, \alpha_2, 0)$,

$$E_\alpha = e^{-i\alpha\cdot x}E(x_1, x_2, x_3), \tag{2.13}$$

$$H_\alpha = e^{-i\alpha\cdot x}H(x_1, x_2, x_3), \tag{2.14}$$

are periodic in the $x_1$ direction of period $\Lambda_1$ and in the $x_2$ direction of period $\Lambda_2$.

Denote

$$\nabla_\alpha = \nabla + i\alpha = \nabla + i(\alpha_1, \alpha_2, 0) \ .$$

It is easy to see from (2.9) and (2.10) that $E_\alpha$ and $H_\alpha$ satisfy

$$\nabla_\alpha \times \Big(d\nabla_\alpha \times E_\alpha\Big) - \omega^2\nabla_\alpha \times (\varepsilon\beta E_\alpha) - \omega^2\varepsilon\beta\nabla_\alpha \times E_\alpha - \omega^2\varepsilon E_\alpha = 0, \tag{2.15}$$

$$\nabla_\alpha \times E_\alpha = (\gamma(x))^2\,\beta(x)E_\alpha + i\omega\mu(x)(\frac{\gamma(x)}{k(x)})^2\,H_\alpha. \tag{2.16}$$

In order to solve (2.15)-(2.16) we need to impose a radiation condition on the scattering problem. Due to the (infinite) periodic structure, the usual Sommerfeld or Silver-Müller radiation condition is no longer valid [50]. The appropriate radiation condition may be derived as follows: Since $E_\alpha$ is $\Lambda$ periodic, we can expand $E_\alpha$ in a Fourier series:

$$E_\alpha(x) = E_\alpha^{in}(x) + \sum_{n\in Z} U_\alpha^{(n)}(x_3)e^{i\alpha_n\cdot x}, \tag{2.17}$$

where $E_\alpha^{in} = E^{in}e^{-i\alpha\cdot x}$, $\alpha_n = (2\pi n_1/\Lambda_1, 2\pi n_2/\Lambda_2, 0)$, and

$$U_\alpha^{(n)}(x_3) = \frac{1}{\Lambda_1\Lambda_2}\int_0^{\Lambda_1}\int_0^{\Lambda_2}(E_\alpha(x) - E_\alpha^{in}(x))e^{-i\alpha_n\cdot x}dx_1dx_2.$$

Define for $j = 1, 2$ the coefficients

$$\beta_j^{(n)}(\alpha) = \begin{cases} \sqrt{\omega^2\varepsilon_j\mu_j - |\alpha_n + \alpha|^2}, & \omega^2\varepsilon_j\mu_j > |\alpha_n + \alpha|^2 \ , \\ i\sqrt{|\alpha_n + \alpha|^2 - \omega^2\varepsilon_j\mu_j}, & \omega^2\varepsilon_j\mu_j < |\alpha_n + \alpha|^2 \ . \end{cases} \tag{2.18}$$

We assume that $\omega^2\varepsilon_j \neq |\alpha_n + \alpha|^2$ for all $n \in Z^2$, $j = 1, 2$. This condition excludes "resonances".

For convenience, we also introduce the following notation:

$$\Lambda_j^+ = \{n \in Z^2 : \ \ Im(\beta_j^{(n)}) = 0\} \ ,$$
$$\Lambda_j^- = \{n \in Z^2 : \ \ Im(\beta_j^{(n)}) \neq 0\} \ .$$

Observe that inside $\Omega_j$ $(j = 1, 2)$, $\varepsilon = \varepsilon_j$, $\mu = \mu_j$, and $\beta = 0$, Maxwell's equations then become

$$(\Delta_\alpha + \omega^2 \varepsilon_j \mu_j) E_\alpha = 0 \ , \tag{2.19}$$

where $\Delta_\alpha = \Delta + 2i\alpha \cdot \nabla - |\alpha|^2$.

Since the medium in $\Omega_j$ $(j = 1, 2)$ is homogeneous, the method of separation of variables implies that $E_\alpha$ can be expressed as a sum of plane waves:

$$E_\alpha|_j = E^{in}_{\alpha,j}(x) + \sum_{n\in Z} A_j^{(n)} e^{\pm i\beta_j^{(n)} x_3 + i\alpha_n \cdot x}, \quad j = 1, 2, \quad \text{in } (-1)^{j+1} x_3 > b, \tag{2.20}$$

$$H_\alpha|_j = H^{in}_{\alpha,j}(x) + \sum_{n\in Z} B_j^{(n)} e^{\pm i\beta_j^{(n)} x_3 + i\alpha_n \cdot x}, \quad j = 1, 2, \quad \text{in } (-1)^{j+1} x_3 > b, \tag{2.21}$$

where the $A_j^{(n)}$ and $B_j^{(n)}$ are constant (complex) vectors and $E^{in}_{\alpha,1}(x) = E^{in}_\alpha(x), H^{in}_{\alpha,1}(x) = H^{in}_\alpha(x)$ in $x_3 > b$ and $E^{in}_{\alpha,2}(x) = H^{in}_{\alpha,2}(x) = 0$ in $x_3 < -b$.

The following radiation condition is employed: Since $\beta_j^n$ is real for at most finitely many $n$, there are only a finite number of propagating plane waves in the sum (2.20), the remaining waves are exponentially decaying (or radiated) as $|x_3| \to \infty$. We will insist that $E_\alpha$ is composed of bounded outgoing plane waves in $\Omega_1$ and $\Omega_2$, plus the incident (incoming) wave in $\Omega_1$.

From (2.17) and (2.18) we deduce

$$E_\alpha^{(n)}(x_3) = \begin{cases} U_\alpha^{(n)}(b) e^{i\beta_1^{(n)}(x_3 - b)}, & \text{in } x_3 > b, \\ U_\alpha^{(n)}(-b) e^{-i\beta_2^{(n)}(x_3 + b)}, & \text{in } x_3 < -b. \end{cases} \tag{2.22}$$

Define

$$\Lambda = \Lambda_1 Z \times \Lambda_2 Z \times \{0\} \subset \mathbf{R}^3 \ .$$

Since the fields $E_\alpha$ are $\Lambda$-periodic, we can move the problem from $\mathbf{R}^3$ to the quotient space $\mathbf{R}^3/\Lambda$. For the remainder of the paper, we shall identify $\Omega$ with the cylinder $\Omega/\Lambda$, and similarly for the boundaries $\Gamma_j \equiv \Gamma_j/\Lambda$. Thus from now on,

*all functions defined on $\Omega, \Omega_j$, and $\Gamma_j$ are implicitly $\Lambda$-periodic.*

Define $div_\alpha$ by $div_\alpha u = \nabla_\alpha \cdot u = (\partial_{x_1} + i\alpha_1)u_1 + (\partial_{x_2} + i\alpha_2)u_2$.

In the future, for simplicity, we shall drop the subscript $\alpha$. Denote by $\mathrm{div}_{\Gamma_j}, \nabla_{\Gamma_j}, \nabla_{\Gamma_j}\times$, and $\mathrm{curl}_{\Gamma_j}$, the surface divergence, the surface gradient, the surface vector rotational, and the surface scalar rotational, respectively. Their meanings should be clear from the contexts. Let $\mathrm{H}^m$ be the $m$th order $\mathrm{L}^2$-based Sobolev spaces of complex valued functions and $\mathrm{H}^m_p(\Omega)$ be the subset of all functions in $\mathrm{H}^m(\Omega)$ which are the restrictions to $\Omega$ of the $\Lambda$-periodic functions in $\mathrm{H}^m_{loc}(\mathbf{R}^2 \times (-b, b))$. The spaces $\mathrm{H}^m_p(\Omega_j)$ and $\mathrm{H}^m_p(\Gamma_j)$ may be defined similarly. Consider further the notation:

$$\mathrm{H}(\mathrm{curl}, \Omega) = \Big\{ v \in \mathrm{L}^2(\Omega)^3, \nabla \times v \in \mathrm{L}^2(\Omega)^3 \Big\} \ ,$$
$$\mathrm{TH}^s(\Gamma_j) = \Big\{ u \in \mathrm{H}^s(\Gamma_j)^3, u \,.\, n_j = 0 \Big\},$$
$$\mathrm{TH}^s(\mathrm{div}, \Gamma_j) = \Big\{ u \in \mathrm{TH}^s(\Gamma_j), \mathrm{div}_{\Gamma_j} u \in \mathrm{H}^s(\Gamma_j) \Big\},$$
$$\mathrm{TH}^s(\mathrm{curl}, \Gamma_j) = \Big\{ u \in \mathrm{TH}^s(\Gamma_j), \mathrm{curl}_{\Gamma_j} u \in \mathrm{H}^s(\Gamma_j) \Big\}.$$

Next, introduce the periodic Green kernel $G_j$, for $j = 1, 2$, which satisfies the radiation condition (2.22) and the Helmholtz equation:

$$\Delta\, u + \omega^2\, \varepsilon_j\, \mu_j\, u = 0 \quad \text{in } \mathbb{R}^3.$$

From [50], consider formally the sum

$$G_j = -\frac{i}{2\Lambda_1\Lambda_2} \sum_{n\in Z^2} \frac{1}{\beta_j^{(n)}} e^{-i\alpha_n\,.\,x}\, e^{i\beta_j^{(n)}|x_3|}. \tag{2.23}$$

We have

**Lemma 2.1.** *The sum* (2.23) *defines an* $L^2_{loc}(\mathbb{R}^3)$ *periodic function which satisfies*

$(i)\quad \Delta\, G_j + \omega^2\, \varepsilon_j\, \mu_j\, G_j = \sum_{n\in Z^2} \delta(\Lambda_n) \quad \text{in } (\mathcal{C}_0^\infty(\mathbb{R}^3))'$,

$(ii)$ $G_j$ *is a* $\mathcal{C}^\infty$ *function in* $\mathbb{R}^3 \setminus \cup_{n\in Z^2}\{\Lambda_n\}$,

$(iii)$ $G_j$ *satisfies the radiation condition* (2.22).

*Here* $\Lambda_n = (n_1\Lambda_1, n_2\Lambda_2, 0), n = (n_1, n_2) \in Z^2$ *and* $\delta(\Lambda_n)$ *is the Dirac measure at* $\Lambda_n$.

Note that if $\beta_j^{(n)} \neq 0, \forall n \in Z^2$, for $x \neq \Lambda_n$, the series in (2.23) converges uniformly in compact sets but cannot be component-wise differentiated with respect to $x_3$ at $x_3 = 0$.

The following identity holds.

**Lemma 2.2.**

$$G_j = \sum_{n\in Z^2} \frac{e^{i\omega\sqrt{\varepsilon_j\mu_j}|x_n|} e^{-i\alpha\,.\,x_n}}{4\pi|x_n|}, \tag{2.24}$$

*where* $x_n = x + \Lambda_n$.

See Morelot [46] for a proof of (2.24) by the Poisson summation formula. An analogous representation of the periodic Green kernel in the case of a single periodic surface was given by Chen and Friedman [25] and Bruno and Reitich [24].

From now on, we denote by $G_j(x, y) = G_j(x - y)$ for $x = (x_1, x_2, x_3), y = (y_1, y_2, y_3) \in \mathbb{R}^3$.

We have the following additional result about the singularity of the kernel $G_j$.

**Lemma 2.3.** *The function*

$$G_j(x, y) - \frac{1}{4\pi|x - y|} + \frac{i}{2\pi}\Big(\alpha_1 \log|x_1 - y_1| + \alpha_2 \log|x_2 - y_2|\Big)$$

*is a continuous function as* $|x - y| \to 0$.

*Proof.* Recalling that $\Delta = \nabla_\alpha\,.\,\nabla_\alpha$, it is easy to see that

$$(\Delta + \omega^2\varepsilon_j\mu_j)\left(G_j - \frac{e^{i\omega\sqrt{\varepsilon_j\mu_j}|x-y|}}{4\pi|x - y|}\right) = -\frac{i\alpha}{2\pi}\,.\,\nabla\left(\frac{e^{i\omega\sqrt{\varepsilon_j\mu_j}|x-y|}}{4\pi|x - y|}\right) + |\alpha|^2 \frac{e^{i\omega\sqrt{\varepsilon_j\mu_j}|x-y|}}{4\pi|x - y|},$$

for any $x = (x_1, x_2, x_3)$, $y = (y_1, y_2, y_3) \in (0, \Lambda_1) \times (0, \Lambda_2) \times \mathbb{R}$. By the standard elliptic theory, the kernel $G_j - e^{i\omega\sqrt{\varepsilon_j\mu_j}}/|x - y|$ has the same singularity when $|x - y| \to 0$ as $R_j$ with

$$\Delta R_j = -\frac{i\alpha}{2\pi}\,.\,\nabla(\frac{1}{|x - y|})\ .$$

Moreover, $R_j$ behaves like $i(2\pi)^{-1}(\alpha_1 \log|x_1 - y_1| + \alpha_2 \log|x_2 - y_2|) + \mathcal{O}(|x - y| \log|x - y|)$. The conclusion follows from the continuity of the function $|x - y| \log|x - y|$ as $|x - y| \to 0$. $\square$

**Lemma 2.4.** *There exist three positive constants $C, C'$, and $C''$, such that*

$$C||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} \geq \Big| \int_{\Gamma_j} \int_{\Gamma_j} G_j(x,y)\theta(x)\overline{\theta}(y)d\gamma(y)d\gamma(x) \Big| \\ \geq C'||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} - C''||\theta||^2_{\mathrm{H}^{-3/2}(\Gamma_j)}, \tag{2.25}$$

*for any $\theta \in \mathrm{H}^{-1/2}(\Gamma_j)$.*

*Proof.* By Lemma 2.3, it suffices to prove that there exist positive constants $C$ and $C'$ such that

$$C||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} \geq \Big| \int_{\Gamma_j} \int_{\Gamma_j} \frac{1}{|x-y|}\theta(x)\overline{\theta}(y)d\gamma(y)d\gamma(x) \Big| \geq C'||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)}, \tag{2.26}$$

for any $\theta \in \mathrm{H}^{-1/2}(\Gamma_j)$. The coercivity estimate is classical if the boundary $\Gamma$ is closed. Let $\tilde{\Gamma}_j$ be a bounded and closed boundary such that $2\,\Gamma_j \subset \tilde{\Gamma}_j$, $\varphi \equiv 1$ on $\Gamma_j$, and $\varphi \equiv 0$ outside of $3\,\Gamma_j/2$ (component-wise). Denote $\tilde{\theta} = \varphi\theta$ for any $\theta \in \mathrm{H}^{-1/2}(\Gamma_j)$. According to [49] it is clear that

$$\Big| \int_{\tilde{\Gamma}_j} \int_{\tilde{\Gamma}_j} \frac{1}{|x-y|}\tilde{\theta}(x)\overline{\tilde{\theta}}(y)d\gamma(y)d\gamma(x) \Big| \geq C||\theta||^2_{\mathrm{H}^{-1/2}(\tilde{\Gamma}_j)}\ ,$$

which along with

$$\Big| \int_{\tilde{\Gamma}_j} \int_{\tilde{\Gamma}_j} \frac{1}{|x-y|}\tilde{\theta}(x)\overline{\tilde{\theta}}(y)d\gamma(y)d\gamma(x) \Big| \leq 2\Big| \int_{\Gamma_j} \int_{\Gamma_j} \frac{1}{|x-y|}\theta(x)\overline{\theta}(y)d\gamma(y)d\gamma(x) \Big|$$

and

$$2||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} \geq ||\tilde{\theta}||^2_{\mathrm{H}^{-1/2}(\tilde{\Gamma}_j)} \geq ||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)}$$

yield the estimate (2.25). □

## 3. Continuous Coupling FEM/BEM Formulations

In this section, we derive coupling FEM/BEM formulations for solving the diffraction problem. The well-posedness of the continuous coupling formulations is established. We also prove that the derived coupling formulations are of Fredholm type and they do not generate spurious eigenfrequencies at the continuous level since they are completely equivalent to Equations (2.15)-(2.16) which along with the radiation condition (2.22) govern the diffraction from periodic chiral structures. In the following, we first state a useful Hodge decomposition lemma, a classical compactness result, and a trace regularity result. We then derive coupling FEM/BEM formulations. We also study questions on existence and uniqueness of the solutions.

### 3.1. Hodge decomposition and compactness

Assume that $\Omega$ is connected and $\Gamma_j$ is simply connected.

**Lemma 3.1.** *(a) Let*

$$\mathbb{M}(\Omega) = \Big\{ u \in \mathrm{H}(\mathrm{curl}, \Omega), \int_\Omega \varepsilon\, u \,.\, \nabla\, q = 0, \forall\, q \in \mathrm{H}^1(\Omega) \Big\}.$$

*The following Hodge decomposition holds:*

$$\mathrm{H}(\mathrm{curl}, \Omega) = \mathbb{M}(\Omega) \overset{\perp}{\oplus} \nabla\, \mathrm{H}^1(\Omega),$$

*where the orthogonality is with respect to the product* $((,))$ *defined by*

$$((u,v)) = \int_\Omega \nabla \times u \,.\, \nabla \times v + \int_\Omega \varepsilon\, u \,.\, v.$$

*(b) The Hodge decomposition holds:*

$$\mathrm{TH}^{-1/2}(\mathrm{div},\Gamma_j) = \nabla_{\Gamma_j}\ \mathrm{H}^{3/2}(\Gamma_j)/C \overset{\perp}{\oplus} \nabla_{\Gamma_\mathrm{j}} \times \mathrm{H}^{1/2}(\Gamma_\mathrm{j})/C,$$

*where the orthogonality is with respect to the duality product between* $\mathrm{TH}^{1/2}(\Gamma_j)$ *and* $\mathrm{TH}^{-1/2}(\Gamma_j)$.

*Proof.* Let $E \in \mathrm{H}(\mathrm{curl},\Omega)$. Since $\Omega$ is connected, *i.e.*, the space of Neumann fields in $\Omega$ is trivial, there exists a unique $u$ satisfying

$$\begin{aligned}&\nabla \times u = \nabla \times E \quad \text{in } \Omega,\\ &\mathrm{div}\ \varepsilon u = 0 \quad \text{in } \Omega,\\ &u \,.\, n_j = 0 \quad \text{on } \Gamma_j.\end{aligned}$$

Further, since $\Delta_{\Gamma_j}^{-1}(\mathrm{div}_{\Gamma_j}(E_{\Gamma_j} - u_{\Gamma_j})) \in \mathrm{H}^{1/2}(\Gamma_j)$, there exists a unique solution $p \in \mathrm{H}^1(\Omega)$ to the boundary value problem

$$\begin{aligned}&\mathrm{div}\varepsilon\nabla p = 0 \quad \text{in } \Omega,\\ &p = \Delta_{\Gamma_j}^{-1}(\mathrm{div}_{\Gamma_j}(E_{\Gamma_j} - u_{\Gamma_j})) \quad \text{on } \Gamma_j.\end{aligned}$$

It is clear that $E = u + \nabla p$ and the uniqueness of the decomposition (a) is obvious.

Since $\Gamma_j$ is simply connected, the decomposition (b) follows immediately from [20]. Note that in the case where $\Gamma_j$ is non-simply connected, the finite dimensional vector space

$$N(\Gamma_j) = \Big\{\theta, \Delta_{\Gamma_j}\theta = 0\Big\} = \Big\{\theta, \mathrm{div}_{\Gamma_j}\theta = 0, \mathrm{curl}_{\Gamma_j}\theta = 0\Big\},$$

is nontrivial and (b) should be replaced with, see for instance ([4], section 4),

$$\mathrm{TH}^{-1/2}(\mathrm{div},\Gamma_j) = \nabla_{\Gamma_j}\ \mathrm{H}^{3/2}(\Gamma_j)/\mathbb{C} \oplus \nabla_{\Gamma_\mathrm{j}} \times \mathrm{H}^{1/2}(\Gamma_\mathrm{j})/\mathbb{C} \oplus \mathrm{N}(\Gamma_\mathrm{j}).$$

This completes the proof of the lemma. □

**Remark 3.1.** A decomposition similar to (a) was originally introduced by Birman and Solomyak [21] to regularize Maxwell's equations in a bounded domain. A decomposition similar to (b) was used in [5].

**Lemma 3.2.** *The imbedding from* $\mathbb{M}(\Omega)$ *to* $L^2(\Omega)^3$ *is compact.*

*Proof.* For any sequence $u_m \in \mathbb{M}(\Omega)$ let $\tilde{u}_m$ be its periodic extension. Denote $\Omega = (0,\Lambda_1) \times (0,\Lambda_2) \times \mathcal{O}$. Let $\tilde{\Omega} = (-\Lambda_1, 2\Lambda_1) \times (-\Lambda_2, 2\Lambda_2) \times \mathcal{O}$ and $\varphi$ be a smooth function with

$$\begin{aligned}&\varphi(x_1,x_2) \equiv 1 \quad (x_1,x_2) \in [0,\Lambda_1] \times [0,\Lambda_2],\\ &\varphi(x_1,x_2) \equiv 0 \quad (x_1,x_2) \in ([-\Lambda_1,-\Lambda_1/2] \cup [3\Lambda_1/2, 2\Lambda_1]) \times ([-\Lambda_2,-\Lambda_2/2] \cup [3\Lambda_2/2, 2\Lambda_2]).\end{aligned}$$

Then

$$\begin{cases}\varphi\, \tilde{u}_m \,.\, n = 0 \quad \text{on } \partial\tilde{\Omega},\\ \varphi\, \tilde{u}_m \in \mathrm{L}^2(\tilde{\Omega})^3, \nabla \times \varphi\, \tilde{u}_m \in \mathrm{L}^2(\tilde{\Omega})^3,\\ \mathrm{div}\varphi\, \tilde{u}_m \in \mathrm{L}^2(\tilde{\Omega}).\end{cases}$$

Further, $\varphi\tilde{u}_m = u_m$ in $\Omega$ and there exists a constant $C$ independent of $m$, such that

$$||\varphi\tilde{u}_m||_{\mathrm{H}(\mathrm{curl},\tilde{\Omega})} \leq C\,||u_m||_{\mathbb{M}(\Omega)}. \tag{3.1}$$

If the sequence $\{\tilde{u}_m\}$ is bounded in $\mathrm{H}(\mathrm{curl},\tilde{\Omega})$ then we can extract by Weber [54] a subsequence that converges strongly in $\mathrm{L}^2(\Omega)^3$. The compactness of the imbedding follows from (3.1). □

**Lemma 3.3.** ([3]) *For any $\eta > 0$, the following estimate holds:*

$$||u \times n_j||_{\mathrm{TH}^{-1/2}(\Gamma_j)} \leq \eta||\nabla \times u||_{\mathrm{L}^2(\Omega)^3} + \frac{1}{\eta}||u||_{\mathrm{L}^2(\Omega)^3}.$$

### 3.2. Periodic integral representations

Denote

$$E = \begin{cases} E_1 & \text{in } \Omega_1, \\ E_i & \text{in } \Omega, \\ E_2 & \text{in } \Omega_2, \end{cases} \qquad H = \begin{cases} H_1 & \text{in } \Omega_1, \\ H_i & \text{in } \Omega, \\ H_2 & \text{in } \Omega_2. \end{cases}$$

We now derive periodic integral representations for $E_j$ and $H_j$ inside $\Omega_j$.

**Lemma 3.4.** *The following periodic integral representation formulas hold:*

$$E_j = E_j^{in} - \nabla \times \int_{\Gamma_1} G_j M_j - \frac{i}{\omega\varepsilon_j}\nabla \int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j} J_j - i\omega\mu_j \int_{\Gamma_j} G_j J_j, \quad x \in \Omega_j, \tag{3.2}$$

$$H_j = H_j^{in} - \nabla \times \int_{\Gamma_j} G_j J_j + \frac{i}{\omega\mu_j}\nabla \int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j} M_j + i\omega\varepsilon_j \int_{\Gamma_j} G_j M_j, \quad x \in \Omega_j, \tag{3.3}$$

*where $M_j = E_j \times n_j|_{\Gamma_j} = E_i \times n_j|_{\Gamma_j}$ and $J_j = H_j \times n_j|_{\Gamma_j} = H_i \times n_j|_{\Gamma_j}$.*

*Proof.* Without loss of generalities, it suffices to establish the periodic integral representation (3.2) for $E_1$ in $\Omega_1$. Let $\Omega_1^b = \Omega_1 \cap \{x_3 < b\}$. Multiplying both sides of the Maxwell equations satisfied by $E_1$ and integrating by parts over $\Omega_1^b$, we get by some standard manipulations [28] that

$$\begin{aligned} E_1(x) = & -\nabla \times \int_{\Gamma_1} G_1 M_1 - \frac{i}{\omega\varepsilon_1}\nabla \int_{\Gamma_1} G_1 \mathrm{div}_{\Gamma_1} J_1 - i\omega\mu_1 \int_{\Gamma_1} G_1 J_1 \\ & +\nabla \times \int_{x_3=b} G_1 E_1 \times e_3 + \frac{i}{\omega\varepsilon_1}\nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}(E_1 \times e_3) \\ & +i\omega\mu_1 \int_{x_3=b} G_1 E_1 \times e_3, \quad x \in \Omega_1^b. \end{aligned}$$

Rewrite the terms on $x_3 = b$

$$\begin{aligned} & \nabla \times \int_{x_3=b} G_1 E_1 \times e_3 + \frac{i}{\omega\varepsilon_1}\nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}(E_1 \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1 E_1 \times e_3 \\ = & \nabla \times \int_{x_3=b} G_1 E_1^{in} \times e_3 + \frac{i}{\omega\varepsilon_1}\nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}(E_1^{in} \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1 E_1^{in} \times e_3 \\ & +\nabla \times \int_{x_3=b} G_1 (E_1 - E_1^{in}) \times e_3 + \frac{i}{\omega\varepsilon_1}\nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}((E_1 - E_1^{in}) \times e_3) \\ & +i\omega\mu_1 \int_{x_3=b} G_1 (E_1 - E_1^{in}) \times e_3 \;. \end{aligned}$$

It is easily seen that

$$E_1^{in}(x) = \nabla \times \int_{x_3=b} G_1 E_1^{in} \times e_3 + \frac{i}{\omega\varepsilon_1} \nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}(E_1^{in} \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1 E_1^{in} \times e_3,$$

for $x \in \Omega_1^b$.

To prove the periodic integral representation (3.2), it is sufficient to show that the quantity

$$\nabla \times \int_{x_3=b} G_1(E_1 - E_1^{in}) \times e_3 + \frac{i}{\omega\varepsilon_1} \nabla \int_{x_3=b} G_1 \mathrm{div}_{x_3=b}((E_1 - E_1^{in}) \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1(E_1 - E_1^{in}) \times e_3$$

goes to 0 as $b \to +\infty$ uniformly in $x$. Write $G_1 = G_1^+ + G_1^-$, where

$$G_1^{\pm} = -\frac{i}{2\Lambda_1\Lambda_2} \sum_{n \in \Lambda_1^{\pm}} \frac{1}{\beta_j^{(n)}} e^{-i\alpha_n \cdot x}\, e^{i\beta_j^{(n)}|x_3|}.$$

From

$$B_1^{(n)} = -\frac{i}{\omega\mu_1} A_1^{(n)} \times (iB_1^{(n)} e_3 + i\alpha_n), \quad \forall\, n \in Z^2,$$

where $A_1^{(n)}$ and $B_1^{(n)}$ are defined by (2.20)-(2.21), we obtain after some simple calculations that

$$\nabla \times \int_{x_3=b} G_1^+(E_1 - E_1^{in}) \times e_3 + \frac{i}{\omega\varepsilon_1} \nabla \int_{x_3=b} G_1^+ \mathrm{div}_{x_3=b}((E_1 - E_1^{in}) \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1^+(E_1 - E_1^{in}) \times e_3 = 0. \tag{3.4}$$

On the other hand, the quantity

$$\nabla \times \int_{x_3=b} G_1^-(E_1 - E_1^{in}) \times e_3 + \frac{i}{\omega\varepsilon_1} \nabla \int_{x_3=b} G_1^- \mathrm{div}_{x_3=b}((E_1 - E_1^{in}) \times e_3) + i\omega\mu_1 \int_{x_3=b} G_1^-(E_1 - E_1^{in}) \times e_3$$

is exponentially decaying as $b \to +\infty$ hence the conclusion follows from (3.4). □

Next, we determine the unknowns $M_j$ and $J_j$ in $\mathrm{TH}^{-1/2}(\mathrm{div}, \Gamma_j)$ as well as the fields $E_i$ and $H_i$ in $\mathrm{H}(\mathrm{curl}, \Omega)$. To derive periodic integral equations on $\Gamma_j$ from the periodic integral representations (3.2)-(3.3), the following lemma is needed.

**Lemma 3.5.** *For any* $v \in \mathrm{TH}^{-1/2}(\mathrm{div}, \Gamma_j)$,

$$\lim_{x \in \Omega_j \to x_0 \in \Gamma_j} n_j(x_0) \times \nabla \times \int_{\Gamma_j} G_j(x,y) v(y)\, d\gamma(y) = -\frac{v(x_0)}{2} + n_j(x_0) \times \int_{\Gamma_j} \nabla_x G_j(x,y) \times v(y)\, d\gamma(y).$$

*Proof.* The key of the proof is to observe by Lemma 2.3 that

$$G_j(x,y) - \frac{1}{4\pi|x-y|} + \frac{i}{2\pi}\Big(\alpha_1 \log|x_1-y_1| + \alpha_2 \log|x_2-y_2|\Big)$$

is a continuous function even as $x-y \to 0$. Hence

$$\begin{aligned}&\lim_{x\in\Omega_j \to x_0 \in \Gamma_j} n_j(x_0) \times \nabla \times \int_{\Gamma_j} \Big(G_j(x,y) - \frac{1}{4\pi|x-y|}\Big) v(y)\, d\gamma(y)\\ &= n_j(x_0) \times \nabla \times \int_{\Gamma_j} \Big(G_j(x_0,y) - \frac{1}{4\pi|x_0-y|}\Big) v(y)\, d\gamma(y).\end{aligned}$$

By Müller [47], we have

$$\begin{aligned}&\lim_{x\in\Omega_j \to x_0 \in \Gamma_j} n_j(x_0) \times \nabla \times \int_{\Gamma_j} \frac{1}{|x-y|} v(y)\, d\gamma(y)\\ &= -\frac{v(x_0)}{2} + n_j(x_0) \times \int_{\Gamma_j} \nabla_x \frac{1}{|x-y|} \times v(y)\, d\gamma(y),\\ &\lim_{x\in\Omega_j \to x_0 \in \Gamma_j} n_j(x_0) \times \int_{\Gamma_j} \frac{1}{|x-y|} v(y)\, d\gamma(y) = n_j(x_0) \times \int_{\Gamma_j} \frac{1}{|x_0-y|} v(y)\, d\gamma(y).\end{aligned}$$

The proof is now complete. □

Taking the limit of (3.2)-(3.3) tangentially on $\Gamma_j$, we obtain by Lemma 3.5 the periodic integral equations on $\Gamma_j$:

$$\begin{aligned}&\frac{1}{2} n_j(x) \times E_i(x)\\ &= n_j(x) \times E_j^{in}(x) - \frac{i}{\omega\varepsilon_j} n_j(x) \times (\nabla_{\Gamma_j} \int_{\Gamma_j} G_j(x,y) \mathrm{div}_{\Gamma_j} J_j(y)\, d\gamma(y)\, d\gamma(x))\\ &\quad - i\omega\mu_j n_j(x) \times (\int_{\Gamma_j} G_j(x,y) J_j(y)\, d\gamma(y)\, d\gamma(x))\\ &\quad - n_j(x) \times (\int_{\Gamma_j} \nabla_x G_j(x,y) \times M_j(y)\, d\gamma(y)\, d\gamma(x))\end{aligned} \tag{3.5}$$

and

$$\begin{aligned}&\frac{1}{2} n_j(x) \times H_i(x)\\ &= n_j(x) \times H_j^{in}(x) + \frac{i}{\omega\mu_j} n_j(x) \times (\nabla_{\Gamma_j} \int_{\Gamma_j} G_j(x,y) \mathrm{div}_{\Gamma_j} M_j(y)\, d\gamma(y)\, d\gamma(x))\\ &\quad + i\omega\varepsilon_j n_j(x) \times (\int_{\Gamma_j} G_j(x,y) M_j(y)\, d\gamma(y)\, d\gamma(x))\\ &\quad - n_j(x) \times (\int_{\Gamma_j} \nabla_x G_j(x,y) \times J_j(y)\, d\gamma(y)\, d\gamma(x)).\end{aligned} \tag{3.6}$$

### 3.3. Derivations of the coupling FEM/BEM formulations

Since the singularity of the kernel $G_j(x,y)$ behaves like $(4\pi|x-y|)^{-1}$, classical results from potential theory [47] yield that each term in (3.5)-(3.6) belongs to $\mathrm{TH}^{-1/2}(\mathrm{curl}, \Gamma_j)$. By the classical duality result: $(\mathrm{TH}^{-1/2}(\mathrm{curl}, \Gamma_j))' = \mathrm{TH}^{-1/2}(\mathrm{div}, \Gamma_j)$, we can make sense of the duality products of (3.5)-(3.6) with test functions in $\mathrm{TH}^{-1/2}(\mathrm{div},\Gamma_j)$. Multiplying both sides of the equation (3.6) by $J_j^t \in \mathrm{TH}^{-1/2}(\mathrm{div},\Gamma_j)$ and integrating it over $\Gamma_j$, we obtain

$$\begin{aligned}\frac{i}{\omega\varepsilon_j}\int_{\Gamma_j}\int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j} J_j \mathrm{div}_{\Gamma_j} J_j^t - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j J_j \,.\, J_j^t - \frac{1}{2}\int_{\Gamma_j} E_i \,.\, J_j^t \\ - \int_{\Gamma_j}\int_{\Gamma_j} \nabla_x G_j \times M_j \,.\, J_j^t = \int_{\Gamma_j} E_j^{in} \,.\, J_j^t, \quad \forall\, J_j^t \in \mathrm{TH}^{-1/2}(\mathrm{div},\Gamma_j). \qquad (3.7)\end{aligned}$$

Using the Hodge decomposition Lemma 3.1, we decompose (3.7) into the following two variational formulations: $\forall\, \varphi_j^t \in \mathrm{H}^{3/2}(\Gamma_j)$ and $\psi_j^t \in \mathrm{H}^{1/2}(\Gamma_j)$,

$$\begin{aligned}\frac{i}{\omega\varepsilon_j}\int_{\Gamma_j}\int_{\Gamma_j} G_j \Delta_{\Gamma_j}\varphi_j \Delta_{\Gamma_j}\varphi_j^t - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j}\varphi_j \,.\, \nabla_{\Gamma_j}\varphi_j^t - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j}\times\psi_j \,.\, \nabla_{\Gamma_j}\varphi_j^t \\ - \int_{\Gamma_j}\int_{\Gamma_j} \nabla_x G_j \times M_j \,.\, \nabla_{\Gamma_j}\varphi_j^t - \frac{1}{2}\int_{\Gamma_j} E_i \,.\, \nabla_{\Gamma_j}\varphi_j^t = \int_{\Gamma_j} E_j^{in} \,.\, \nabla_{\Gamma_j}\varphi_j^t \qquad (3.8)\end{aligned}$$

and

$$\begin{aligned}-i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j}\times\psi_j \,.\, \nabla_{\Gamma_j}\times\psi_j^t - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j}\varphi_j \,.\, \nabla_{\Gamma_j}\times\psi_j^t \\ - \int_{\Gamma_j}\int_{\Gamma_j} \nabla_x G_j \times M_j \,.\, \nabla_{\Gamma_j}\times\psi_j^t - \frac{1}{2}\int_{\Gamma_j} E_i \,.\, \nabla_{\Gamma_j}\times\psi_j^t = \int_{\Gamma_j} E_j^{in} \,.\, \nabla_{\Gamma_j}\times\psi_j^t, \qquad (3.9)\end{aligned}$$

where the unknowns are $\varphi_j \in \mathrm{H}^{3/2}(\Gamma_j)$ and $\psi_j \in \mathrm{H}^{1/2}(\Gamma_j)$. The unknown function

$$J_j = \nabla_{\Gamma_j}\varphi_j + \nabla_{\Gamma_j}\times\psi_j$$

is in $TH^{-1/2}(\mathrm{div},\Gamma_j)$.

In the chiral medium, we solve the following problem for $E_i \in \mathrm{H}(\mathrm{curl},\Omega)$ in a weak sense:

$$\nabla\times d\nabla\times E_i - \omega^2\varepsilon\beta\nabla\times E_i - \omega^2\nabla\times(\varepsilon\beta E_i) - \omega^2\varepsilon E_i = 0 \quad \text{in } \Omega, \qquad (3.10)$$

$$E_i\times n_j = M_j \quad \text{on } \Gamma_j. \qquad (3.11)$$

Multiplying both sides of (3.10) by $E^t \in \mathrm{H}(\mathrm{curl},\Omega)$ and integrating by parts over $\Omega$ yield

$$\begin{aligned}\int_\Omega d\nabla\times E_i \,.\, \nabla\times E^t - \omega^2\int_\Omega \varepsilon E_i \,.\, E^t - \omega^2\int_\Omega \varepsilon\beta E_i \,.\, \nabla\times E^t \\ -\omega^2\int_\Omega \varepsilon\beta\nabla\times E_i \,.\, E^t - i\omega\int_{\Gamma_1} J_1 \,.\, E^t - i\omega\int_{\Gamma_2} J_2 \,.\, E^t = 0, \qquad (3.12)\end{aligned}$$

for any $E^t \in \mathrm{H}(\mathrm{curl},\Omega)$. By the Hodge decomposition Lemma 3.1, we write

$$E_i = u_i + \nabla p_i,$$

where $u_i \in \mathbb{M}(\Omega)$ and $p_i \in \mathrm{H}^1(\Omega)$. Replacing $E_i$ with $u_i + \nabla p_i$ in the variational equation (3.12), we obtain

$$\begin{aligned}\int_\Omega d\nabla\times u_i \,.\, \nabla\times u^t - \omega^2\int_\Omega \varepsilon u_i \,.\, u^t - \omega^2\int_\Omega \varepsilon\beta u_i \,.\, \nabla\times u^t - \omega^2\int_\Omega \varepsilon\beta\nabla p_i \,.\, \nabla\times u^t \\ -\omega^2\int_\Omega \varepsilon\beta\nabla\times u_i \,.\, u^t - i\omega\int_{\Gamma_1} J_1 \,.\, u^t - i\omega\int_{\Gamma_2} J_2 \,.\, u^t = 0, \quad \forall\, u^t \in \mathbb{M}(\Omega), \qquad (3.13)\end{aligned}$$

and

$$\begin{aligned}
&-\omega^2 \int_\Omega \varepsilon \nabla p_i \,.\, \nabla p^t - \omega^2 \int_\Omega \varepsilon\beta \nabla \times u_i \,.\, \nabla p^t \\
&-i\omega \int_{\Gamma_1} J_1 \,.\, \nabla p^t - i\omega \int_{\Gamma_2} J_2 \,.\, \nabla p^t = 0, \quad \forall\, p^t \in \mathrm{H}^1(\Omega). \qquad (3.14)
\end{aligned}$$

From now on, we denote $u_{\Gamma_j} = u_{i,\Gamma_j} = -n_j \times (n_j \times u_i)$ on $\Gamma_j$.

**Theorem 3.1.** *If $E$ and $H$ are solutions of the Maxwell equations* (2.15)-(2.16) *together with the radiation condition* (2.22)*, then $u_i, p_i, J_j, \varphi_j$, and $\psi_j$ defined by $E_i = u_i + \nabla p_i, J_j = H_i \times n_j|_{\Gamma_j} = \nabla_{\Gamma_j}\varphi_j + \nabla_{\Gamma_j} \times \psi_j$ are solutions of the variational formulation* (3.13)-(3.14)-(3.8)-(3.9).

*The converse is also true. If $u_i, p_i, \varphi_j, \psi_j$, and $J_j = \nabla_{\Gamma_j}\varphi_j + \nabla_{\Gamma_j} \times \psi_j$ are solutions of* (3.13)-(3.14)-(3.8)-(3.9) *and satisfy that*

$$\begin{aligned}
\frac{1}{2} J_j = H_j^{in} \times n_j &- (\nabla \times \int_{\Gamma_j} G_j J_j) \times n_j \\
&+ \frac{i}{\omega\mu_j} \nabla_{\Gamma_j} \int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j}((u_{\Gamma_j} + \nabla_{\Gamma_j} p_i) \times n_j) \times n_j \\
&+ i\omega\varepsilon_j \int_{\Gamma_j} G_j((u_{\Gamma_j} + \nabla_{\Gamma_j} p_i) \times n_j) \times n_j, \qquad (3.15)
\end{aligned}$$

*then*

$$E = \begin{cases} E_1 & \text{in } \Omega_1, \\ E_i & \text{in } \Omega_i, \\ E_2 & \text{in } \Omega_2, \end{cases} \qquad H = \begin{cases} H_1 & \text{in } \Omega_1, \\ H_i & \text{in } \Omega_i, \\ H_2 & \text{in } \Omega_2, \end{cases} \qquad (3.16)$$

*where $E_j$ and $H_j$ are determined from the periodic integral representations* (3.2)-(3.3) *and $H_i = -i(\omega\mu)^{-1}\nabla \times u_i$, are solutions of the Maxwell equations* (2.15)-(2.16) *along with the radiation condition* (2.22).

*Proof.* By the Hodge decomposition Lemma 3.1, the periodic integral representations (3.2)-(3.3) and some integrations by parts, we easily establish that if $E$ and $H$ are solutions of the Maxwell equations (2.15)-(2.16) along with the radiation condition (2.22). Thus $u_i, p_i, J_j, \varphi_j$, and $\psi_j$ defined by $E_i = u_i + \nabla p_i, J_j = H_i \times n_j|_{\Gamma_j} = \nabla_{\Gamma_j}\varphi_j + \nabla_{\Gamma_j} \times \psi_j$, are solutions of the variational formulation (3.13)-(3.14)-(3.8)-(3.9).

Now, assume that $u_i, p_i, \varphi_j, \psi_j$, and $J_j = \nabla_{\Gamma_j}\varphi_j + \nabla_{\Gamma_j} \times \psi_j$ are solutions of (3.13)-(3.14)-(3.8)-(3.9) and also satisfy the periodic integral equation (3.15). Adding equations (3.13) and (3.14), we get once again by the Hodge decomposition Lemma 3.1 that

$$\begin{aligned}
&\int_\Omega d\nabla \times E_i \,.\, \nabla \times E^t - \omega^2 \int_\Omega \varepsilon E_i \,.\, E^t - \omega^2 \int_\Omega \varepsilon\beta E_i \,.\, \nabla \times E^t \\
&\quad -\omega^2 \int_\Omega \varepsilon\beta \nabla \times E_i \,.\, E^t - i\omega \int_{\Gamma_1} J_1 \,.\, E^t - i\omega \int_{\Gamma_2} J_2 \,.\, E^t = 0,
\end{aligned}$$

for any $E^t \in \mathrm{H}(\mathrm{curl}, \Omega)$ with $E_i = u_i + \nabla p_i$ in $\Omega$. Consequently,

$$\begin{aligned}
&\nabla \times d\nabla \times E_i - \omega^2 \varepsilon\beta\nabla \times E_i - \omega^2 \nabla \times (\varepsilon\beta E_i) - \omega^2 \varepsilon E_i = 0 \quad \text{in } \Omega, \\
&d\nabla \times E_i \times n_j - \omega^2 \varepsilon\beta E_i \times n_j = i\omega J_j \quad \text{on } \Gamma_j.
\end{aligned}$$

From (3.8)-(3.9), we obtain that the fields $E_1$ and $E_2$ given by the periodic integral representations (3.2), where

$$M_j = (u_i + \nabla p_i) \times n_j \quad \text{on } \Gamma_j,$$

are solutions of the Maxwell equations

$$\nabla \times \nabla \times E_j - \omega^2 \varepsilon_j \mu_j E_j = 0 \quad \text{in } \Omega_j,$$

along with the radiation condition (2.22). In addition, if (3.15) holds, then the fields $E_j$ satisfy

$$(\nabla \times E_j) \times n_j = i\omega\mu_j J_j \quad \text{on } \Gamma_j.$$

But $E_j \times n_j = E_i \times n_j$ on $\Gamma_j$. Thus, from the jump conditions (2.11), it follows that $E$ and $H$ of the form (3.16) with $H_i = -i(\omega\mu)^{-1}\nabla \times u_i$ are solutions of the Maxwell equations (2.15)-(2.16) together with the radiation condition (2.22). The proof is now complete. □

To derive coupling FEM/BEM variational formulations for solving the diffraction problem, we also need the following two lemmas. These lemmas are known in case of a closed boundary $\Gamma$ and the usual Green kernel of the Helmholtz equation in $\mathbb{R}^3$ [7].

**Lemma 3.6.** *If $J_j, u_{\Gamma_j}$, and $p_i$ satisfy the periodic integral equation* (3.15), *then*

$$\begin{aligned}
\frac{1}{2}\int_{\Gamma_j} J_j \,.\, u^t_{\Gamma_j} &= \frac{i}{\omega\mu_j}\int_{\Gamma_j}\int_{\Gamma_j} G_j \,\mathrm{curl}_{\Gamma_j} u_{\Gamma_j}\, \mathrm{curl}_{\Gamma_j} u^t_{\Gamma_j} \\
&- i\omega\varepsilon_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j} \times p_i \,.\, u^t_{\Gamma_j} \times n_j - i\omega\varepsilon_j \int_{\Gamma_j}\int_{\Gamma_j} G_j u_{\Gamma_j} \times n_j \,.\, u^t_{\Gamma_j} \times n_j \\
&- \int_{\Gamma_j}\int_{\Gamma_j} (\partial_{n_j(x)} G_j J_j - \nabla_x G_j (n_j(x) - n_j(y)) \,.\, J_j) \,.\, u^t_{\Gamma_j} \\
&+ \int_{\Gamma_j} (H^{in}_j \times n_j) \,.\, u^t_{\Gamma_j}, \quad \forall\, u^t_{\Gamma_j} \in \mathrm{TH}^{-1/2}(\mathrm{curl}, \Gamma_j), \qquad (3.17)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2}\int_{\Gamma_j} J_j \,.\, \nabla_{\Gamma_j} p^t &= -i\omega\varepsilon_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j} \times p_i \,.\, \nabla_{\Gamma_j} \times p^t \\
&- \int_{\Gamma_j}\int_{\Gamma_j} (\partial_{n_j(x)} G_j J_j - \nabla_x G_j (n_j(x) - n_j(y)) \,.\, J_j) \,.\, \nabla_{\Gamma_j} p^t \\
&- i\omega\varepsilon_j \int_{\Gamma_j}\int_{\Gamma_j} G_j u_{\Gamma_j} \times n_j \,.\, \nabla_{\Gamma_j} \times p^t + \int_{\Gamma_j} (H^{in}_j \times n_j) \,.\, \nabla_{\Gamma_j} p^t, \quad \forall\, p^t \in \mathrm{H}^{1/2}(\Gamma_j). \quad (3.18)
\end{aligned}$$

*Proof.* It suffices to establish (3.17). Multiplying $\nabla_{\Gamma_j} \int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j}(u_{\Gamma_j} \times n_j)$ by $u^t_{\Gamma_j} \times n_j$ for any $u^t_{\Gamma_j} \in \mathrm{TH}^{-1/2}(\mathrm{curl}, \Gamma_j)$ and integrating by parts over $\Gamma_j$ gives

$$\begin{aligned}
&\int_{\Gamma_j} \nabla_{\Gamma_j} \int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j}(u_{\Gamma_j} \times n_j) u^t_{\Gamma_j} \times n_j \\
&= -\int_{\Gamma_j}\int_{\Gamma_j} G_j \mathrm{div}_{\Gamma_j}(u_{\Gamma_j} \times n_j) \mathrm{div}_{\Gamma_j}(u^t_{\Gamma_j} \times n_j) = -\int_{\Gamma_j}\int_{\Gamma_j} G_j \mathrm{curl}_{\Gamma_j} u_{\Gamma_j} \mathrm{curl}_{\Gamma_j} u^t_{\Gamma_j}. \qquad (3.19)
\end{aligned}$$

The formula (3.17) follows from an integration by parts of the periodic integral equation (3.6) along with (3.19). □

We also need the following technical lemma.

**Lemma 3.7.** *For any $\varphi, \psi \in \mathrm{H}^{1/2}(\Gamma_j)$, and $v_{\Gamma_j} \in \mathrm{TH}^{-1/2}(\Gamma_j)$, the following identities hold:*

$$\int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j} \times \varphi \,.\, \nabla_{\Gamma_j}\psi = \int_{\Gamma_j}\int_{\Gamma_j} (n_j(x) - n_j(y)) \times \nabla_y G_j \,.\, \nabla_{\Gamma_j}\psi\ \varphi, \tag{3.20}$$

$$\int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j} \times \varphi \,.\, v_{\Gamma_j} = \int_{\Gamma_j}\int_{\Gamma_j} (n_j(x) - n_j(y)) \times \nabla_y G_j \,.\, v_{\Gamma_j}\ \varphi, \tag{3.21}$$

$$\int_{\Gamma_j}\int_{\Gamma_j} \nabla G_j \,.\, ((\nabla_{\Gamma_j} \times \varphi) \times (\nabla_{\Gamma_j} \times \psi)) = \omega^2 \varepsilon_j \mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j\ \psi\ ((n_j(x) - n_j(y)) \,.\, \nabla_{\Gamma_j}\varphi), \tag{3.22}$$

$$\int_{\Gamma_j}\int_{\Gamma_j} \nabla G_j \,.\, ((v_{\Gamma_j} \times n_j) \times \nabla_{\Gamma_j} \times \psi) = \omega^2 \varepsilon_j \mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j\ \psi\ (n_j(x) - n_j(y)) \,.\, v_{\Gamma_j}. \tag{3.23}$$

We are now ready to state and prove the following theorem.

**Theorem 3.2.** *The variational formulation* (3.13)-(3.14)-(3.8)-(3.9) *together with the periodic integral equations* (3.15) *yield the following coupling FEM/BEM formulations:*

($A$)*: obtained by replacing the terms $\int_{\Gamma_j} J_j \,.\, u^t$ and $\int_{\Gamma_j} J_j \,.\, \nabla p^t$ with their expressions from* (3.17)-(3.18)*;*

($B$)*: obtained by dividing each of the terms $\int_{\Gamma_j} J_j \,.\, u^t$ and $\int_{\Gamma_j} J_j \,.\, \nabla p^t$ into two halves and then replacing $\frac{1}{2}\int_{\Gamma_j} J_j \,.\, u^t$ and $\frac{1}{2}\int_{\Gamma_j} J_j \,.\, \nabla p^t$ with their expressions from* (3.17)-(3.18).

Note that an important advantage of ($B$) is that the coupling formulation is symmetric.

Furthermore, we may derive the third coupling FEM/BEM variational formulation. Similar to (3.12), the following variational formulation may be obtained for the magnetic field $H$:

$$\begin{aligned}\int_\Omega d'\nabla \times H_i \,.\, \nabla \times H^t - \omega^2 \int_\Omega \mu H_i \,.\, H^t - \omega^2 \int_\Omega \mu\beta H_i \,.\, \nabla \times H^t \\ -\omega^2 \int_\Omega \mu\beta \nabla \times H_i \,.\, H^t - i\omega \int_{\Gamma_1} M_1 \,.\, H^t - i\omega \int_{\Gamma_2} M_2 \,.\, H^t = 0,\end{aligned} \tag{3.24}$$

for any $H^t \in \mathrm{H}(\mathrm{curl}, \Omega)$, where

$$d' = \frac{1 - \omega^2\beta^2\varepsilon\mu}{\varepsilon}, \quad H = \begin{cases} H_1 & \text{in } \Omega_1, \\ H_i & \text{in } \Omega_i, \\ H_2 & \text{in } \Omega_2. \end{cases}$$

Represent by the Hodge decomposition Lemma 3.1, $H_i = v_i + \nabla q_i$, where $v_i \in \mathbb{M}(\Omega)$ and $q_i \in \mathrm{H}^1(\Omega)$. It follows from the periodic integral equation (3.5) and the identities (3.17)-(3.18) that

$$\begin{aligned}\frac{1}{2}\int_{\Gamma_j} M_j \,.\, v^t_{\Gamma_j} = {} & \frac{i}{\omega\varepsilon_j}\int_{\Gamma_j}\int_{\Gamma_j} G_j\, \mathrm{curl}_{\Gamma_j} v_{\Gamma_j}\, \mathrm{curl}_{\Gamma_j} v^t_{\Gamma_j} - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j} \times q_i \,.\, v^t_{\Gamma_j} \times n_j \\ & - \int_{\Gamma_j}\int_{\Gamma_j} (\partial_{n_j(x)} G_j M_j - \nabla_x G_j (n_j(x) - n_j(y)) \,.\, M_j) \,.\, u^t_{\Gamma_j} \\ & - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j v_{\Gamma_j} \times n_j \,.\, v^t_{\Gamma_j} \times n_j \\ & + \int_{\Gamma_j} (E^{in}_j \times n_j) \,.\, v^t_{\Gamma_j}, \quad \forall\, v^t_{\Gamma_j} \in \mathrm{TH}^{-1/2}(\mathrm{curl}, \Gamma_j),\end{aligned} \tag{3.25}$$

$$\begin{aligned}\frac{1}{2}\int_{\Gamma_j} M_j\,.\,\nabla_{\Gamma_j} q^t = &-i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j \nabla_{\Gamma_j}\times q_i\,.\,\nabla_{\Gamma_j}\times q^t - i\omega\mu_j \int_{\Gamma_j}\int_{\Gamma_j} G_j v_{\Gamma_j}\times n_j\,.\,\nabla_{\Gamma_j}\times q^t\\ &-\int_{\Gamma_j}\int_{\Gamma_j} (\partial_{n_j(x)} G_j M_j - \nabla_x G_j (n_j(x)-n_j(y))\,.\,M_j)\,.\,\nabla_{\Gamma_j} q^t\\ &+\int_{\Gamma_j} (E_j^{in}\times n_j)\,.\,\nabla_{\Gamma_j} q^t, \quad \forall\, q^t\in \mathrm{H}^{1/2}(\Gamma_j). \end{aligned} \tag{3.26}$$

Therefore, we obtain the third coupling FEM/BEM variational formulation.

**Theorem 3.3.** *The variational formulation* (3.13)-(3.14)-(3.8)-(3.9) *together with the periodic integral equations* (3.15) *yield the following coupling FEM/BEM formulation:*

$(C)$*: obtained by replacing* $H_i$ *by* $v_i+\nabla q_i$ *in* (3.24)*,* $E_i$ *by* $u_i+\nabla p_i$ *in* (3.12)*, and the terms* $\int_{\Gamma_j} J_j\,.\,E^t$ *and* $\int_{\Gamma_j} M_j\,.\,H^t$ *with their expressions from* (3.17)-(3.18) *and* (3.25)-(3.26)*.*

### 3.4. Existence and uniqueness results

In this subsection, we show that the coupling FEM/BEM variational formulations $(A),(B)$, and $(C)$ are of Fredholm type. Hence, for all but possibly a discrete sequence of parameters, there exist unique solutions to $(A),(B)$, and $(C)$. The results also yield a new proof of the uniqueness theorem for the diffraction problem.

**Theorem 3.4.** *Each one of the variational formulations* $(A),(B)$*, and* $(C)$ *is of Fredholm type.*

*Proof.* It is sufficient to prove the theorem for the variational formulation $(B)$. The same arguments will prove the theorem for the other two formulations $(A)$ and $(C)$.

Denote the left hand side terms of $(B)$ by $a_1(u,u^t), a_2(p,p^t), a_3(\varphi_j,\varphi_j^t)$, and $a_4(\psi_j,\psi_j^t)$, respectively. We take $u^t=\overline{u}, p^t=\overline{p}, \varphi^t=\varphi$, and $\psi^t=\overline{\psi}$ and consider the quantity

$$a_1(u,\overline{u}) - a_2(p,\overline{p}) - i\omega a_3(\varphi_j,\overline{\varphi_j}) + i\omega a_4(\psi_j,\overline{\psi_j}).$$

Note that

$$\int_{\Gamma_j} \nabla p\,.\,\nabla_{\Gamma_j}\times\overline{\psi_j} = \int_{\Gamma_j} \nabla_{\Gamma_j}\times\psi_j\,.\,\nabla\overline{p} = 0.$$

Next, Lemma 3.7 (3.20)-(3.21) and the fact that the kernel $(n_j(x)-n_j(y))\times\nabla_x G_j$ is of order one yield

$$\int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\times p\,.\,\overline{u}_{\Gamma_j},\quad \int_{\Gamma_j}\int_{\Gamma_j} G_j u_{\Gamma_j}\times n_j\,.\,\nabla_{\Gamma_j}\overline{p},\quad \int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\times p\,.\,\nabla_{\Gamma_j}\overline{p},$$
$$\int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\times\psi_j\,.\,\nabla_{\Gamma_j}\overline{\varphi_j},\quad \text{and} \int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\varphi_j\,.\,\nabla_{\Gamma_j}\times\overline{\psi_j}$$

are compact. Next, by the Cauchy-Schwartz inequality, for any $\eta$

$$\Big|\int_\Omega \varepsilon\beta(u\,.\,\nabla\times\overline{u} - \nabla\times u\,.\,\overline{u})\Big| \le \eta\|\nabla\times u\|^2_{\mathrm{L}^2(\Omega)^3} + C(\eta)\|u\|^2_{\mathrm{L}^2(\Omega)^3}.$$

Now, we estimate the term $\int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\varphi_j\,.\,\nabla_{\Gamma_j}\overline{\varphi_j}$. According to Lemma 2.4

$$\Big|\int_{\Gamma_j}\int_{\Gamma_j} G_j\nabla_{\Gamma_j}\varphi_j\,.\,\nabla_{\Gamma_j}\overline{\varphi_j}\Big| \le C\|\varphi_j\|^2_{\mathrm{H}^{1/2}(\Gamma_j)}.$$

By the trace regularity result stated in Lemma 3.3, we have

$$\begin{aligned}&\Big|\int_{\Gamma_j}\int_{\Gamma_j} G_j u_{\Gamma_j}\times n_j\,.\,\overline{u}_{\Gamma_j}\times n_j\Big|\\ &\leq C||u_{\Gamma_j}||^2_{\mathrm{TH}^{-1/2}(\Gamma_j)} \leq \eta||\nabla\times u||^2_{\mathrm{L}^2(\Omega)^3} + C(\eta)||u||^2_{\mathrm{L}^2(\Omega)^3},\end{aligned}$$

and

$$\begin{aligned}&\Big|\int_{\Gamma_j} u_{\Gamma_j}\,.\,\nabla\overline{\varphi}_j\Big| \leq ||u_{\Gamma_j}||_{\mathrm{TH}^{-1/2}(\Gamma_j)}||\varphi_j||_{\mathrm{H}^{3/2}(\Gamma_j)},\\ &\leq\Big(\eta||\nabla\times u||_{\mathrm{L}^2(\Omega)^3} + \frac{1}{\eta}||u||_{\mathrm{L}^2(\Omega)^3}\Big)||\varphi_j||_{\mathrm{H}^{3/2}(\Gamma_j)},\\ &\leq \frac{1}{\eta}(\eta||\nabla\times u||_{\mathrm{L}^2(\Omega)^3})^2 + \eta||\varphi_j||^2_{\mathrm{H}^{3/2}(\Gamma_j)} + \frac{1}{\eta}\Big(\frac{1}{\eta}||u||_{\mathrm{L}^2(\Omega)^3}\Big)^2 + \eta||\varphi_j||^2_{\mathrm{H}^{3/2}(\Gamma_j)}\\ &\leq \eta||\nabla\times u||^2_{\mathrm{L}^2(\Omega)^3} + 2\eta||\varphi_j||^2_{\mathrm{H}^{3/2}(\Gamma_j)} + \frac{1}{\eta^3}||u||^2_{\mathrm{L}^2(\Omega)^3}.\end{aligned}$$

Combining the above estimates and observing that

$$\begin{aligned}&\Re e\Big\{\int_\Omega \varepsilon\beta\nabla p\,.\,\nabla\times\overline{u} - \int_\Omega \varepsilon\beta\nabla\times u\,.\,\nabla\overline{p}\Big\} = 0,\\ &\Re e\Big\{i\Big[\int_{\Gamma_j}\nabla_{\Gamma_j}\times\psi_j\,.\,\overline{u} + \int_{\Gamma_j} u_{\Gamma_j}\,.\,\nabla_{\Gamma_j}\times\overline{\psi}_j\Big]\Big\} = 0,\\ &\Re e\Big\{i\Big[\int_{\Gamma_j}\nabla_{\Gamma_j}\varphi_j\,.\,\nabla\overline{p} + \int_{\Gamma_j}\nabla p\,.\,\nabla_{\Gamma_j}\overline{\varphi_j}\Big]\Big\} = 0,\end{aligned}$$

and the fact that the term

$$\frac{1}{\mu_j}\int_{\Gamma_j}\int_{\Gamma_j} G_j|\,\mathrm{curl}_{\Gamma_j} u_{\Gamma_j}|^2$$

has the favorable sign, we obtain from Lemma 2.4 that for any $u \in \mathbb{M}(\Omega), p \in \mathrm{H}^1(\Omega), \varphi_j \in \mathrm{H}^{3/2}(\Gamma_j)$, and $\psi_j \in \mathrm{H}^{1/2}(\Gamma_j)$,

$$\begin{aligned}&\Re e\Big\{a_1(u,\overline{u}) - a_2(p,\overline{p}) + i\omega a_3(\varphi_j,\overline{\varphi_j}) - i\omega a_4(\psi_j,\overline{\psi_j})\Big\}\\ &\geq C_1\Big\{||u||^2_{\mathbb{M}(\Omega)} + ||p||^2_{\mathrm{H}^1(\Omega)} + ||\varphi_j||^2_{\mathrm{H}^{3/2}(\Gamma_j)} + ||\psi_j||^2_{\mathrm{H}^{1/2}(\Gamma_j)}\Big\}\\ &\quad -C_2\Big\{||u||^2_{\mathrm{L}^2(\Omega)^3} + ||p||^2_{\mathrm{L}^2(\Omega)} + ||\varphi_j||^2_{\mathrm{H}^{1/2}(\Gamma_j)} + ||\psi_j||^2_{\mathrm{L}^2(\Gamma_j)}\Big\},\end{aligned}$$

where $C_1$ and $C_2$ are two positive constants.

Since the imbedding from $\mathbb{M}(\Omega)$ to $\mathrm{L}^2(\Omega)^3$ is compact (Lemma 3.2), the Fredholm alternative holds for $(B)$. The proof is now complete. □

## 4. Discrete Problems

This section is devoted to the study of discretization of the coupling FEM/BEM formulations. Our main result is a uniform convergence theorem for the coupling approach.

### 4.1. Convergence analysis

We discretize the coupling FEM/BEM variational formulations by using a family of finite element subspaces $V_h$ in $\mathrm{H}(\mathrm{curl},\Omega)$, where the parameter $h$ is the maximum diameter of the elements for a given finite element mesh. The domain $\Omega$ can be meshed by using curvilinear tetrahedra. Assume that the subspace $V_h$ satisfies the Hodge decomposition given in Lemma 3.1. Then any vector $E_h \in V_h$ can be represented as $E_h = u + \nabla p$, where $u \in \mathbb{M}(\Omega)$ and $p \in \mathrm{H}^1(\Omega)$. We also require that

$$\frac{1}{||E_h||_{\mathrm{H}(\mathrm{curl},\Omega)}} ||R_h u - u||_{\mathrm{L}^2(\Omega)^3} \to 0, \quad h \to 0,$$

where $R_h : \mathrm{H}^2(\Omega)^3 \mapsto V_h$ is an interpolation operator. The family of finite element subspaces used to discretize the vector unknown $u$ is the projection of $V_h$ on $\mathbb{M}(\Omega)$. An example which satisfies the assumptions is the family of Nédélec's finite elements (tetrahedra) in H(curl) [48] . The Nédélec element has the property that $\nabla S_h \subset V_h$, where $S_h$ is the usual $P_1$-Lagrange finite element approximation. Natural approximations for $\varphi_j \in \mathrm{H}^{3/2}(\Gamma_j)$ and $\psi_j \in \mathrm{H}^{1/2}(\Gamma_j)$ are: (i) $P_1$-Lagrange finite element approximation for $\psi$ and then $\nabla_{\Gamma_j} \times \psi_j$ is the space of Raviart-Thomas; and (ii) any $\mathcal{C}^1$ finite element for $\varphi_j$.

Now, let $\mathcal{X}_h \subset \mathcal{X} = \mathbb{M}(\Omega) \times \mathrm{H}^1(\Omega) \times \mathrm{H}^{3/2}(\Gamma_j) \times \mathrm{H}^{1/2}(\Gamma_j)$ be the discretized subspace. By essentially identical arguments as in [7], the Babuska-Brezzi condition may be verified.

**Lemma 4.1.** *There is a positive constant $C$ independent of $h$ such that*

$$\sup_{(u_h^t, p_h^t, \varphi_h^t, \psi_h^t) \in \mathcal{X}_h \setminus \{0\}} \frac{|\mathcal{A}((u_h, p_h, \varphi_h, \psi_h), (u_h^t, p_h^t, \varphi_h^t, \psi_h^t))|}{|||(u_h^t, p_h^t, \varphi_h^t, \psi_h^t)|||}$$
$$\geq C\, |||(u_h, p_h, \varphi_h, \psi_h)|||, \quad \forall\, (u_h, p_h, \varphi_h, \psi_h) \in \mathcal{X}_h.$$

From the above lemma, the convergence result below follows.

**Theorem 4.1.** *There exists $h_0 > 0$, such that, for $0 < h < h_0$, the discrete solution*

$$E_h = u_h + \nabla p_h$$

*is well defined with the following error estimate:*

$$||E_i - E_h||_{\mathrm{H}(\mathrm{curl},\Omega)} \leq C \inf_{\mathbf{F}_h \in \mathcal{X}_h} ||E_i - F_h||_{\mathrm{H}(\mathrm{curl},\Omega)}, \tag{4.1}$$

*where $C$ is a positive constant independent of $h$.*

**Remark 4.1.** Note that in general the estimate (4.1) may not be improved. This is essentially due to the fact that the solution is only in $\mathrm{H}(\mathrm{curl}, \Omega)$ for bounded measurable material parameters $\varepsilon, \mu$ and $\beta$. Better convergence results would be possible with additional smoothness assumptions on the solutions.

### 4.2. Approximation of the periodic integral operators

In practice, one cannot compute the kernels $(G_j)_{j=1,2}$ from the full infinite series expansions (2.23). It is thus necessary to obtain appropriate error estimates when truncations of the series expansions take place. In the following, we show that by extracting the principle singularity $(4\pi|x-y|)^{-1}$ from $G_j(x, y)$, the uniform error estimates remain valid, provided that sufficiently many terms in the expansions of the operators

$$G_j(x, y) - \frac{1}{4\pi|x-y|}$$

are taken. Write

$$G_j(x,y)|_{x_3=y_3} = -\frac{i}{2\Lambda_1\Lambda_2}\sum_{n\in Z^2}\frac{e^{-i\alpha_n\,.\,(x-y)}}{\sqrt{n_1^2+n_2^2}} + \frac{i}{2\Lambda_1\Lambda_2}\sum_{n\in Z^2}\Big(\frac{1}{\beta_j^{(n)}} - \frac{1}{\sqrt{n_1^2+n_2^2}}\Big)e^{-i\alpha_n\,.\,(x-y)}.$$

Then

$$G_j(x,y)|_{x_3=y_3} = \frac{1}{4\pi|x-y|} + R_j(x,y) + K_j(x,y),$$

where

$$R_j(x,y) = -\frac{i}{2\Lambda_1\Lambda_2}\sum_{n\in Z^2}\frac{e^{-i\alpha_n\,.\,(x-y)}}{\sqrt{n_1^2+n_2^2}} - \frac{1}{4\pi|x-y|} = \sum_{n\in Z^2}\gamma_j^{(n)}e^{-i\alpha_n\,.\,(x-y)},$$

$$K_j(x,y) = \frac{i}{2\Lambda_1\Lambda_2}\sum_{n\in Z^2}\Big(\frac{1}{\beta_j^{(n)}} - \frac{1}{\sqrt{n_1^2+n_2^2}}\Big)e^{-i\alpha_n\,.\,(x-y)}.$$

The kernel $R_j(x,y)$ has a singularity like $i\alpha\pi^{-1}\log|x-y|$ as $|x-y|\to 0$ and the kernel $K_j(x,y)$ is continuous as $|x-y|\to 0$.

**Lemma 4.2.** *There exists a positive constant $M_0$, such that for $M > M_0$*

$$\Big|\int_{\Gamma_j}\int_{\Gamma_j}\Big(\sum_{|n_1|\geq M+1,|n_2|\geq M+1}\gamma_j^{(n)}e^{-i\alpha_n\,.\,(x-y)}\Big)\theta(x)\overline{\theta}(y)\;d\gamma(x)\;d\gamma(y)\Big| \leq CM^{-1}||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} \tag{4.2}$$

*for any $\theta\in\mathrm{H}^{-1/2}(\Gamma_j)$, where $C$ is a positive constant independent of $M$.*

We recall that there are two positive constants $C_1$ and $C_2$ with

$$C_1||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)} \leq \Big|\int_{\Gamma_j}\int_{\Gamma_j}\frac{1}{|x-y|}\theta(x)\overline{\theta}(y)\;d\gamma(x)\;d\gamma(y)\Big| \leq C_2||\theta||^2_{\mathrm{H}^{-1/2}(\Gamma_j)}.$$

Let the truncated kernel $G_j^M$ be defined by

$$G_j^M(x,y) = \frac{1}{4\pi|x-y|} + \sum_{|n_1|\leq M,|n_2|\leq M}\gamma_j^{(n)}e^{-i\alpha_n\,.\,(x-y)} + \frac{i}{2\Lambda_1\Lambda_2}\sum_{|n_1|\leq M,|n_2|\leq M}\Big(\frac{1}{\beta_j^{(n)}} - \frac{1}{\sqrt{n_1^2+n_2^2}}\Big)e^{-i\alpha_n\,.\,(x-y)}.$$

By replacing $G_j$ with $G_j^M$ in the coupling FEM/BEM variational formulations $(A), (B)$, and $(C)$, the following error estimate holds.

**Theorem 4.2.** *There exist $h_0$ and $M_0$, such that for $0 < h < h_0$ and $M > M_0$*

$$||E_i - E_h||_{\mathrm{H}(\mathrm{curl},\Omega)} \;\leq\; C\Big\{\inf_{\mathbf{F}_h\in\mathcal{X}_h}||E_i - F_h||_{\mathrm{H}(\mathrm{curl},\Omega)} + M^{-1}||E_i||_{\mathrm{H}(\mathrm{curl},\Omega)}\Big\},$$

*where $C$ is a constant independent of $h$ and $M$.*

**Remark 4.2.** By assuming a complex frequency: $\omega = \omega' + i\omega''$ ($\omega'' > 0$), Morelot [46] proved that the estimate

$$\Big| \sum_{|n_1|\geq M+1, |n_2|\geq M+1} \frac{1}{\beta_j^{(n)}} e^{-i\alpha_n \cdot x} e^{i\beta_j^{(n)}|x_3|} \Big| \leq C \frac{e^{-\omega'' M \min(\Lambda_1, \Lambda_2)}}{\omega''},$$

holds uniformly in compact sets, where the constant $C$ is independent of $M$. Note that Morelot's estimate breaks down when $\omega'' = 0$. We also refer to [46] for a computation of the kernel $G_j$ by using the Ewald transform.

## 5. Concluding Remarks

We have presented and analyzed several coupling FEM/BEM formulations for solving the diffraction from periodic chiral structures. It has been shown that the proposed numerical approximations attain unique solutions with uniform convergence properties. An interesting future project is to decouple the finite element and integral equations solutions by using an iterative procedure. The integral equations could then be solved by a fast algorithm, for example a multipole method, independently of the finite element solutions. The fast algorithm would significantly reduce the CPU time for the integral equation portion of the code.

**Acknowledgments.** The research of G. Bao was supported in part by the NSF grants DMS-0604790, CCF-0514078, EAR-0724527, the ONR grant N000140210365, the National Science Foundation of China grant 10428105.

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