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A FINITE ELEMENT METHOD WITH PERFECTLY MATCHED ABSORBING LAYERS FOR THE WAVE SCATTERING BY A PERIODIC CHIRAL STRUCTURE ^{*1)}

Deyue Zhang

(School of Mathematics, Jilin University, Changchun 130012, China School of Computer Science and Technology, Jilin University, Changchun 130012, China Email: Zhangdeyue@126.com)

Fuming Ma

(School of Mathematics, Jilin University, Changchun 130012, China Email: mfm@mail.jlu.edu.cn)

Abstract

Consider the diffraction of a time-harmonic wave incident upon a periodic chiral structure. The diffraction problem may be simplified to a two-dimensional one. In this paper, the diffraction problem is solved by a finite element method with perfectly matched absorbing layers (PMLs). We use the PML technique to truncate the unbounded domain to a bounded one which attenuates the outgoing waves in the PML region. Our computational experiments indicate that the proposed method is efficient, which is capable of dealing with complicated chiral grating structures.

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1. Introduction

Consider a time-harmonic electromagnetic plane wave incident on a periodic chiral structure which is periodic in x_1 - direction and invariant in x_3 - direction. The medium inside the structure is chiral and separates two homogeneous regions. The scattering problem may be simplified to a two-dimensional one. In this paper, we propose and analyze a finite element method with perfectly matched absorbing layers for the scattering problem.

Recently, there has been a considerable interest in the study of scattering and diffraction by chiral media. In general, the electromagnetic fields inside the chiral medium are governed by Maxwell equations together with the Drude-Born-Fedorov equations in which the electric and magnetic fields are coupled. The chiral media is characterized by the electric permittivity ε , the magnetic permeability μ and the chirality measure β . On the other hand, periodic structures (gratings) have received increasing attentions through the years because of importance applications in integrated optics, optical lenses, et al.

Scattering theory in chiral structures has recently received considerable attention in the applied mathematical community. We refer to Ammari and Bao [1], Ammari and Nédélec [2] for the existence and uniqueness to the scattering problem for bi-periodic chiral media. A good introduction to the electromagnetic diffraction through chiral structures can be found in Lakhtakia [3] and Lakhtakia, Varadan and Varadan [4] (non-periodic chiral structures).

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This work is a continuation of our recent analysis of diffraction problem of Zhang and Ma [5]. In [5], we simplify the diffraction problem into a two-dimensional one and established the well-posedness. We also propose a finite element method and give the numerical analysis for the scattering problem.

The purpose of this paper is to develop efficient numerical methods for solving the scattering problem. In doing so, the main difficulty is to truncate the domain into a bounded computational domain. The finite element method studied in [5] is based on variational formulation on a bounded domain, with periodic condition in the x_1 -direction and the transparent boundary condition on the top and bottom boundaries. The transparent boundary condition is obtained by insisting that the solutions be composed of bounded outgoing plane waves, plus the incident wave in the domain above the structure. The derived transparent boundary condition is represented as a quasi-differential operator and is nonlocal. In practical computations, the infinite series must be truncated. In [6], for the wave scattering by periodic (achiral) structures, Chen and Wu use perfectly matched layer (PML) technique to deal with the difficulty. In this paper, we will develop the PML method to solve the scattering problem for chiral structures.

Under the assumption that the exterior solution is composed of outgoing waves only, the basic idea of the PML technique is to surround the computational domain with a finite thickness layer of a specially designed model medium, which would either slow down or attenuate all the waves that propagate from inside the computational domain. Since the work of Berenger [7], which proposed a PML for use with the time dependent Maxwell equations, various constructions of PML absorbing layers have been proposed and studied in the literature. We refer to Turkel and Yefet [8] for a review on various proposed models, and Lassas and Somersalo [9] for the study of mathematical properties of the PML equations.

The layout of the paper is as follows. In the next section, we state the model problem and a variational formulation. We discuss the energy distribution of diffracted waves in Section 3. In Section 4, we introduce our PML formulation, and establish the existence, uniqueness and convergence of the PML formulation. Finally, in Section 5, we present several numerical examples to illustrate the advantages of our method.

2. The Scattering Problem

Let us consider the propagation of time-harmonic electromagnetic waves. The electromagnetic fields are governed by the time-harmonic (time dependence $e^{-i\omega t}$) Maxwell's equations

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

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

where $\mathbf{E}, \mathbf{H}, \mathbf{D}$ and \mathbf{B} denote the electric field, the magnetic field, the electric and magnetic displacement vectors in \mathbb{R}^3 , respectively. For chiral media, $\mathbf{E}, \mathbf{H}, \mathbf{D}$ and \mathbf{B} satisfy with the Drude-Born-Fedorov constitutive equations:

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

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

where $x = (x_1, x_2, x_3)$, ε is the electric permittivity, μ is the magnetic permeability, and β is the chirality admittance. To put equations (2.1)-(2.4) together, we deduce

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

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

where

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

Throughout, we make the additional assumption that $(k(x)\beta(x))^2 \neq 1, x \in \mathbb{R}^3$.

We assume that the structure is periodic in the x_1 -direction of period Λ and constant in the x_3 -direction. In other words, $\varepsilon(x_1 + n\Lambda, x_2) = \varepsilon(x_1, x_2)$, $\mu(x_1 + n\Lambda, x_2) = \mu(x_1, x_2)$, $\beta(x_1 + n\Lambda, x_2) = \beta(x_1, x_2)$, and the electromagnetic fields E and H depend only on x_1 and x_2 . We also make the general assumptions:

(1) For some fixed positive b and sufficiently small $\delta > 0$,

$$\begin{aligned} \varepsilon(x_1, x_2) &= \varepsilon_1, \ \mu(x_1, x_2) = \mu_1, \ \beta(x_1, x_2) = 0, & \text{for } x_2 \ge b - \delta, \\ \varepsilon(x_1, x_2) &= \varepsilon_2, \ \mu(x_1, x_2) = \mu_2, \ \beta(x_1, x_2) = 0, & \text{for } x_2 \le -b + \delta, \end{aligned}$$

where $\varepsilon_1, \varepsilon_2, \mu_1$ and μ_2 are positive constants;

(2) $\varepsilon(x), \mu(x)$ and $\beta(x)$ are real valued L^{∞} functions, $\varepsilon(x) \ge \varepsilon_0, \mu(x) \ge \mu_0$ and $\beta \ge 0$, where ε_0 and μ_0 are positive constants;

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

Remark 2.1. The third condition is essential. Fortunately it appears to be common in the literature and justifiable since β is generally small. The second assumption is a technical one. For materials that absorb energy, analogous condition can be made properly.

We introduce some useful notations. Let

$$\begin{split} &\Gamma_1 = \{ x \in \mathbb{R}^2 ; 0 < x_1 < \Lambda, \ x_2 = b \}, \quad \Gamma_2 = \{ x \in \mathbb{R}^2 ; 0 < x_1 < \Lambda, \ x_2 = -b \}, \\ &\Omega_1 = \{ x \in \mathbb{R}^2 ; 0 < x_1 < \Lambda, \ x_2 > b \}, \quad \Omega_2 = \{ x \in \mathbb{R}^2 ; 0 < x_1 < \Lambda, \ x_2 < -b \}, \\ &\Omega = \{ x \in \mathbb{R}^2 ; 0 < x_1 < \Lambda, \ -b < x_2 < b \}. \end{split}$$

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

$$H^{1}_{qp}(\Omega) = \{ w \in H^{1}(\Omega) : w(0, x_{2}) = e^{-i\alpha\Lambda}w(\Lambda, x_{2}) \text{ for } -b < x_{2} < b \}.$$

Similarly, we define the space $H_{qp}^{1/2}(\Gamma_j)$. For convenience, we drop the subscript qp. For $f \in H^{1/2}(\Gamma_j)$, define the operator T_j by

$$(T_j f)(x_1) = \sum_{n \in \mathbb{Z}} i \beta_j^n f^n e^{i(\alpha_n + \alpha)x_1}, \quad 0 < x_1 < \Lambda, \ j = 1, 2,$$

where

$$f^{n} = \frac{1}{\Lambda} \int_{0}^{\Lambda} f(x) e^{-i(\alpha_{n} + \alpha)x_{1}} dx_{1}, \quad \beta_{j}^{n} = e^{i\gamma_{j}/2} |\omega^{2}\varepsilon_{j}\mu_{j} - (\alpha_{n} + \alpha)^{2}|^{1/2},$$
$$\gamma_{j} = \arg(\omega^{2}\varepsilon_{j}\mu_{j} - (\alpha_{n} + \alpha)^{2}), \quad 0 \le \gamma_{n} \le 2\pi, \qquad \alpha_{n} = 2n\pi/\Lambda,$$



Fig. 2.1. Geometry of the grating problem.

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

Remark 2.2. In our case, for j = 1, 2, $\text{Im}(\varepsilon_j) = 0$ and $\text{Im}(\mu_j) = 0$, then for $n \in \mathbb{Z}$

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

Thus β_i^n (j = 1, 2) is real for at most finitely many n.

Consider a plane wave $\mathbf{E}_{\mathrm{I}} = \mathbf{s} \, e^{i\mathbf{q}\cdot x}, \mathbf{H}_{\mathrm{I}} = \mathbf{p} \, e^{i\mathbf{q}\cdot x}$ incident on the structure, where

$$\mathbf{q} = (\alpha, -\beta_1, 0) = \omega \sqrt{\varepsilon_1 \mu_1} (\sin \theta, -\cos \theta, 0)$$

is the incident wave vector. The vectors \mathbf{s} and \mathbf{p} satisfy

$$\mathbf{s} = (\mathbf{p} \times \mathbf{q}) / \omega \varepsilon_1, \quad \mathbf{q} \cdot \mathbf{q} = \omega^2 \varepsilon_1 \mu_1, \quad \mathbf{p} \cdot \mathbf{q} = 0.$$

We are interested in quasi-periodic solutions of equations (2.5) and (2.6). We shall insist that the electromagnetic fields **E** and **H** are composed of only bounded outgoing plane waves, plus the incident incoming wave above the structure.

Let $\mathbf{E} = (e_1, e_2, e)^T$, $\mathbf{H} = (h_1, h_2, h)^T$. Then, e_1, e_2, h_1 and h_2 can be expressed in terms of e and h, and two coupled equations for e and h can be achieved. Denoting by ψ the component e or h, it follows from the knowledge of the fundamental solution inside Ω_1 and Ω_2 , ψ can be expressed as a sum of plane waves:

$$\psi \mid_{\Omega_1} = \psi_{\mathbf{I}} + \sum_{n \in \mathbb{Z}} a_1^n e^{i(\alpha_n + \alpha)x_1 + i\beta_1^n x_2}, \qquad \psi \mid_{\Omega_2} = \sum_{n \in \mathbb{Z}} a_2^n e^{i(\alpha_n + \alpha)x_1 - i\beta_2^n x_2}.$$
(2.7)

We also have boundary conditions on Γ_j for e and h. Then, the scattering problem is simplified to a two-dimensional one (see [5]):

$$-\nabla \cdot \left(\frac{1}{\mu}\nabla e\right) + i\omega\nabla \cdot (\beta\nabla h) - \omega^2 \varepsilon \frac{\gamma^2}{k^2} e - i\omega\gamma^2 \beta h = 0, \quad \text{in } \Omega, \tag{2.8}$$

$$-\nabla \cdot \left(\frac{1}{\varepsilon}\nabla h\right) - i\omega\nabla \cdot (\beta\nabla e) - \omega^2 \mu \frac{\gamma^2}{k^2} h + i\omega\gamma^2 \beta e = 0, \quad \text{in } \Omega,$$
(2.9)

$$(T_1 - \frac{\partial}{\partial \nu})e = 2i\beta_1 s_3 e^{i\alpha x_1 - i\beta_1 b}, \quad (T_1 - \frac{\partial}{\partial \nu})h = 2i\beta_1 p_3 e^{i\alpha x_1 - i\beta_1 b}, \quad \text{on } \Gamma_1, \quad (2.10)$$

$$(T_2 - \frac{\partial}{\partial \nu})e = 0, \quad (T_2 - \frac{\partial}{\partial \nu})h = 0, \quad \text{on } \Gamma_2.$$
 (2.11)

Let $u = (e, h)^T$ and $v = (p, q)^T$. Define the following sesquilinear form

$$A(u,v) = \int_{\Omega} \frac{1}{\mu} \nabla e \cdot \nabla \bar{p} \, dx + \int_{\Omega} \frac{1}{\varepsilon} \nabla h \cdot \nabla \bar{q} \, dx - i\omega \int_{\Omega} \beta \nabla h \cdot \nabla \bar{p} \, dx + i\omega \int_{\Omega} \beta \nabla e \cdot \nabla \bar{q} \, dx$$
$$-i\omega \int_{\Omega} \gamma^{2} \beta h \, \bar{p} \, dx + i\omega \int_{\Omega} \gamma^{2} \beta e \, \bar{q} \, dx - \int_{\Omega} \frac{\gamma^{2}}{\mu} e \, \bar{p} \, dx - \int_{\Omega} \frac{\gamma^{2}}{\varepsilon} h \, \bar{q} \, dx$$
$$-\sum_{j=1}^{2} \frac{1}{\mu_{j}} \int_{\Gamma_{j}} T_{j}(e) \, \bar{p} \, dx_{1} - \sum_{j=1}^{2} \frac{1}{\varepsilon_{j}} \int_{\Gamma_{j}} T_{j}(h) \, \bar{q} \, dx_{1}.$$
(2.12)

The weak formulation of the scattering problem then reads as follows: Given incoming plane wave $e_{\rm I} = s_3 e^{i\alpha x_1 - i\beta_1 x_2}$ and $h_{\rm I} = p_3 e^{i\alpha x_1 - i\beta_1 x_2}$, seek $u \in H^1(\Omega) \times H^1(\Omega)$, such that

$$A(u,v) = -\frac{1}{\mu_1} \int_{\Gamma_1} 2i\beta_1 e_{\rm I} \,\bar{p} \,dx_1 - \frac{1}{\varepsilon_1} \int_{\Gamma_1} 2i\beta_1 \,h_{\rm I} \,\bar{q} \,dx_1, \quad \forall v \in H^1(\Omega) \times H^1(\Omega).$$
(2.13)

The following result is concerned with existence and uniqueness of solutions to (2.13). We refer to Zhang and Ma [5] for a proof.

Theorem 2.1. For all but possibly a discrete set of frequencies ω , the variational problem (2.13) admits a unique solution u in $H^1(\Omega) \times H^1(\Omega)$.

3. Energy Distribution

In this section we study the energy distribution for the diffraction problem. The result will be used in Section 5 for verifying the accuracy of our algorithm. In general, the energy is distributed away from the grating structure through the propagating plane waves which consist of propagating reflected modes in Ω_1 and transmitted modes in Ω_2 . It is measured by the coefficients of each term in (2.7).

According to the simple calculation in [10], the coefficients of propagating reflected plane waves are

$$\begin{cases} r_e^n = e^{(n)}(b)e^{-i\beta_1^n b}, & n \neq 0, \ n \in \Lambda_1^+, \\ r_e^0 = e^{(0)}(b)e^{-i\beta_1 b} - s_3 e^{-2i\beta_1 b}, & n = 0, \\ \\ r_h^n = h^{(n)}(b)e^{-i\beta_1^n b}, & n \neq 0, \ n \in \Lambda_1^+, \\ \\ r_h^0 = h^{(0)}(b)e^{-i\beta_1 b} - p_3 e^{-2i\beta_1 b}, & n = 0, \end{cases}$$

where $\Lambda_1^+ = \{n \in \mathbb{Z}; \operatorname{Im}(\beta_1^n) = 0\}$. Hence, the energy of each reflected mode may be defined by

$$\frac{\beta_1^n |r_e^n|^2}{\beta_1}, \qquad \frac{\beta_1^n |r_h^n|^2}{\beta_1} \tag{3.1}$$

and the total energy of all reflected modes is given by

$$e_r = \sum_{n \in \Lambda_1^+} \frac{\beta_1^n |r_e^n|^2}{\beta_1}, \qquad h_r = \sum_{n \in \Lambda_1^+} \frac{\beta_1^n |r_h^n|^2}{\beta_1}$$

Similarly, the coefficients of each propagating transmitted mode are

$$t_e^n = e^{(n)}(-b)e^{-i\beta_2^n b}, \qquad t_h^n = h^{(n)}(-b)e^{-i\beta_2^n b}, \qquad n \in \Lambda_2^+,$$

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where $\Lambda_2^+ = \{n \in \mathbb{Z}; \text{ Im}(\beta_2^n) = 0\}$. The energy of each transmitted mode is defined by

$$\frac{\mu_1 \beta_2^n |t_e^n|^2}{\mu_2 \beta_1}, \qquad \frac{\varepsilon_1 \beta_2^n |t_h^n|^2}{\varepsilon_2 \beta_1} \tag{3.2}$$

and the total energy of all transmitted modes is given by

$$e_t = \sum_{n \in \Lambda_2^+} \frac{\mu_1 \beta_2^n |t_e^n|^2}{\mu_2 \beta_1}, \qquad h_t = \sum_{n \in \Lambda_2^+} \frac{\varepsilon_1 \beta_2^n |t_h^n|^2}{\varepsilon_2 \beta_1}.$$

Remark 3.1. To indicate the physical nature of each propagating mode, we introduce new notations r_e^n, r_h^n, t_e^n and t_h^n for coefficients a_j^n in (2.7).

Remark 3.2. In optics literature, the numbers of (3.1) and (3.2) are called reflected and transmitted efficiencies, respectively. They represent the proportion of energy distributed in each propagating mode. The sum of reflected and transmitted efficiency is referred to as grating efficiency.

The following result states that in the case of no energy absorption the total energy is conserved, *i.e.*, the incident energy is the same as the total energy of the propagating waves.

Theorem 3.1. Assume that $\varepsilon(x)$, ε_1 , ε_2 , $\mu(x)$, μ_1 , μ_2 are real and positive, and $\beta(x) \ge 0$. Then

$$\frac{1}{\mu_1}(e_r + e_t) + \frac{1}{\varepsilon_1}(h_r + h_t) = \frac{1}{\mu_1}|\mathbf{s}_3|^2 + \frac{1}{\varepsilon_1}|\mathbf{p}_3|^2.$$
(3.3)

Proof. By taking p = e, q = h in (2.15), we deduce that

$$\int_{\Omega} \frac{1}{\mu} |\nabla e|^2 dx + \int_{\Omega} \frac{1}{\varepsilon} |\nabla h|^2 dx - \int_{\Omega} \frac{\gamma^2}{\mu} |e|^2 dx - \int_{\Omega} \frac{\gamma^2}{\varepsilon} |h|^2 dx$$
$$+ 2\omega \operatorname{Im} \left(\int_{\Omega} \beta \nabla h \cdot \nabla \bar{e} \, dx \right) + 2\omega \operatorname{Im} \left(\int_{\Omega} \gamma^2 \beta h \, \bar{e} \, dx \right)$$
$$- \sum_{j=1}^2 \frac{1}{\mu_j} \int_{\Gamma_j} T_j(e) \, \bar{e} \, dx_1 - \sum_{j=1}^2 \frac{1}{\varepsilon_j} \int_{\Gamma_j} T_j(h) \, \bar{h} \, dx_1$$
$$= -\frac{1}{\mu_1} \int_{\Gamma_1} 2i\beta_1 \mathrm{s}_3 e^{i\alpha x_1 - i\beta_1 b} \bar{e} \, dx_1 - \frac{1}{\varepsilon_1} \int_{\Gamma_1} 2i\beta_1 \mathrm{p}_3 e^{i\alpha x_1 - i\beta_1 b} \bar{h} \, dx_1.$$
(3.4)

Taking the imaginary part of (3.4), we get

$$\frac{1}{\mu_{1}} \sum_{n \in \Lambda_{1}^{+}} \beta_{1}^{n} |e^{(n)}|^{2} + \frac{1}{\mu_{2}} \sum_{n \in \Lambda_{2}^{+}} \beta_{2}^{n} |e^{(n)}|^{2} + \frac{1}{\varepsilon_{1}} \sum_{n \in \Lambda_{1}^{+}} \beta_{1}^{n} |h^{(n)}|^{2} + \frac{1}{\varepsilon_{2}} \sum_{n \in \Lambda_{2}^{+}} \beta_{2}^{n} |h^{(n)}|^{2} \\
= \operatorname{Im}\left(\frac{1}{\mu_{1}} \int_{\Gamma_{1}} 2i\beta_{1} \mathrm{s}_{3} e^{i\alpha x_{1} - i\beta_{1}b} \bar{e} \, dx_{1} + \frac{1}{\varepsilon_{1}} \int_{\Gamma_{1}} 2i\beta_{1} \mathrm{p}_{3} e^{i\alpha x_{1} - i\beta_{1}b} \bar{h} \, dx_{1}\right).$$
(3.5)

The proof is completed by noticing that

$$\begin{aligned} |r_e^0|^2 &= |e^{(0)}(b)|^2 + |\mathbf{s}_3|^2 - 2\mathrm{Re}\{\mathbf{s}_3 e^{-i\beta_1 b} \bar{e}^{(0)}\},\\ |r_h^0|^2 &= |h^{(0)}(b)|^2 + |\mathbf{p}_3|^2 - 2\mathrm{Re}\{\mathbf{p}_3 e^{-i\beta_1 b} \bar{h}^{(0)}\}. \end{aligned}$$

Remark 3.3. From Maxwell equations, it is easy to see

$$\begin{aligned} &\frac{\mu_1}{\varepsilon_1} |\mathbf{p}_3|^2 + |\mathbf{s}_3|^2 = |\mathbf{s}_1|^2 + |\mathbf{s}_2|^2 + |\mathbf{s}_3|^2 = |\mathbf{s}|^2, \\ &(e_r + e_t) + \frac{\mu_1}{\varepsilon_1} (h_r + h_t) = E_r + E_t, \end{aligned}$$

where E_r and E_t are the energy of reflected and transmitted electric fields, respectively. Thus, the total energy is conserved, i.e.,

$$E_r + E_t = |\mathbf{s}|^2. \tag{3.6}$$

4. PML Formulation

In this section we shall introduce variational formulations for the scattering problem using the PML technique.

We assume that the variational problem (2.13) has a unique solution. Then the general theory in Babuška and Aziz [11, Chap.5] implies that there exists a constant $\lambda > 0$ such that the following inf-sup condition holds:

$$\sup_{\neq v \in H^1(\Omega) \times H^1(\Omega)} \frac{|A(w,v)|}{||v||_1} \ge \lambda ||w||_1, \quad \forall w \in H^1(\Omega) \times H^1(\Omega).$$

$$(4.1)$$

To simply the notation, $|| \cdot ||_l$ will be used for the norm $|| \cdot ||_{H^l \times H^l}$.

Now we turn to the introduction of absorbing PML layers. We surround our computational domain Ω with two PML layers of thickness δ_1 and δ_2 in Ω_1 and Ω_2 , respectively. Let $s(x_2) = s_1(x_2) + is_2(x_2)$ be the model medium property which satisfies

$$s_1, s_2 \in C(\mathbb{R}), \quad s_1 \ge 1, s_2 \ge 0, \quad \text{and } s(x_2) = 1 \text{ for } -b \le x_2 \le b.$$
 (4.2)

Following the general idea in designing PML absorbing layers, we introduce the PML regions

$$\begin{split} \Omega_1^{\text{PML}} &= \{ (x_1, x_2) : 0 < x_1 < \Lambda, \quad b < x_2 < b + \delta_1 \}, \\ \Omega_2^{\text{PML}} &= \{ (x_1, x_2) : 0 < x_1 < \Lambda, \quad -b - \delta_2 < x_2 < -b \}, \end{split}$$

and the PML differential operators

0

$$\mathcal{L}^{1} := \frac{\partial}{\partial x_{1}} \left(\frac{1}{\mu(x)} s(x_{2}) \frac{\partial}{\partial x_{1}} \right) + \frac{\partial}{\partial x_{2}} \left(\frac{1}{\mu(x)} \frac{1}{s(x_{2})} \frac{\partial}{\partial x_{2}} \right) + \omega^{2} \varepsilon(x) \left(\frac{\gamma(x)}{k(x)} \right)^{2} s(x_{2}),$$
$$\mathcal{L}^{2} := \frac{\partial}{\partial x_{1}} \left(\frac{1}{\varepsilon(x)} s(x_{2}) \frac{\partial}{\partial x_{1}} \right) + \frac{\partial}{\partial x_{2}} \left(\frac{1}{\varepsilon(x)} \frac{1}{s(x_{2})} \frac{\partial}{\partial x_{2}} \right) + \omega^{2} \mu(x) \left(\frac{\gamma(x)}{k(x)} \right)^{2} s(x_{2}).$$

The PML equations in the PML region are

$$\mathcal{L}^{1}(\hat{e} - e_{\mathrm{I}}) = 0 \quad \text{in } \Omega_{1}^{\mathrm{PML}}, \qquad \mathcal{L}^{1}\hat{e} = 0 \quad \text{in } \Omega_{2}^{\mathrm{PML}}, \tag{4.3}$$
$$\mathcal{L}^{2}(\hat{h} - h_{\mathrm{I}}) = 0 \quad \text{in } \Omega_{1}^{\mathrm{PML}}, \qquad \mathcal{L}^{2}\hat{h} = 0 \quad \text{in } \Omega_{2}^{\mathrm{PML}}. \tag{4.4}$$

Define the differential operator

$$\mathcal{L} = \left(\begin{array}{cc} \mathcal{L}^1 & L \\ -L & \mathcal{L}^2 \end{array} \right),$$

where

$$L = -i\omega\nabla \cdot (\beta(x)\nabla) + i\omega(\gamma(x))^2\beta(x).$$

Let $D = \{(x_1, x_2) : 0 < x_1 < \Lambda, -b - \delta_2 < x_2 < b + \delta_1\}$. Due to the assumption (4.2), we can now formulate the PML model which we are going to solve in this paper:

$$\mathcal{L}\hat{u} = -g \quad \text{in} \quad D, \tag{4.5}$$

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with the quasi-periodic boundary condition $\hat{u}(0, x_2) = e^{-i\alpha\Lambda}\hat{u}(\Lambda, x_2)$ for $-b - \delta_2 < x_2 < b + \delta_1$, and the Dirichlet condition

$$\begin{split} \hat{u} &= u_{\mathrm{I}} \quad \text{on} \quad \Gamma_{1}^{\mathrm{PML}} = \{ (x_{1}, x_{2}) : 0 < x_{1} < \Lambda, x_{2} = b + \delta_{1} \}, \\ \hat{u} &= 0 \quad \text{on} \quad \Gamma_{2}^{\mathrm{PML}} = \{ (x_{1}, x_{2}) : 0 < x_{1} < \Lambda, x_{2} = -b - \delta_{2} \}. \end{split}$$

Here $\hat{u} = (\hat{e}, \ \hat{h})^T, \ u_{\mathrm{I}} = (e_{\mathrm{I}}, \ h_{\mathrm{I}})^T$, and

$$g = \begin{cases} -\mathcal{L}u_{\mathrm{I}} & \text{in } \Omega_{\mathrm{I}}^{\mathrm{PML}}, \\ 0 & \text{elsewhere.} \end{cases}$$

Define the space

 $H^1_{qp}(D) = \{ w \in H^1(D) : w_\alpha = w e^{-i\alpha x_1} \text{ is periodic in } x_1 \text{ with period } \Lambda \}.$

For convenience, we also drop the subscript qp. Introduce the following sesquilinear form

$$\begin{split} A_{D}(u,v) &= \int_{D} \left(\frac{1}{\mu(x)} s(x_{2}) \frac{\partial e}{\partial x_{1}} \frac{\partial \bar{p}}{\partial x_{1}} + \frac{1}{\mu(x)} \frac{1}{s(x_{2})} \frac{\partial e}{\partial x_{2}} \frac{\partial \bar{p}}{\partial x_{2}} - \frac{\gamma^{2}(x)}{\mu(x)} s(x_{2}) e \bar{p} \right) dx \\ &+ \int_{D} \left(\frac{1}{\varepsilon(x)} s(x_{2}) \frac{\partial h}{\partial x_{1}} \frac{\partial \bar{q}}{\partial x_{1}} + \frac{1}{\varepsilon(x)} \frac{1}{s(x_{2})} \frac{\partial h}{\partial x_{2}} \frac{\partial \bar{q}}{\partial x_{2}} - \frac{\gamma^{2}(x)}{\varepsilon(x)} s(x_{2}) h \bar{q} \right) dx \\ &+ i\omega \int_{D} \beta(x) \nabla e \cdot \nabla \bar{q} \, dx + i\omega \int_{D} \gamma^{2}(x) \beta(x) e \bar{q} \, dx \\ &- i\omega \int_{D} \beta(x) \nabla h \cdot \nabla \bar{p} \, dx - i\omega \int_{D} \gamma^{2}(x) \beta(x) h \, \bar{p} \, dx. \end{split}$$

Define $H_E^1(D) = \{w \in H^1(D), w = 0 \text{ on } \Gamma_1^{\text{PML}} \cup \Gamma_2^{\text{PML}}\}$. Then the weak formulation of the PML model reads as follows: Find $\hat{u} \in H^1(D) \times H^1(D)$ such that $\hat{u} = u_{\text{I}}$ on $\Gamma_1^{\text{PML}}, \hat{u} = 0$ on Γ_2^{PML} , and

$$A_{\scriptscriptstyle D}(\hat{u},v) = \int_D g \,\bar{v} \, dx, \quad \forall \, v \in H^1_E(D) \times H^1_E(D). \tag{4.6}$$

To prove the existence and uniqueness of the above problem and derive an error estimate between \hat{u} and u, we first find an equivalent formulation of (4.6) in the domain Ω . Similar to the arguments in [6], we deduce that

$$\hat{u} = u_{\rm I} + \sum_{n \in \mathbb{Z}} \frac{\zeta_1^n(x_2)}{\zeta_1^n(b)} \hat{u}_{\alpha}^{(n)}(b) e^{i(\alpha_n + \alpha)x_1} \quad \text{in} \quad \Omega_1^{\rm PML},
\hat{u} = \sum_{n \in \mathbb{Z}} \frac{\zeta_2^n(x_2)}{\zeta_2^n(-b)} \hat{u}_{\alpha}^{(n)}(-b) e^{i(\alpha_n + \alpha)x_1} \quad \text{in} \quad \Omega_2^{\rm PML},$$
(4.7)

where

$$\begin{aligned} \zeta_1^n(x_2) &= \exp\{-i\beta_1^n \int_{x_2}^{b+\delta_1} s(\tau)d\tau\} - \exp\{i\beta_1^n \int_{x_2}^{b+\delta_1} s(\tau)d\tau\},\\ \zeta_2^n(x_2) &= \exp\{-i\beta_2^n \int_{-b-\delta_2}^{x_2} s(\tau)d\tau\} - \exp\{i\beta_2^n \int_{-b-\delta_2}^{x_2} s(\tau)d\tau\} \end{aligned}$$

Introduce the following Dirichlet to Neumann operator T_j^{PML} in [6]

$$\left(T_j^{\text{PML}}f\right)(x_1) = \sum_{n \in \mathbb{Z}} i\beta_j^n \coth(-i\beta_j^n \sigma_j) f^n e^{i(\alpha_n + \alpha)x_1},\tag{4.8}$$

where $\operatorname{coth}(\tau) = (e^{\tau} + e^{-\tau})/(e^{\tau} - e^{-\tau})$ and

$$\sigma_1 = \int_b^{b+\delta_1} s(\tau) d\tau, \qquad \sigma_2 = \int_{-b-\delta_2}^{-b} s(\tau) d\tau.$$
(4.9)

Then we know easily from (4.7) that

$$\frac{\partial(\hat{u}-u_{\rm I})}{\partial\nu} - T_1^{\rm PML}(\hat{u}-u_{\rm I}) = 0 \quad \text{on} \quad \Gamma_1, \qquad \frac{\partial\hat{u}}{\partial\nu} - T_2^{\rm PML}\hat{u} = 0 \quad \text{on} \quad \Gamma_2.$$
(4.10)

This motivates us to introduce the sesquilinear form

$$A^{\rm PML}(u,v) = \int_{\Omega} \frac{1}{\mu} \nabla e \cdot \nabla \bar{p} \, dx + \int_{\Omega} \frac{1}{\varepsilon} \nabla h \cdot \nabla \bar{q} \, dx - i\omega \int_{\Omega} \beta \nabla h \cdot \nabla \bar{p} \, dx + i\omega \int_{\Omega} \beta \nabla e \cdot \nabla \bar{q} \, dx - i\omega \int_{\Omega} \gamma^2 \beta h \, \bar{p} \, dx + i\omega \int_{\Omega} \gamma^2 \beta e \, \bar{q} \, dx - \int_{\Omega} \frac{\gamma^2}{\mu} e \, \bar{p} \, dx - \int_{\Omega} \frac{\gamma^2}{\varepsilon} h \, \bar{q} \, dx - \sum_{j=1}^2 \frac{1}{\mu_j} \int_{\Gamma_j} T_j^{\rm PML}(e) \, \bar{p} \, dx_1 - \sum_{j=1}^2 \frac{1}{\varepsilon_j} \int_{\Gamma_j} T_j^{\rm PML}(h) \, \bar{q} \, dx_1,$$
(4.11)

and introduce the following variational problem: Find $\varpi \in H^1(\Omega) \times H^1(\Omega)$ such that

$$A^{\text{PML}}(\varpi, v) = -\frac{1}{\mu_1} \int_{\Gamma_1} i\beta_1 (1 + \coth(-i\beta_1\sigma_1)) e_{\mathrm{I}} \bar{p} \, dx_1 -\frac{1}{\varepsilon_1} \int_{\Gamma_1} i\beta_1 (1 + \coth(-i\beta_1\sigma_1)) h_{\mathrm{I}} \bar{q} \, dx_1, \quad \forall \ v \in H^1(\Omega) \times H^1(\Omega), \quad (4.12)$$

where we have used the fact that

$$\frac{\partial u_{\mathrm{I}}}{\partial \nu} - T_{1}^{\mathrm{PML}} u_{\mathrm{I}} = -i\beta_{1}(1 + \coth(-i\beta_{1}\sigma_{1}))u_{\mathrm{I}} \quad \text{on} \quad \Gamma_{1}.$$

Then we have the following lemma, which establishes the relation of this variational problem to the PML model problem (4.6).

Lemma 4.1. Any solution \hat{u} of the problem (4.6) restricted to Ω is a solution of (4.12). Conversely, any solution ϖ of the problem (4.12) can be uniquely extended to the whole domain D to be a solution of (4.6).

Proof. This proof is standard based on the construction given in (4.7). We omit the details.

Let $\Delta_j^n = |k_j^2 - (\alpha_n + \alpha)^2|^{1/2}$ and $U_j = \{n : k_j^2 > (\alpha_n + \alpha)^2\}, j = 1, 2$. Then we have $\beta_j^n = \Delta_j^n$ for $n \in U_j$, and $\beta_j^n = i\Delta_j^n$ for $n \notin U_j$. Let

$$\Delta_j^- = \min\{\Delta_j^n : n \in U_j\}, \qquad \Delta_j^+ = \min\{\Delta_j^n : n \notin U_j\}.$$
(4.13)

The following lemmas play a key role in the subsequent analysis. We refer to Chen and Wu [6] for the proof.

Lemma 4.2. For any $\varphi, \psi \in H^1(\Omega)$, we have

$$\left| \int_{\Gamma_j} (T_j \varphi - T_j^{\mathrm{PML}} \varphi) \bar{\psi} dx_1 \right| \le M_j \| \varphi \|_{L^2(\Gamma_j)} \| \psi \|_{L^2(\Gamma_j)},$$

where

$$M_j = \max\left(\frac{2\Delta_j^-}{e^{2\sigma_j^I\Delta_j^-} - 1}, \frac{2\Delta_j^+}{e^{2\sigma_j^R\Delta_j^+} - 1}\right)$$

and σ_j^R, σ_j^I are the real and imaginary parts of σ_j defined in (4.9), namely, $\sigma_j = \sigma_j^R + i\sigma_j^I$.

Lemma 4.3. For any $\psi \in H^1(\Omega)$, we have

$$|\psi||_{L^{2}(\Gamma_{j})} \leq ||\psi||_{H^{1/2}(\Gamma_{j})} \leq \hat{C}||\psi||_{H^{1}(\Omega)},$$

with $\hat{C} = \sqrt{1 + (2b)^{-1}}$. Here if $\psi(x_1, \pm b) = \sum_{n \in \mathbb{Z}} \psi_{\alpha}^{(n)}(\pm b) e^{i(\alpha_n + \alpha)x_1}$ on Γ_j , then

$$\|\psi\|_{H^{1/2}(\Gamma_j)} = \left(\Lambda \sum_{n \in \mathbb{Z}} (1 + |\alpha_n + \alpha|^2)^{1/2} |\psi_{\alpha}^{(n)}(\pm b)|^2\right)^{1/2}$$

From the above two lemmas, we can obtain the following theorem.

Theorem 4.1. Let $\lambda > 0$ be the constant in the inf-sup condition (4.1) and

$$(M_1 + M_2)\hat{C}^2/\chi < \lambda,$$

where $\chi = \min_{j=1,2} \{\mu_j, \varepsilon_j\}$. Then the PML variational problem has a unique solution \hat{u} . Moreover, we have the following error estimate:

$$|||u - \hat{u}|||_{\Omega} := \sup_{0 \neq v \in H^{1}(\Omega) \times H^{1}(\Omega)} \frac{|A(u - \hat{u}, v)|}{||v||_{1}}$$

$$\leq (\hat{C}M_{1}/\chi)||\hat{u} - u_{\mathrm{I}}||_{L^{2}(\Gamma_{1}) \times L^{2}(\Gamma_{1})} + (\hat{C}M_{2}/\chi)||\hat{u}||_{L^{2}(\Gamma_{2}) \times L^{2}(\Gamma_{2})}.$$
(4.14)

Proof. By Lemma 4.1 we only need to show that the variational problem (4.12) has a unique solution. The key point is to show the inf-sup condition for the sesquilinear form $A^{^{PML}}$ defined in (4.11). From Lemmas 4.2 and 4.3 and the assumption $(M_1 + M_2)\hat{C}^2/\chi < \lambda$, we have

$$\begin{split} |A^{^{\mathrm{PML}}}(u,v)| &\geq |A(u,v)| - \sum_{j=1}^{2} \left\{ \frac{1}{\mu_{j}} \left| \int_{\Gamma_{j}} (T_{j}e - T_{j}^{^{\mathrm{PML}}}e)\bar{p}dx_{1} \right| + \frac{1}{\varepsilon_{j}} \left| \int_{\Gamma_{j}} (T_{j}h - T_{j}^{^{\mathrm{PML}}}h)\bar{q}dx_{1} \right| \right\} \\ &\geq |A(u,v)| - \sum_{j=1}^{2} \left(\frac{M_{j}}{\mu_{j}} ||e||_{L^{2}(\Gamma_{j})} ||p||_{L^{2}(\Gamma_{j})} + \frac{M_{j}}{\varepsilon_{j}} ||h||_{L^{2}(\Gamma_{j})} ||q||_{L^{2}(\Gamma_{j})} \right) \\ &\geq |A(u,v)| - \frac{\hat{C}^{2}}{\chi} \sum_{j=1}^{2} M_{j} \left(||e||_{H^{1}(\Omega)} ||p||_{H^{1}(\Omega)} + ||h||_{H^{1}(\Omega)} ||q||_{H^{1}(\Omega)} \right) \\ &\geq |A(u,v)| - \frac{\hat{C}^{2}}{\chi} (M_{1} + M_{2}) ||u||_{1} ||v||_{1}, \qquad \forall u, v \in H^{1}(\Omega) \times H^{1}(\Omega). \end{split}$$

By (2.10), (2.11), (4.11), (4.12) and Lemma 4.1, we conclude that for any $v \in H^1(\Omega) \times H^1(\Omega)$

$$A(u - \hat{u}, v) = -\frac{1}{\mu_{1}} \int_{\Gamma_{1}} 2i\beta_{1} e_{\mathrm{I}} \bar{p} \, dx_{1} - \frac{1}{\varepsilon_{1}} \int_{\Gamma_{1}} 2i\beta_{1} h_{\mathrm{I}} \bar{q} \, dx_{1} + \frac{1}{\mu_{1}} \int_{\Gamma_{1}} i\beta_{1} (1 + \coth(-i\beta_{1}\sigma_{1})) e_{\mathrm{I}} \bar{p} \, dx_{1} + \frac{1}{\varepsilon_{1}} \int_{\Gamma_{1}} i\beta_{1} (1 + \coth(-i\beta_{1}\sigma_{1})) h_{\mathrm{I}} \bar{q} dx_{1} + A^{\mathrm{PML}}(\hat{u}, v) - A(\hat{u}, v) = \frac{1}{\mu_{1}} \int_{\Gamma_{1}} (T_{1} - T_{1}^{\mathrm{PML}})(\hat{e} - e_{\mathrm{I}}) \bar{p} \, dx_{1} + \frac{1}{\mu_{2}} \int_{\Gamma_{2}} (T_{2} - T_{2}^{\mathrm{PML}}) \hat{e} \bar{p} \, dx_{1} + \frac{1}{\varepsilon_{1}} \int_{\Gamma_{1}} (T_{1} - T_{1}^{\mathrm{PML}})(\hat{h} - h_{\mathrm{I}}) \bar{q} \, dx_{1} + \frac{1}{\varepsilon_{2}} \int_{\Gamma_{2}} (T_{2} - T_{2}^{\mathrm{PML}}) \hat{h} \bar{q} \, dx_{1}.$$
(4.15)

This completes the proof of the theorem upon using Lemmas 4.2 and 4.3.

From the classical FEM theory, it is readily to achieve the convergence for the finite element approximation of the PML problems (4.6). We omit the details here.



Fig. 5.1. The real part of electric field $\operatorname{Re}(e)$ and magnetic field $\operatorname{Re}(h)$ for Example 1.

Table 5.1: The comparison between numerical and exact solutions for Example 1. N_k is the number of nodal points. $e_k = ||e - \hat{e}_h||_{H^1(\Omega)}, h_k = ||h - \hat{h}_h||_{H^1(\Omega)}, \varepsilon_k = ||(e, h) - (\hat{e}_h, \hat{h}_h)||_1, \varepsilon_{r,k}$ is relative estimate.

k	N_k	e_k	h_k	ε_k	$\varepsilon_{r,k}$
0	28	2.5738	2.2288	3.4047	0.7251
1	93	0.7846	0.6333	1.0082	0.2181
2	337	0.3120	0.1706	0.3556	0.0769
3	1281	0.1392	0.0779	0.1595	0.0345
4	4993	0.0684	0.0382	0.0783	0.0169
5	19713	0.0341	0.0190	0.0390	0.0084

5. Implementation and Numerical Examples

The implementation of the algorithm in this section is based on the PDE toolbox of MAT-LAB. We use the a posteriori error estimate from Theorem 4.1 to determine the PML parameters. We choose the PML medium property as the power function (see [6]), and we need to specify only the thickness δ_j of the layers and the medium parameters σ_j . In our implementation we choose δ_j and σ_j such that $M_j \Lambda^{1/2} \leq 10^{-8}$, which makes the PML error negligible compared with the finite element discretization errors. We use uniform mesh and linear element in the Finite Element Method.

In this following, we present computational results for a set of test problems. In general, we assume the medium is non-magnetic, i.e., $\mu = 1$.

Example 1. We consider the simplest periodic chiral structure, a homogeneous chiral slab. Assume that plane waves

$$e_{\mathbf{I}} = e^{ik_1(x_1\sin\theta - x_2\cos\theta)}, \quad h_{\mathbf{I}} = \frac{1}{2}e^{ik_1(x_1\sin\theta - x_2\cos\theta)}$$

are incident on the slab ($x_2 = 0$ and $x_2 = d$), which separates two homogeneous media whose dielectric coefficients are ε_1 and ε_2 , respectively. In this situation, exact solutions are available (see [12]), which allow us to test the accuracy of the numerical algorithm.

In our experiment, the parameters are chosen as $\beta = 0.2$, $\varepsilon = 1/2$, $\varepsilon_1 = \varepsilon_2 = 1$, $\omega = 2$, d = -1/2, $\theta = \pi/6$ and $\delta = 1$. Table 5.1 compares the numerical solutions and exact solutions, and indicates that $||u - \hat{u}_h||_1 \approx CN_k^{-1/2}$. Fig. 5.1 shows the graphs of the real part of the electric field e and magnetic field h.



Fig. 5.2. Geometry of the domain in Example 2.



Fig. 5.3. Grating efficiency of Example 2.

Example 2. We consider the chiral grating with period $\Lambda = 2$ whose surface has corners, as shown in Fig. 5.2. Assume that plane waves

$$e_{\mathbf{I}} = e^{ik_1(x_1\sin\theta - x_2\cos\theta)}, \quad h_{\mathbf{I}} = 0$$

are incident at $\theta = \pi/4$ on the structure.

The parameters are chosen as $\varepsilon = 2.25$, $\varepsilon_1 = \varepsilon_2 = 1$, $\omega = \pi$, $\beta = 0.1$. The thickness of the PML layers $\delta = 1$. The grating efficiency of the reflected and transmitted waves as well as the total grating efficiency are displayed in Fig. 5.3. It is evident from the figure that the total energy is conserved. Figs. 5.4-5.6 show the real part, the imaginary part and amplitude of the electric field and magnetic field. Comparison with the achiral grating problem in which h = 0, it is clear from the Figures that the magnetic field is no longer trivial. This is so-called 'Optical Activity'.

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Fig. 5.4. The real part of electric field $\operatorname{Re}(e)$ and magnetic field $\operatorname{Re}(h)$ for Example 2.



Fig. 5.5. The imaginary part of electric field Im(e) and magnetic field Im(h) for Example 2.



Fig. 5.6. The amplitude of electric field |e| and magnetic field |h| for Example 2.

Example 3. Finally, we consider a chiral grating with two sharp angles indicated in Fig. 5.7. The parameters are taken as follows: $\beta_1 = 0.2$, $\beta_2 = 0.1$, $\varepsilon_1 = 2.56$, $\varepsilon_2 = 4.84$, $\varepsilon_0 = \varepsilon_3 = 1$, $\omega = 2.5$, and $\Lambda = 1$. The incident plane waves are

$$e_{\rm I} = (4/5)e^{ik_1(x_1\sin\theta - x_2\cos\theta)}, \quad h_{\rm I} = (3/5)e^{ik_1(x_1\sin\theta - x_2\cos\theta)}$$

with $\theta = \pi/6$. We take $\delta = \Lambda = 1$. The grating efficiency of the reflected and transmitted waves as well as the total grating efficiency are displayed in Fig. 5.8. The amplitudes of the electric field and magnetic field are illustrated in Fig. 5.9.



Fig. 5.7. Geometry of the domain in Example 3.



Fig. 5.8. Grating efficiency of Example 3.



Fig. 5.9. The amplitude of electric field |e| and magnetic field |h| for Example 3.

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