### Numerical solution for non-periodic scattering problems in the 3D periodic structure

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# Abstract

This paper is devoted to solving non-periodic acoustic scattering problems from periodic structure in three-dimensional (3D) space. These problems, which have a substantial role in mathematical physics, are modeled by the Helmholtz equation on an unbounded domain. The main step is to use the Floquet-Bloch transform, which has been known as a powerful tool for 2D scattering problems. However, the straightforward extension of the method used in the 2D problems is not suitable for the 3D case because singularities of the Bloch transformed field are no longer in a finite number of points; in fact, they lie on the union of circles. Then, a new highorder numerical method needs to be proposed for the 3D problem. Hence, we apply a highorder method based on a nonuniform mesh by generating the fine mesh near the singular circles. Eventually, the exponential convergence of the proposed method is proved.

**Keywords:** Non-periodic scattering problems, 3D periodic surface, Floquet-Bloch transform, finite element method.

## 1 Introduction

In this article, we propose a high-order method for solving non-periodic scattering problems with an unbounded periodic structure. The classical methods used for quasi-periodic scattering problems no longer work for non-periodic problems. Then, it is necessary to find a way out of the mentioned difficulty. In this case, the Floquet-Bloch transform can establish a link between a non-periodic problem in an unbounded domain and a family of quasi-periodic problems in a bounded domain. In [1], the Floquet-Bloch transform has been applied for this kind of problem, but the reported convergence rate is low.

Assume that  $\Gamma$  is a  $\Lambda$ -periodic Lipschitz surface lying in the 3D space and  $\Omega$  is the unbounded domain above  $\Gamma$ . Moreover, let  $\Gamma_{\rm H}$  be a flat surface parallel to  $\Gamma$ , i.e.,  $\Gamma_{\rm H} = \mathbb{R}^2 \times \{{\rm H}\}$ and  $\Omega_{\rm H}$  denotes the domain between  $\Gamma$  and  $\Gamma_{\rm H}$ as depicted in Fig. 1.

The main objective of this paper is to find



Figure 1: Illustration of domain (left image) and periodic structure (right image)

the total field  $\boldsymbol{u}$  that satisfies the following Helmholtz problem

$$\Delta u + k^2 u = 0, \quad \text{in } \Omega \subset \mathbb{R}^3, \tag{1}$$

$$u = 0$$
 on  $\Gamma$ . (2)

For a non-periodic incident field  $u^i$ , the total field is related to the scattered field  $u^s$  as  $u := u^i + u^s$ . The upward propagating radiation condition of  $u^s$  yields another boundary condition

$$\frac{\partial u}{\partial x_3} - T^+ u = \frac{\partial u^i}{\partial x_3} - T^+ u^i, \quad \text{on } \Gamma_{\rm H}, \quad (3)$$

in which the Dirichlet-to-Neumann (DtN) map  $T^+$  introduced in [1]. In [3], it has been indicated that the DtN map is continuous from  $H_r^{\frac{1}{2}}(\Gamma_{\rm H})$  into  $H_r^{-\frac{1}{2}}(\Gamma_{\rm H})$  for |r| < 1.

#### 2 Floquet-Bloch transform

The Floquet-Bloch transform is a generalization of Fourier transform, which is defined as follows

$$v = (\mathcal{J}_{\Omega} u)(oldsymbol{lpha}, oldsymbol{x}) := rac{|\det \Lambda|^{1/2}}{2\pi} \sum_{oldsymbol{j} \in \mathbb{Z}^2} u(oldsymbol{ ilde{x}} + \Lambda oldsymbol{j}, x_3) e^{-ioldsymbol{lpha} \cdot \Lambda oldsymbol{j}},$$

where  $\boldsymbol{x} = (\tilde{\boldsymbol{x}}, x_3) \in \Omega_H^{\Lambda}$  ( $\Omega_H^{\Lambda}$  has been illustrated in Fig. 1) and  $\boldsymbol{\alpha} \in W^* := [0, 1]^2$ . It is straightforward to check that the Floquet-Bloch transform of u is  $\boldsymbol{\alpha}$ -quasi-periodic in  $\boldsymbol{x}$  and 1-periodic in  $\boldsymbol{\alpha}$ .

Taking the Floquet-Bloch transform from Eqs. (1)-(3) and using the periodized versions of transformed field v and  $\mathcal{J}_{\Omega}u^{i}$ , i.e.,

$$v_{\boldsymbol{\alpha}} := e^{-i\boldsymbol{\alpha}\cdot\tilde{\boldsymbol{x}}}v(\boldsymbol{\alpha}, \boldsymbol{x}), \quad \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) := e^{-i\boldsymbol{\alpha}\cdot\tilde{\boldsymbol{x}}}\mathcal{J}_{\Omega}u^{i}(\boldsymbol{\alpha}, \boldsymbol{x})$$

indicate that  $v_{\pmb{\alpha}}$  satisfies in the following variational problem

$$a_{\alpha}(v_{\alpha},\varphi) = \int_{\Gamma_{\mathrm{H}}^{\Lambda}} \mathcal{F}(\alpha,\cdot) \ \overline{\varphi} \,\mathrm{d}S, \ \forall \varphi \in V_{per}, \ (4)$$



Figure 2: Singular circles for different k

where

$$\begin{aligned} a_{\alpha}(v_{\alpha},\varphi) &:= \int_{\Omega_{\mathrm{H}}^{\Lambda}} [\nabla v_{\alpha} \cdot \nabla \overline{\varphi} - 2i\alpha \cdot \widetilde{\nabla} v_{\alpha} \overline{\varphi} \\ -(k^{2} - |\alpha|^{2}) v_{\alpha} \overline{\varphi}] \,\mathrm{d}x - \int_{\Gamma_{\mathrm{H}}^{\Lambda}} T_{\alpha}^{+}(v_{\alpha}) \overline{\varphi} \,\mathrm{d}S, \\ \mathcal{F}(\alpha, \cdot) &:= \frac{\partial \psi_{\alpha}}{\partial x_{3}} - T_{\alpha}^{+}(\psi_{\alpha}), \end{aligned}$$

in which  $\widetilde{\nabla} v_{\alpha} = (\partial v_{\alpha} / \partial x_1, \partial v_{\alpha} / \partial x_2)^{\top}$  and the DtN map  $T_{\alpha}^+$  is defined by

$$T^{+}_{\boldsymbol{\alpha}}(\phi) = i \sum_{\boldsymbol{j} \in \mathbb{Z}^2} \sqrt{k^2 - |\boldsymbol{j} - \boldsymbol{\alpha}|^2} \ \widehat{\phi}_{\boldsymbol{j}} \ e^{i(\boldsymbol{j} \cdot \boldsymbol{\tilde{x}})}, \quad (5)$$

where  $\widehat{\phi}$  denotes the Fourier coefficient of  $\phi$ .

To obtain numerical solution, we applied the finite element method for variational formulation (4) for any fixed  $\boldsymbol{\alpha}$  since this method is known as a robust method for simulating wave propagation modeling. Then, tetrahedral elements are used to generate a mesh for  $\Omega_H^{\Lambda}$ . Afterward, the transformed field  $v_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}, \cdot)$  is approximated by the piecewise linear basic functions on considered domain.

# 3 Singularity of $v_{\alpha}$ with respect to $\alpha$

Because of the square root singularities of the DtN map in Eq. (5), it turns out the transformed field  $v_{\alpha}(\alpha, \cdot)$  depends analytically on  $\alpha$  except for a finite number of circles with the centers  $j \in \mathbb{Z}^2$  and radius k. Notice that when the wave number k gets larger, the geometry of singular circles becomes more complicated, as shown in Fig. 2. Now, we need to consider the following decomposition

$$v_{\alpha}(\alpha, \cdot) = w(\alpha, \cdot) + \sum_{j \in \mathbf{J}} \sqrt{k^2 - |j - \alpha|^2} w_j(\alpha, \cdot),$$

where  $\mathbf{J} := \{j \in \mathbb{Z}^2 : \exists \boldsymbol{\alpha} \in [0,1]^2, s.t., |\boldsymbol{j} - \boldsymbol{\alpha}| = k\}$  is a finite set, and  $w_j(\boldsymbol{\alpha}, \cdot)$  and  $w(\boldsymbol{\alpha}, \cdot)$  depend analytically on  $\boldsymbol{\alpha}$ .



Figure 3: Nonuniform mesh for different k

## 4 High-order numerical method

The next step is to evaluate the original total field u by the inverse Bloch transform as follows:

$$u = \mathcal{J}^{-1}v = \frac{|\det \Lambda|^{1/2}}{2\pi} \int_0^1 \int_0^1 v(\boldsymbol{\alpha}, \boldsymbol{x}) e^{i\boldsymbol{\alpha}.\Lambda \boldsymbol{j}} \, \mathrm{d}\boldsymbol{\alpha}, \ \boldsymbol{x} \in \Omega_H^{\Lambda}$$

In comparison with the 2D case in [2] where singularities only lie on at most three points in a bounded interval, the 3D case is much more difficult. Our idea for computing the above double integral is based on the nonuniform mesh so that we generate fine mesh in the neighborhood of the singular circles (see Fig. 3). On the coarse elements, the Gaussian quadrature rule is applied. Moreover, we use the midpoint rule on fine elements near singularities.

**Theorem 1** Suppose that  $u_{N,M,\varepsilon}$  is the numerical solution of the mentioned problem which is obtained by the finite element method with mesh size  $\varepsilon$ . Then, the error between  $u_{N,M,\varepsilon}$  and the exact solution u is bounded by

$$||u_{N,M,\varepsilon} - u||_{L^2(\Omega)} \le \widetilde{C} \left[\varepsilon^2 + \delta^{-C_1M} + 2^{-C_2N}\right],$$

where N is the number of divisions for nonuniform mesh in  $\alpha$  space, M denotes order of Gaussian quadrature rule and  $\delta > 1$ .

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