Near-field imaging of locally perturbed periodic surfaces

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Abstract

This paper concerns the inverse scattering problem to reconstruct a locally perturbed periodic surface. Different from scattering problems with quasi-periodic incident fields and periodic surfaces, the scattered fields are no longer quasi-periodic. Thus the classical method for quasi-periodic scattering problems no longer works. The method based on the Floquet–Bloch transform provides an efficient numerical algorithm to solve the direct scattering problem, and a possibility to reconstruct both the unknown periodic part and the unknown local perturbation from the near-field data.

By transforming the original scattering problem into one defined in an infinite rectangle, the information of the surface is included in the coefficients. The numerical scheme contains two steps. The first step is to obtain an initial guess from a sampling method. The second step is to reconstruct the surface. As is proved in the paper, for some incident fields, the corresponding scattered fields carry little information of the perturbation. In this case, we use these scattered fields to reconstruct the periodic surface. Then we could apply the data that carries more information of the perturbation to reconstruct the local perturbation. The Newton-CG method is applied to solve the associated optimization problems. Numerical examples are given at the end of this paper to show the efficiency of our numerical method.

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(Some figures may appear in colour only in the online journal)

1. Introduction

In this paper, we introduce a numerical method for the inverse scattering problem from a locally perturbed periodic surface. Both the periodic part and the local perturbation of the surface are unknown. The aim is to reconstruct both of them from the near-field measurement data.

Since the periodic surface is perturbed, the classical framework for the quasi-periodic scattering problems (i.e. quasi-periodic incident fields with periodic domains) no longer works. An efficient way to solve these problems is the Floquet–Bloch transform. With the help of this Fourier-like transform, the original problem, which is defined in a 2D unbounded domain, can be written into a new one defined in a 3D bounded domain. This method has been applied to perturbed periodic structures in [3] and waveguide problems in [7]. For scattering problems with non-periodic incident fields and periodic surfaces, we refer to [11, 12, 14]. For problems with locally perturbed periodic surfaces, see [10, 13]. In the paper [17], a high order numerical method has been proposed based on the Floquet–Bloch transform and this method is used in this paper to produce the measured data.

The work in this paper is an extension of joint work of the second author with Prof Armin Lechleiter in [15]. In that paper, the periodic surface is assumed to be known. A numerical method has been proposed to discover both the location and the shape of a local perturbation. The sampling method introduced by Ito et al (see [8]) was extended to find out the location, and a Newton-CG method was applied to reconstruct the shape. However, the setting in this paper is more difficult, i.e. the periodic surface is no longer known. Thus we have to find the perturbation on an unknown periodic surface, and also reconstruct both the periodic surface and the perturbation. In this case, the sampling method in [15] does not work any more, which makes the problem much more challenging.

In this paper, we develop a numerical method for the inverse problem. The first task is to find out the location of both the periodic surface and the perturbation. Since the previous sampling method does not work, we apply the algorithm introduced in [16], which is a fast imaging method to reconstruct rough surfaces. The algorithm provides a rough guess of the locally perturbed surface, thus we could estimate the vertical location of the whole surface, and also figure out the location of the perturbation from a relatively large domain. Then we apply the Newton’s method to reconstruct the shapes of both the periodic surface and the local perturbation. The reconstruction contains two steps. The first step is to reconstruct the periodic surface. It is proved that for certain incident fields, the measured data does contain very little information of the local perturbation. Thus in this case, the measured scattered field could be adopted to reconstruct the periodic surface. Based on the former approximation of the periodic surface, we apply the method in [15] to recover the local perturbation.

The rest of this paper is organized as follows. In section 2, we recall the mathematical model of the direct scattering problem and the Floquet–Bloch transform based formulation. In section 3, the estimation is considered for the difference between the scattered fields with and without perturbation. The inverse problem is formulated in section 4, and the Fréchet derivative and its adjoint operator are studied. In section 5, we conclude the algorithm for inverse problems, including the sampling method for the initial guess and the iterative method for the further reconstruction. In section 6, we present three numerical results obtained from our algorithm.
2. Direct scattering problem

2.1. Mathematical model

Given a bounded $2\pi$-periodic function $\zeta$, it defines a periodic surface

$$\Gamma := \{(x_1, \zeta(x_1)) : x_1 \in \mathbb{R}\}.$$  

Let the function $p$ be a compactly supported perturbation. For simplicity, suppose $\text{supp}(p) \subset (-\pi, \pi) + 2\pi J$, where $J \in \mathbb{Z}$ is an integer. Let $\zeta_p := \zeta + p$ be the perturbed function and define

$$\Gamma_p := \{(x_1, \zeta_p(x_1)) : x_1 \in \mathbb{R}\}.$$  

The domain above $\Gamma$ and above $\Gamma_p$ are set to be $\Omega$ and $\Omega_p$, respectively.

**Remark 1.** For simplicity, all the theoretical arguments in sections 2–4 are proved in the case that $J = 0$. These results can be easily extended to any $J \in \mathbb{Z}$ with the translation $x \mapsto x - 2\pi J$.

In this paper, we assume that the surface $\Gamma_p$ is sound-soft. Given an incident field $u'$ that satisfies $\Delta u' + k^2 u' = 0$ in $\mathbb{R}^2$, it propagates onto $\Gamma_p$ and then generates the scattered field $u'$ (or equivalently, the total field $u = u' + u$). For the mathematical model we refer to figure 1.

First, $u$ satisfies

$$\Delta u + k^2 u = 0 \quad \text{in} \quad \Omega_p.$$  

(1)

Second, as the surface $\Gamma_p$ is sound-soft,

$$u = 0 \quad \text{on} \quad \Gamma_p.$$  

(2)

Moreover, the scattered field $u'$ is propagating upwards. The upward propagation radiation condition (UPRC) is typically written as a double layer potential, see [5], and an alternative definition was introduced in [2, 1]. Let $H$ be a real number that is larger than $\|\zeta\|_{\infty}$ and $\|\zeta_p\|_{\infty}$, then the UPRC is written as

$$u'(x_1, x_2) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\xi x_1 + k\xi x_2} \widehat{u'}(\xi, H) d\xi, \quad x_2 \geq H,$$

where $\widehat{u'}(\xi, H)$ is the Fourier transform of $u'(x_1, H)$. Define the Dirichlet-to-Neumann map $T^+$ by

$$(T^+ \varphi)(x_1) = \frac{i}{2\pi} \int_{\mathbb{R}} \sqrt{k^2 - \xi^2} \ e^{i\xi x_1} \hat{\varphi}(\xi) d\xi, \quad \varphi = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\xi x_1} \hat{\varphi}(\xi) d\xi.$$  

Let $\Gamma_H := \{(x_1, H) : x_1 \in \mathbb{R}\}$, then the UPRC is equivalent to

$$\frac{\partial u}{\partial x_2}(x_1, H) = T^+ \left[u|_{\Gamma_H}\right] + f \quad \text{on} \quad \Gamma_H, \quad \text{where} \quad f = \frac{\partial u'}{\partial x_2}(x_1, H) - T^+ \left[u'|_{\Gamma_H}\right].$$  

(3)

Define the domain $\Omega_H^p := \mathbb{R} \times (-\infty, H) \cap \Omega_p$ and we consider the problem (1)–(3) in a weighted Sobolev space $H^1_\ell(\Omega_H^p)$, where the space $H^1_\ell(\Omega_H^p)$ is defined by

$$H^1_\ell(\Omega_H^p) := \left\{ \varphi \in \mathcal{D}'(\Omega_H^p) : (1 + |x|^2)^{\ell/2} \varphi \in H^1(\Omega_H^p) \right\}.$$  

(4)

$\tilde{H}^1_\ell(\Omega_H^p)$ is the subspace of $H^1_\ell(\Omega_H^p)$ such that all the elements vanish on $\Gamma_p$. Similarly, we can define the weighted spaces $H^{1/2}_{\ell/2}(\Gamma_H)$ and $H^{-1/2}_{\ell/2}(\Gamma_H)$. From [1], the operator $T^+$ is bounded and continuous from $H^{1/2}_{\ell/2}(\Gamma_H)$ to $H^{-1/2}_{\ell/2}(\Gamma_H)$ for all $|\ell| < 1$. 

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The weak formulation of the scattering problem (1)–(3) is to find $u \in \tilde{H}^1_r(\Omega_p^H)$ such that
\[
\int_{\Omega_p^H} \left[ \nabla u \cdot \nabla \overline{v} - k^2 u \overline{v} \right] \, dx - \int_{\Gamma_p^H} T^+ \left( u|_{\Gamma_p^H} \right) \overline{v} \, ds = \int_{\Gamma_p^H} f \overline{v} \, ds
\]
for all $v \in \tilde{H}^1_r(\Omega_p^H)$ with compact support in $\Omega_p^H$. The unique solvability of the variational problem (5) has been proved in [1].

**Theorem 2.** Given an incident field $u'$ such that $f \in H^{-1/2}_r(\Gamma_H)$ with $|r| < 1$, then the variational problem (5) has a unique solution $u \in \tilde{H}^1_r(\Omega_H^p)$.

**Remark 3.** Although the unique solvability is proved for bounded surfaces, in this paper, the functions $\zeta$ and $\zeta_p$ are assumed to be at least Lipschitz continuous.

### 2.2. Floquet–Bloch transform

During the numerical process of the inverse problem, a Floquet–Bloch transform based numerical method is applied to solve the direct scattering problem. Thus in this section, we give a brief introduction to this method. Let $h$ and $H$ be two real numbers such that $h < \min \{ \zeta, \zeta_p \} < \max \{ \zeta, \zeta_p \} < H$ and define $D := \mathbb{R} \times (h, H)$. Define the periodic cell $W$ and its dual-cell $W^*$ by
\[
W = (-\pi, \pi], \quad W^* = (-1/2, 1/2].
\]
Then let $D^{2\pi} = D \cap W \times \mathbb{R}$, $\Gamma^{2\pi}_h = W \times \{h\}$ and $\Gamma^{2\pi}_H = W \times \{H\}$. Define the Bloch transform with period $2\pi$ in $D$ by
\[
J_D \varphi(\alpha, x) = \sum_{j \in \mathbb{Z}} \varphi \left( x + \begin{pmatrix} 2\pi j \\ 0 \end{pmatrix} \right) e^{2\pi i j \alpha}.
\]
The function space $H^r_0(W^*; H^s_0(D^{2\pi}))$ is the closure of $C^\infty_0(W^* \times D^{2\pi})$ with the following norm for $r \in \mathbb{N}$:
\[
\| \varphi \|_{H^r_0(W^*; H^s_0(D^{2\pi}))} = \left[ \sum_{r=0}^\infty \int_{W^*} \| \partial^{2r}_{\alpha} \psi(\alpha, \cdot) \|_{H^s_0(D^{2\pi})}^2 \right]^{1/2}.
\]
This definition can be extended to all $r \geq 0$ by interpolation between Hilbert spaces and to $r \in \mathbb{R}$ by duality arguments. The following property of the Bloch transform has been investigated in [13].

**Theorem 4.** The Bloch transform is an isomorphism between $H^r_0(D)$ and $H^r_0(W^*; H^s_0(D^{2\pi}))$. Further, when $s = r = 0$, $J_D$ is an isometry with the inverse.
\( (J_D^{-1}\varphi)(x + \left(\frac{2\pi j}{0}\right)) = \int_{\Gamma_{\Omega}} \varphi(\alpha, x)e^{2\pi j\alpha} d\alpha, \quad x \in \Omega, \), \quad (6)

and the inverse transform equals to the adjoint operator of \( J_D \).

Now we apply the Floquet–Bloch transform to the scattering problem (5). Following [13], the first task is to transform the original problem, which is defined in the non-periodic domain \( \Omega^P \), to a problem defined in a periodic domain. In this paper, \( D \) is the periodic domain. Let \( H_0 \) be a real number that lies in the interval \((\min\{\zeta, \zeta_p\}, H)\) and define the following two diffeomorphisms for \( x \in \Omega^P \):

\[ \Phi : x \mapsto \left( x_1, x_2 + \frac{(x_2 - H_0)^3}{(h - H_0)^3} (\zeta - x_2) \right) \quad \Phi_\alpha : x \mapsto \left( x_1, x_2 + \frac{(x_2 - H_0)^3}{(h - H_0)^3} (\zeta - x_2) \right) \]

Then extend them by the identity operator for \( x_2 \geq H_0 \). As \( \text{supp}(\zeta - \zeta_p) \subset W \), \( \text{supp}(\Phi_\alpha - \zeta_p) \subset D^{2\pi} \).

Let \( u_D = u \circ \Phi_\alpha \), it can be easily checked that \( u_D \) satisfies the following variational equation:

\[ \int_D [A_\zeta \nabla u_D \cdot \nabla \overline{v_D} - k^2 c_\zeta u_D \overline{v_D}] dx - \int_{\Gamma_H} T^+ (u_D|_{\Gamma_H}) \overline{v_D} ds = \int_{\Gamma_H} f \overline{v_D} ds, \]

for all \( v_D = \nu \circ \Phi_\alpha \in \overline{H}^1(D) \), where

\[ A_\zeta(x) = \left| \det \nabla \Phi_\alpha(x) \right| \left( \left( \nabla \Phi_\alpha(x) \right)^{-1} \left( \nabla \Phi_\alpha(x) \right)^{-1} \right)^T \in L^\infty(D, \mathbb{R}^{2 \times 2}); \]

\[ c_\zeta(x) = \left| \det \nabla \Phi_\alpha(x) \right| \in L^\infty(D). \]

We define the matrix \( A_\zeta \) and \( c_\zeta \) by \( \Phi_\alpha \) in a similar way, i.e.

\[ A_\zeta(x) = \left| \det \nabla \Phi_\alpha(x) \right| \left( \left( \nabla \Phi_\alpha(x) \right)^{-1} \left( \nabla \Phi_\alpha(x) \right)^{-1} \right)^T \in L^\infty(D, \mathbb{R}^{2 \times 2}); \]

\[ c_\zeta(x) = \left| \det \nabla \Phi_\alpha(x) \right| \in L^\infty(D). \]

As \( \text{supp}(\Phi_\alpha - \zeta_p) \subset D^{2\pi} \), the supports of both \( A_\zeta - A_\zeta \) and \( c_\zeta - c_\zeta \) are subsets of \( D^{2\pi} \). Let \( w := J_D u_D \), then it satisfies

\[ \int_{\Omega^X} a_\alpha(w(\alpha, \cdot), z(\alpha, \cdot)) d\alpha + b(J_\Omega w, J_{\Omega}^1 z) = \int_{\Gamma_{\Omega^X}} F(\alpha, \cdot) z(\alpha, \cdot) d\alpha d\sigma, \]

where

\[ a_\alpha(u, v) = \int_{\Omega^P} [A_\zeta \nabla u \cdot \nabla \overline{v} - k^2 c_\zeta u \overline{v}] dx - \int_{\Gamma_H} (T^+ u) \overline{v} ds; \]

\[ b(u, v) = \int_{\Omega^P} [(A_\zeta - A_\zeta) \nabla u \cdot \nabla \overline{v} - k^2 c_\zeta u \overline{v}] dx; \]

\[ F(\alpha, \cdot) = \frac{\partial (J_\Omega u')}{\partial x_\alpha} - T^+ (J_\Omega u')(\alpha, \cdot); \]

\[ T^+ \varphi = i \sum_{j \in \mathbb{Z}} k^2 - j - \alpha^2 \varphi(j) e^{i(j-\alpha)x}, \quad \varphi = \sum_{j \in \mathbb{Z}} \varphi(j) e^{i(j-\alpha)x}. \]
Following the arguments in [10, 13], it is easy to prove that when the functions \( \zeta \) and \( \zeta_p \) are Lipschitz continuous, the variational problem (8) is equivalent to (5). When (5) has a unique solution of \( H_0^1(\Omega_H^p) \) for some \( |r| < 1 \), the problem (8) has a unique solution in \( H_0^1(\Omega^p; H_0^1(D^{2\pi})) \). Moreover, if the incident field \( u' \in H_0^1(\Omega_H^p) \) and the surfaces are \( C^{2,1} \), then the solution belongs to the space \( H_0^1(\Omega^p; \widetilde{H}_0^\infty(D^{2\pi})) \). In [13], a convergent numerical method based on (8) has been proposed for the numerical solution, and a high order method has been proposed in [17].

**Remark 5.** The information on the periodic function \( \zeta \) is included in \( A_c \) and \( c_c \), and the information of \( p \) is included in \( A_{c_p} \) and \( c_{c_p} \). During the iteration process, when \( \zeta \) and \( p \) are updated, the matrices \( A_c \), \( A_p \) and the functions \( c_c \), \( c_p \) are also updated. Thus we do not need to change the meshes during this process.

3. Approximation of the scattering problems with periodic surfaces

This section considers the difference between the scattered fields with and without a local perturbation. Let \( u_0 \) be the total field corresponding to the same incident field \( u' \) and periodic surface \( \Gamma \), then \( u_0 \) satisfies the variational equation:

\[
\int_{\Omega_H} \left[ \nabla u_0 \cdot \nabla \bar{\sigma} - k^2 u_0 \bar{\sigma} \right] dx - \int_{\Gamma_H} T^+ \left( u_0 \right|_{\Gamma_H} ) \bar{\sigma} ds = \int_{\Gamma_H} f \bar{\sigma} ds.
\]

From theorem 2, if \( f \in H_r^{-1/2}(\Gamma_H) \) for some \( |r| < 1 \), then the solution \( u_0 \in H_0^1(\Omega_H) \). In this paper, we assume that \( r \in (0, 1) \). As \( u_0 \in H_0^1(\Omega_H) \), there exists a constant \( C \) that does not depend on \( u_0 \) and \( x_1 \) such that

\[ |u_0(x_1, x_2)| \leq C(1 + x_1^{r/2 - 2/4}). \]

We apply the translation to the first variable, i.e. to replace \( x_1 \) by \( x_1 + 2\pi L \) for some \( L \in \mathbb{Z} \setminus \{0\} \), and let \( u_{0L}(x_1, x_2) := u'(x_1 + 2\pi L, x_2) \) be the incident field. As the surface is \( 2\pi \)-periodic, the total field with the incident field \( u_{0L} \), denoted by \( u_{0L}^L \), is actually the function \( u_0(x_1 + 2\pi L, x_2) \). \( u_{0L}^L \) satisfies the following variational equation

\[
\int_{\Omega_H} \left[ \nabla u_{0L}^L \cdot \nabla \bar{\sigma} - k^2 u_{0L}^L \bar{\sigma} \right] dx - \int_{\Gamma_H} T^+ \left( u_{0L}^L \right|_{\Gamma_H} ) \bar{\sigma} ds = \int_{\Gamma_H} f_L \bar{\sigma} ds
\]

with \( f_L(x_1, x_2) := f(x_1 + 2\pi L, x_2) \) on \( \Gamma_H \). As

\[ |u_0(x_1 + 2\pi L, x_2)| \leq C|2\pi L|^{-r/2 - 2/4}, \quad (x_1, x_2) \in \Omega_H^{2\pi}, \]

the following estimate holds:

\[ |u_{0L}^L(x_1, x_2)| \leq C|2\pi L|^{-r/2 - 2/4}, \quad (x_1, x_2) \in \Omega_H^{2\pi}. \]

Let \( u_L' \) be the solution of (5) with \( f \) replaced by \( f_L \). Similar to the previous section, we can define a diffeomorphism \( \Phi_p \) that maps \( \Omega_H^p \) to \( \Omega_H \) and \( \Phi_p = I_2 \) is supported in \( \Omega_H \cap W \times \mathbb{R} \). Let \( u_F^L := u_L' \circ \Phi_p \), it is easily checked that \( u_F^L \) satisfies

\[
\int_{\Omega_H} \left[ A_p \nabla u_F^L \cdot \nabla \bar{\sigma} - k^2 c_p u_F^L \bar{\sigma} \right] dx - \int_{\Gamma_H} T^+ \left( u_F^L \right|_{\Gamma_H} ) \bar{\sigma} ds = \int_{\Gamma_H} f_L \bar{\sigma} ds, \quad (9)
\]
where
\[ A_p(x) = |\text{det} \nabla \Phi_p(x)| \left[ (\nabla \Phi_p(x))^{-1} \left( (\nabla \Phi_p(x))^{-1} \right)^\top \right] \in L^\infty(D, \mathbb{R}^{2 \times 2}); \]
\[ c_p(x) = |\text{det} \nabla \Phi_p(x)| \in L^\infty(D). \]

Moreover, \( \text{supp}(A_p - I_2), \text{supp}(c_p - 1) \subset \Omega_H \cap W \times \mathbb{R}(:= \Omega_H^\sigma) \). Then the difference \( u^t_0 := u^t_L - u^t_0 \) satisfies the following variational equation, i.e.
\[ \int_{\Omega_H} [A_p \nabla u^t_0 \cdot \nabla \tilde{v} - k^2 c_p u^t_0 \tilde{v}] - \int_{\Gamma_R} \left( u^t_0 \right)^{\top} \tau ds = \tilde{b}(u^t_0, \tilde{v}) \tag{10} \]
for any \( \tilde{v} \in H^1(\Omega_H) \) with compact support, where
\[ \tilde{b}(\cdot, \cdot) = \int_{\Omega_H} \left( (I_2 - A_p) \nabla u^t_0 \cdot \nabla \tilde{v} - k^2 (1 - c_p) u^t_0 \tilde{v} \right) \text{d}x. \tag{11} \]

Here \( \tilde{b}(\cdot, \cdot) \) can be viewed as a bounded sesquilinear form satisfying
\[ |\tilde{b}(u, \tilde{v})| \leq C \|u\|_{H^1(\Omega_H^\sigma)} \|\tilde{v}\|_{H^1(\Omega_H^\sigma)}, \]
where \( C \) is a constant depending only on \( \zeta \) and \( \zeta_p \). Thus the right hand side of (10) satisfies
\[ |\tilde{b}(u^t_0, \tilde{v})| \leq C \|u^t_0\|_{H^1(\Omega_H^\sigma)} \|\tilde{v}\|_{H^1(\Omega_H^\sigma)} \leq C |2\pi L|^{-r/2} \|\tilde{v}\|_{H^1(\Omega_H)} \]
From the equivalence between (5) and (7), the equation (10) is uniquely solvable in \( H^1(\Omega_H) \) when the right hand side is an antilinear functional on \( H^1(\Omega_H) \). Thus
\[ \|u^t_L - u^t_0\|_{H^1(\Omega_H)} \leq C |2\pi L|^{-r/2}. \]

Based on the above analysis, the total field \( u^t_0 \) is a good approximation of \( u^t_L \) if \( L \) is sufficiently large. Particularly, let \( \sigma \) be the noise level of the inverse problem and suppose that \( L \in \mathbb{Z} \) has a large enough absolute value such that \( C |2\pi L|^{-r/2} < \delta \), then \( u^t_L \) could be treated as the ‘exact solution’ of the non-perturbed periodic surface with the incident field \( u^t_L \). Let
\[ \tilde{u}^t_L(x_1, x_2) := u^t_L(x_1 - 2\pi L, x_2), \]
then \( \tilde{u}^t_L \) is a good approximation of \( u^t_0 \). In this case, the solution \( \tilde{u}^t_L \) could be applied to reconstruct the periodic surface in the inverse problem.

4. Inverse problem and the Newton-CG method

The inverse problem is to reconstruct the unknown function \( \zeta^p \) from the measurement Cauchy data \( U \) on a horizontal line \( \Gamma_H \). Here \( U \) is defined as
\[ U := (u^t, \partial_n u^t) \big|_{\Gamma_R} + \sigma (u^t, \partial_n u^t) \big|_{\Gamma_R}, \tag{12} \]
where \( \sigma \) is some noise added to the measurement data.

Further, \( \zeta \in C^{2,1}(\mathbb{R}) \) is supposed to be a 2\( \pi \)-periodic function and \( p \in C^{2,1}(\mathbb{R}) \) is supposed to be a function that is compactly supported in \( W + 2\pi J \) for some \( J \in \mathbb{Z} \).

Remark 6. For the inverse problem, \( J \) is an unknown integer and one task is to find out the exact value of \( J \). As explained later, the integer \( J \) could be obtained by a sampling method (see [16]). In this section, we treat it as a known one. For any \( J \neq 0 \), we can simply apply the trans-
lation $x \mapsto x - 2\pi J$ to move the perturbation to the center of the domain. Thus for simplicity, we still assume that $J = 0$ in this section.

Define the spaces

$$
X := \{ \zeta \in C^{2,1}(\mathbb{R}) : \zeta \text{ is } 2\pi \text{ - periodic} \};
$$

$$
Y := \{ p \in C^{2,1}(\mathbb{R}) : \text{ supp}(p) \subset W \}.
$$

In the following, we assume that $(\zeta, p) \in X \times Y$ and $\zeta_p := \zeta + p$. The inverse problem is to find out $(\zeta, p) \in X \times Y$ such that the near-field Cauchy data corresponding to $(\zeta, p)$ is the best approximation of $U$.

4.1. Scattering operator and its properties with respect to rough surfaces

We recall the inverse scattering problems from rough surfaces introduced in [4]. Let $BC^{1,1}(\mathbb{R})$ be the space of bounded, Lipschitz continuous function. Suppose $f \in BC^{1,1}(\mathbb{R})$ and the surface $\Gamma_f$ is defined by $f$. We can also define the domain $\Omega_f$ by the domain above $\Gamma_f$, and $\Omega_f^H$ by the domain between $\Gamma_f$ and $\Gamma_H$, where $H$ is a real number that is larger than $\|f\|_\infty$. Given an incident field $u^i$, we define the following scattering operator

$$
S : BC^{1,1}(\mathbb{R}) \rightarrow L^2(\Gamma_H)
$$

$$
f \mapsto u^i|_{\Gamma_H}.
$$

Then the inverse problem can be written as an optimization problem, i.e. to find $f \in BC^{1,1}(\mathbb{R})$ such that

$$
\|S(f) - U\|_{L^2(\Gamma_H)}^2 = \min_{f^* \in BC^{1,1}(\mathbb{R})} \|S(f^*) - U\|_{L^2(\Gamma_H)}^2. \tag{13}
$$

Let

$$
F(f) := \|S(f) - U\|_{L^2(\Gamma_H)}^2, \tag{14}
$$

then the inverse problem is to find out the minimizer of the functional $F$ in the domain $BC^{1,1}(\mathbb{R})$. To solve the minimization problem, we have to study the properties of the scattering operator $S$ first.

**Theorem 7.** The operator $S$ is differentiable, and its derivative $DS$ is represented as

$$
DS : BC^{1,1}(\mathbb{R}) \rightarrow L^2(\Gamma_H)
$$

$$
h \mapsto u'|_{\Gamma_H}, \tag{15}
$$

where $u' \in H^1(\Omega_f^H)$ satisfies

$$
\Delta u' + k^2 u' = 0 \text{ in } \Omega_f^H; \tag{17}
$$

$$
u' = -\frac{\partial u}{\partial x_2} h \text{ on } \Gamma_f; \tag{18}
$$

$$
\frac{\partial u'}{\partial x_2} = T^* u' \text{ on } \Gamma_H. \tag{19}
$$

Here $u$ is the total field of the scattering problem (1)–(3).
For the proof of this theorem we refer to [4, 9].

In order to use the Newton’s method, we also need the adjoint operator of the Fréchet derivative $DS$, which is explained in the following theorem.

**Theorem 8.** The adjoint operator of $DS(f)$, denoted by $[DS(f)]^*$ is given by

$$[DS(f)]^* \varphi = -\text{Re} \left[ \frac{\partial u}{\partial \nu} \frac{\partial \varphi}{\partial \nu} \right] \nu_2,$$

(20)

where $\nu$ is the normal derivative upwards, $u$ is the total field and $z$ satisfies

$$\Delta z + k^2 z = 0 \quad \text{in } \Omega^f, \quad (21)$$

$$z = 0 \quad \text{on } \Gamma^f; \quad (22)$$

$$\frac{\partial z}{\partial x_2} - T^+ z = \mathbf{\varphi} \quad \text{on } \Gamma_H. \quad (23)$$

**Remark 9.** During the iteration steps, the problems (17)–(19) and (21)–(23) will be solved several times. We can always apply the method introduced in section 2.2 to transform the problems first into the one defined in the unbounded rectangle $D$ by the transform $\Phi_\zeta$, and then apply the Floquet–Bloch transform to obtain the new problem defined in the bounded domain $W^* \times D^{2\pi}$. For details of the solution of (21)–(23) we refer to remark 12 in [15].

### 4.2. Discretization for locally perturbed periodic surfaces

First, the functions $\zeta$ and $p$ are approximated by the linear combination of linearly independent functions. Let $\{\varphi_1, \varphi_2, \ldots, \varphi_M\}$ be a set of linearly independent functions in the space $X$ and $\{\psi_1, \psi_2, \ldots, \psi_N\}$ be a set of linearly independent functions in the space $Y$. Define the finite-dimensional subspaces of $X$ and $Y$ by:

$$X_M := \text{span}\{\varphi_1, \ldots, \varphi_M\} \subset X \quad \text{and} \quad Y_N := \text{span}\{\psi_1, \ldots, \psi_N\} \subset Y.$$ 

For the coefficients $C^M = (c_1^M, \ldots, c_M^M) \in \mathbb{R}^M$ and $D^N = (d_1^N, \ldots, d_N^N) \in \mathbb{R}^N$, then the elements $\zeta_M \in X_M$ and $p_N \in Y_N$ could be written as

$$\zeta_M(t) = \sum_{m=1}^{M} c_m^M \varphi_m(t), \quad p_N(t) = \sum_{n=1}^{N} d_n^N \psi_n(t).$$

For the function $\zeta \in X$, there is a $C^M \in \mathbb{R}^M$ such that $\zeta_M$ is the approximation in $X_M$ of $\zeta$. The argument also holds for $p_N \in Y_N$ and $p \in Y$.

Define the operators $A$ and $B$ by

$$A : \mathbb{R}^M \to X_M, \quad B : \mathbb{R}^N \to Y_N,$$

$$C^M \mapsto \zeta_M, \quad D^N \mapsto p_N,$$

then the operator $P$ can be defined as

$$P : \mathbb{R}^M \times \mathbb{R}^N \to L^2(\Gamma_H)$$

$$(C^M, D^N) \mapsto S \circ (A(C^M) + B(D^N)),$$

which maps the coefficients of both the periodic function and the local perturbation to the scattered field. Further, we can define a functional $F$ in the finite dimensional space $\mathbb{R}^M \times \mathbb{R}^N$ by
\( F(C^M, D^N) := \|P(C^M, D^N) - U\|_{L^2(\Gamma)}^2 \). \hfill (24)

The inverse problem can be reformulated by the following finite dimensional problem:

**Discrete inverse problem:** find \((C^M, D^N) \in \mathbb{R}^M \times \mathbb{R}^N\) such that

\[
F(C^M, D^N) = \min_{(C^M', D^N') \in \mathbb{R}^M \times \mathbb{R}^N} F(C^M', D^N'). \hfill (25)
\]

We apply the Newton-CG method to solve the discretized inverse problem. The linearized equation is

\[
P(C^M, D^N) + (DP)(C^M, D^N)(\delta C^M, \delta D^N) = U, \hfill (26)
\]

where \(\delta C^M = (\delta c^M_1, \ldots, \delta c^M_M) \in \mathbb{R}^M\) and \(\delta D^N = (\delta d^N_1, \ldots, \delta d^N_N) \in \mathbb{R}^N\), \((DP)(C^M, D^N)\) is the Fréchet derivative of \(P\) at \((C^M, D^N)\). Define

\[
M_A(C^M)(\delta C^M) := (DP)(C^M, D^N)(\delta C^M, 0);
\]

\[
M_B(D^N)(\delta D^N) := (DP)(C^M, D^N)(0, \delta D^N),
\]

then the linearized equation is written as

\[
P(C^M, D^N) + M_A(C^M)(\delta C^M) + M_B(D^N)(\delta D^N) = U. \hfill (27)
\]

First, we have to calculate the derivative of \(P\). As an operator defined in the finite dimensional space \(\mathbb{R}^M \times \mathbb{R}^N\), from direct calculation,

\[
\frac{\partial P}{\partial c_m^M} = (DS)(A(C^M) + B(D^N))\varphi_m; \quad \frac{\partial P}{\partial d_n^N} = (DS)(A(C^M) + B(D^N))\psi_n.
\]

Thus

\[
M_A(C^M)(\delta C^M) = \sum_{m=1}^M \delta c_m^M \frac{\partial P}{\partial c_m^M} = (DS)(A(C^M) + B(D^N)) \left[ \sum_{m=1}^M \delta c_m^M \varphi_m \right];
\]

\[
M_B(D^N)(\delta D^N) = \sum_{n=1}^N \delta d_n^N \frac{\partial P}{\partial d_n^N} = (DS)(A(C^M) + B(D^N)) \left[ \sum_{n=1}^N \delta d_n^N \psi_n \right].
\]

Given any \(\delta C^M \in \mathbb{R}^M\) and \(\varphi \in L^2(\Gamma_H)\),

\[
(\delta C^M, M_A(C^M)\varphi) = (M_A(C^M)(\delta C^M), \varphi)
= (DS)(A(C^M) + B(D^N)) \left[ \sum_{m=1}^M \delta c_m^M \varphi_m \right] \varphi
= \sum_{m=1}^M \delta c_m^M \left( \varphi_m, (DS)(A(C^M) + B(D^N))^* \varphi \right).
\]

Let \(Q = [(DS)(A(C^M) + B(D^N))^*]\), then
Similarly, we can also get
\[
M_B(D^N)\varphi = ((\psi_1, Q\varphi), \ldots, (\psi_N, Q\varphi)).
\] (29)

In the numerical implementation, we solve the discrete inverse problem separately, i.e. first fix \(D^N\) and solve the minimization problem (25) to find out the solution \(C^M\). Then we fix \(C^M\) and solve the problem with respect to \(D^N\).

To solve the minimization problems we apply the Newton-CG method. To minimize the function \(F(C^M, D^N)\) with fixed \(D^N\), we apply the following Newton-CG method.

---

**Algorithm 1.** Newton-CG method—part I.

Input: Data \(U; \varepsilon > 0; j = 0; \text{fixed } D^N \in \mathbb{R}^N\).

Initialization: \(C^M_0 \in \mathbb{R}^M\).

1: while \(|P(C^M_j, D^N) - U|_{L^2(\Omega_\omega)} > \varepsilon_1|U|_{L^2(\Omega_\omega)}\) do
2: \hspace{1em} CGNE iteration scheme to solve \(M_A(C^M_j)(H^M) = U - P(C^M_j, D^N)\)
3: \hspace{1em} \(C^M_{j+1} = C^M_j + H^M;\)
4: \hspace{1em} \(j = j + 1;\)
5: end while

Similarly, we can also minimize the function \(F(C^M, D^N)\) with fixed \(C^M\) by the following algorithm:

---

**Algorithm 2.** Newton-CG method—part II.

Input: Data \(U; \varepsilon > 0; j = 0; \text{fixed } C^M \in \mathbb{R}^M\).

Initialization: \(D^N_0 \in \mathbb{R}^N\).

1: while \(|P(C^M_j, D^N) - U|_{L^2(\Omega_\omega)} > \varepsilon_2|U|_{L^2(\Omega_\omega)}\) do
2: \hspace{1em} CGNE iteration scheme to solve \(M_B(D^N_j)(H^N) = U - P(C^M_j, D^N)\)
3: \hspace{1em} \(D^N_{j+1} = D^N_j + H^N;\)
4: \hspace{1em} \(j = j + 1;\)
5: end while

Note that the method to solve the equations \(M_A(C^M_j)(H^M) = U - P(C^M_j, D^N)\) and \(M_B(D^N_j)(H^N) = U - P(C^M_j, D^N)\) numerically, we adopt the CGNE iteration algorithm, for details we refer to algorithm 7.1, [6].

In the rest of this paper, we choose nonlinear independent functions in \(X\) and \(Y\) as follows.

For the space \(X\), we use \(M (M = 2m + 1 \text{ for some } m \in \mathbb{N})\) trigonometrical functions, i.e.

\[
\varphi_0(t) = 1; \varphi_j(t) = \cos(jt); \varphi_{j+m}(t) = \sin(jt), \quad j = 1, 2, \ldots, m.
\]

For the space \(Y\), the quartic spline functions are adopted (see remark 4.1, [18]). For the positive integer \(N\), let \(h = 2R/(M + 5)\) and \(t_j = (j + 2)h - R\), then the spline function is defined by \(\psi_j(t) = \psi(t - t_j)/h\) for \(j = 1, 2, \ldots, N\), where

\[
\psi(t) := \sum_{\ell=0}^{k+1} \frac{(-1)^j}{k!} \left( \begin{array}{c} k + 1 \cr \ell \end{array} \right) \left( t + \frac{k + 1}{2} - j \right)_+^k,
\]
where $\mathcal{A} = z_4$ for $z \geq 0$ and equals to 0 when $z < 0$. The parameters are chosen as $R = 4$ and $k = 4$.

Thus let a vector $\mathcal{C}_j^M = (c_j^0, c_j^1, \ldots, c_j^m, c_j^{m+1}, \ldots, c_j^{2m})$, the periodic surface is defined by the function

$$\zeta(t) = \sum_{\ell=0}^{M} c_j^\ell \varphi_{\ell}(t) = c_j^0 + \sum_{\ell=1}^{m} c_j^\ell \cos(\ell t) + \sum_{\ell=1}^{m} c_j^{\ell+m} \sin(\ell t).$$

Similarly, if $\mathcal{D}_j^N = (d_j^0, d_j^1, \ldots, d_j^N)$, the local perturbation is defined by

$$p(t) = \sum_{\ell=1}^{N} d_j^\ell \psi_\ell(t).$$

5. Numerical implementation

5.1. Sampling method

In this section, we use the sampling method introduced in [16] to give an initial guess of the perturbed periodic surface, especially for the first term $c_j^0$ of $\mathcal{C}_j^M$ and the integer $J$ of the perturbation.

Suppose that the location $y$ of an incident point source $u(x, y)$ is on a horizontal line $\Gamma_H := \{(x_1, H) : x_1 \in \mathbb{R}\}$ above the surface, we measure the Cauchy data $(u', \partial_x u')$ generated by the point source and the perturbed periodic surface on $\Gamma_H$. Here, $\partial_x u'$ denotes the normal derivative of $u'$ on $\Gamma_H$ with the direction $(0, 1)$.

With the help of the fundamental solution to the two-dimensional Helmholtz equation given by

$$\Phi_k(x, y) := -\frac{i}{4} \hat{H}_0^{(1)}(k|x - y|), \quad x \neq y,$$

we introduce the following imaging function

$$I(z) = \int_{\Gamma_H} \left| \int_{\Gamma_H} \left( \partial_x u'(x, y) \Phi_k(x, z) - u'(x, y) \partial_x \Phi_k(x, z) \right) ds(x) - \frac{i}{4\pi} \int_{\mathbb{R}} e^{i\mathcal{A}(y' - z')} ds(x) \right|^2 ds(y),$$

(30)

where $y' = (y_1, -y_2)$ and $z' = (z_1, -z_2)$. From the analysis in [16], we can expect that the imaging function $I(z)$ takes a large value when $z \in \Gamma_H$ and decays as $z$ is away from $\Gamma_H$. In this way, we give an initial guess of the perturbed surface.

In the numerical computation, we choose $2P + 1$ incident point sources which are located at $y_j = (jh_{\text{inc}}, H)$, $j = -P, \ldots, 0, \ldots, P$, here $h_{\text{inc}}$ is a fixed interval between two adjacent points. The measurement line $\Gamma_H$ is truncated to be $\Gamma_{H,A} := \{x \in \Gamma_H : |x_1| < A\}$ which will be discretized uniformly into $2Q$ subintervals so the step size is $h_{\text{mea}} = A/Q$. In addition, the lower-half circle $\mathbb{S}_-$ in the second integral in (30) will also be uniformly discretized into $R$ grids with the step size $\Delta \theta = \pi/R$. Then for each sampling point $z$ we get the following discrete form of (30)
The initial guess for the first term $c_0^0$ of $C_0^M$ can be deduced by the following formula

$$c_0^0 = c + (d - c) - \frac{1}{M_1M_2} \sum_{j=1}^{M_1} \max_j.$$ (32)

5.2. Iteration method

From the last subsection, we find out the exact value of the integer $J$. By translation on the first variable, i.e. to let $x_1$ be replaced with $x_1 + 2\pi J$, the perturbation is moved to $W$. Thus we could simply set $J = 0$ in this section. We present the iteration method to reconstruct the periodic function $\zeta$ and the compactly supported function $p$ in this section.

From section 3, for an incident field $u' \in H^r_0(\Omega_0^p)$ with some $r \in (0, 1)$, the measured data $U_L$ with the incident field $u'(\cdot + 2\pi L \cdot)$ for $L \in \mathbb{Z} \setminus \{0\}$ could be applied to reconstruct the periodic function $\zeta$. The measured data with incident field $u'$, denoted by $U_0$, is then applied to reconstruct the local perturbation $p$. So we conclude the algorithm for the inverse scattering problem.

**Algorithm 3.** Numerical method for the inverse problem.

Input: Cauchy data $(u'_i, \partial_i u'_i)$ generated by point sources located at $x_i$;

Given: Domain $D$, $\mathcal{M}$ is a regular mesh for $D$.

1. Decide $J$ and $c_0^0$ from the sampling method. Move the perturbation to the center by $x_1 \mapsto x_1 - 2\pi J$.

   Generate the measured data $U_0$ and $U_L$ with incident fields $u'(x_1, x_2)$ and $u'(x_1 + 2\pi L \cdot, x_2)$.

   Set the initial guess: $C_0^M := (c_0^0, 0, \ldots, 0)$, $D_0^N = \mathbf{0}$.

2. Solve the minimization problem for the fixed $D_0^N$ by algorithm 1:

   $$F(C_0^M, D_0^N) = \|P(C_0^M, D_0^N) - U_L\| \to \min.$$ 

3. Solving the minimization problem for the fixed $C^M$ by algorithm 2:

   $$F(C_0^M, D^N) = \|P(C_0^M, D^N) - U_0\| \to \min.$$ 

Then $(C_0^M, D^N)$ is the final result of the numerical scheme.
6. Numerical results

In this section, we present three examples for our numerical method. We define two different periodic surfaces and local perturbations:

\[
\begin{align*}
\zeta_1(t) &= 1.5 + \frac{\sin t}{24} - \frac{\cos 2t}{16}; \\
\zeta_2(t) &= 1.5 + \frac{\cos t}{8} ; \\
\zeta_3(t) &= \begin{cases} 1.35, & 2\pi/3 \leq |t| \leq \pi; \\
1.65, & |t| \leq \pi/3; \\
\text{linear,} & \text{otherwise.}
\end{cases} \\
p_1(t) &= 0.00025((t + 6\pi)^2 - 9)^3 \sin \left(\frac{\pi(t + 3)}{3}\right) X[-3\pi,3\pi](t); \\
p_2(t) &= -\frac{1}{8} \cos t X[-\pi,\pi](t); \\
p_3(t) &= \begin{cases} 0, & 2\pi/3 \leq |t| \leq \pi; \\
-0.3, & |t| \leq \pi/3; \\
\text{linear,} & \text{otherwise.}
\end{cases}
\end{align*}
\]

We apply algorithm 3 to the following three examples (see figure 2):

**Example 1.** The periodic surface \(\Gamma\) is defined by \(\zeta_1\) and the local perturbation is defined by \(p_1\).

**Example 2.** The periodic surface \(\Gamma\) is defined by \(\zeta_2\) and the local perturbation is defined by \(p_2\).

**Example 3.** The periodic surface \(\Gamma\) is defined by \(\zeta_3\) and the local perturbation is defined by \(p_3\). Note that in this example, both the periodic surface and the local perturbation are piecewise linear.

For both incident point sources and Herglotz wave functions, the measurement data are collected on \(\Gamma_{A,H}\) with \(A = 25\pi, H = 3\) and it is divided into \(2Q = 1500\) subintervals with the step length \(h_{\text{mea}} = \pi/300\). Let \(u_e\) be the exact data (either the scattered field or its normal derivative) on \(\Gamma_{A,H}\), then the measured data is defined as:

\[U_{\text{meas}} := u_e + \sigma \max(u_e) \text{randn},\]

where \(\sigma = 5\%\) is the noise level and \(\text{randn}\) presents random numbers from the standard normal distribution.

6.1. Sampling method

For the sampling method, we choose the sampling area to be a rectangle as \([-20\pi, 20\pi] \times [1.2, 1.9]\). The number of sampling points in \(x_1\)-direction and \(x_2\)-direction are set to be \(M_1 = 1600\) and \(M_2 = 400\), respectively. For the first surface, we put 41 incident point sources at \(y_j = (j\pi, 3)\) with \(j = -20, -19, \ldots, 20\). For the second and third surfaces, we put 21 incident point sources at \(y_j = (2j\pi, 3)\) with \(j = -10, -9, \ldots, 10\). The wavenumber is chosen to be \(k = 3\) for both examples.
Use the indicator function introduced in (31), we can get a rough reconstruction of the original perturbed periodic surfaces in figures 3 and 4. In each figure, we first present the profile of the original surface. Then the reconstructed result is given directly by the indicator function.
function $I_{A}(z)$. Finally, in order to give the initial guess of $c_{0}^{0}$ and the integer $J$ of the perturbation, we try to find out the points $z_{\text{max}}$ which get the largest value $I_{A}(z)$ in each vertical line and plot them in the last position of each figure.

By the end of the sampling step, we determine the values of $J$ and $c_{0}^{0}$. Roughly speaking, $J$ represents the location of the perturbation while $c_{0}^{0}$ gives the vertical location of the periodic surface. From figures 3–5, the locations of the perturbations are easily obtained, i.e. $J = -3$ for example 1, $J = 2$ for example 2 and $J = 0$ for example 3. The initial guess of $c_{0}^{0}$ is computed due to (32). By straightforward calculations, we get $c_{0}^{0} = 1.4987$, $c_{0}^{0} = 1.5216$ and

Figure 4. (a) The first surface; (b) and (c) the reconstructions.
\[ c_0^B = 1.5296. \] All of these two results are very good approximations of the constant terms of \( \zeta_1, \zeta_2 \) and \( \zeta_3 \).

6.2. Newton’s method

For the Newton’s method, the Herglotz wave function is applied as the incident field (see figure 6), i.e.

\[ u'(x_1, x_2) = \int_{-\pi/2}^{\pi/2} \exp \left( ik(x_1 \sin t - x_2 \cos t) \right) g(t) dt; \]
where
\[ g(t) = 2^{12}t^6(1-t)^6 \chi_{[0,1)}(t). \]

**Remark 10.** We could not use the point source as the incident fields since the fundamental solution \( \Phi(x, y) = \frac{1}{4\pi}H_0^{(1)}(k|x-y|) \) belongs to the space \( H^r_1(\Omega_H^p) \) only if \( r < 0 \). From [13], the direct solver introduced in section 2.2 does not converge.

The incident field \( u' \in H^r_1(\Omega_H^p) \) for any \( r \in (0, 1) \). Let \( L = 4 \), then we use two incident fields \( u' \) and \( u'_L := u' + 2\pi L \cdot \). Let \( u' \) and \( u'_L \) be the scattered fields corresponding to the incident fields \( u' \) and \( u'_L \), and \( u, u_L \) be the corresponding total fields. From the estimation in section 3, the error between \( u'_L := u \circ \Phi_p \) and \( u'_L' \), which is the total field with incident field \( u'_L \) and the periodic surface, is bounded by:
\[ \|u'_L - u'_L'\|_{H^r(\Omega_H^p)} \leq C|8\pi|^{-r-1/2} \leq 0.008C. \]
Note that the noise level is $\sigma = 5\%$, $u_{L}$ could be treated as a good approximation of $u_{L0}$ although the constant $C$ is unknown.

The parameters in the Newton-CG algorithm are chosen as follows:

$$h = 1.5, \quad M = 9, \quad N = 8, \quad \varepsilon_1 = 0.05, \quad \varepsilon_2 = 0.08.$$ 

We apply algorithm 3 to reconstruct the perturbation with the known values $J$ and $c_{0}^{0}$ from the sampling method. The reconstructions for examples 1–3 are shown in figures 7–9, respectively. From the left pictures of the three figures, the periodic surfaces are well reconstructed; based on the results for the periodic surfaces, we can also reconstruct the local perturbations very well. However, due to the error from the direct solver, we have to use finer meshes to produce measured data for example 3. Note that as Newton-type methods converge very fast when the initial value is given close enough to a local minimum, a good choice of the initial guess plays an important role in the numerical scheme. With the help of the sampling method, we are able to find a good enough initial guess for the periodic surface. With a good enough approximation of the first element $c_{0}^{0}$ in $C_{0}^{M}$, we have already known the location of
the periodic surface, then Newton-CG method converges when both the periodic surface and the local perturbation have relatively small oscillations.

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