Numerical solution of inverse scattering for near-field optics

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A novel regularized recursive linearization method is developed for a two-dimensional inverse medium scattering problem that arises in near-field optics, which reconstructs the scatterer of an inhomogeneous medium located on a substrate from data accessible through photon scanning tunneling microscopy experiments. Based on multiple frequency scattering data, the method starts from the Born approximation corresponding to weak scattering at a low frequency, and each update is obtained by continuation on the wavenumber from solutions of one forward problem and one adjoint problem of the Helmholtz equation.

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Scattering problems are basic in many scientific areas such as radar and sonar, geophysical exploration, and medical imaging [1,2]. However, there is a well-known resolution limit to the sharpness of details that can be observed by conventional far-field optical microscopy, roughly one half of the wavelength, referred to as the diffraction limit [3]. Near-field optics is an effective approach to break the diffraction limit and obtain images with subwavelength resolution, which has diverse applications, including near-field optical microscopy, nondestructive imaging of small-scale biological samples, and nanotechnology [4]. It has been observed experimentally that near-field optics has superresolving capability. To theoretically understand this capability, it is necessary to solve the inverse scattering problem. This work is concerned with the mathematical modeling and numerical solution for the inverse scattering of an important experimental modality in near-field optics, photon scanning tunneling microscopy (PSTM). In this modality, as seen in Fig. 1, a sample is illuminated from below by a plane incident wave, and the scattered wave is detected by passing a tapered fiber probe over the sample in the near-field zone [5].

Consider a model of PSTM with a sample located on a homogeneous substrate, as shown in Fig. 1. The substrate is assumed to be relatively thick so that only one face needs to be considered, thus defining an interface between two half-spaces. The index of refraction in the lower half-space (substrate) has a constant value n_0, and the index of refraction in the upper half-space varies within the domain of the sample but otherwise has the value of unity. The sample is illuminated from below (transmission geometry) by a time-harmonic plane wave, with wavenumber k. Throughout, by assuming nonmagnetic materials and transverse electric polarization, the model Maxwell equations reduce to the two-dimensional Helmholtz equation:

$$\Delta u + n^2 k^2 (1+q) u = 0, \tag{1}$$

where u is the total field, q is the sample permittivity, and

$$n(\mathbf{x}) = \begin{cases} 1 & \text{for } x_2 > 0, \\ n_0 & \text{for } x_2 < 0. \end{cases}$$

Denote the reference field u^{ref} as the solution of the homogeneous equation:

$$\Delta u^{\text{ref}} + n^2 k^2 u^{\text{ref}} = 0, \tag{2}$$

which may be analytically solved [6].

The total field consists of the reference field u^{ref} and the scattered field u^{s}:

$$u = u^{\text{ref}} + u^{\text{s}}. \tag{3}$$

It follows from Eqs. (1)–(3) that the scattered field satisfies

$$\Delta u^{\text{s}} + n^2 k^2 (1+q) u^{\text{s}} = -k^2 q u^{\text{ref}}. \tag{4}$$

In addition, the scattered field is required to satisfy a radiation condition at the infinity [7].

The *inverse scattering problem* is to reconstruct the sample permittivity q from the measurements of the scattered field u^{s}, for the given reference field u^{ref}. The scattered field is measured in the constant height configuration by an idealized point detector at $\mathbf{x}_j, j=1,\ldots,m$. In addition to nonlinearity and ill-

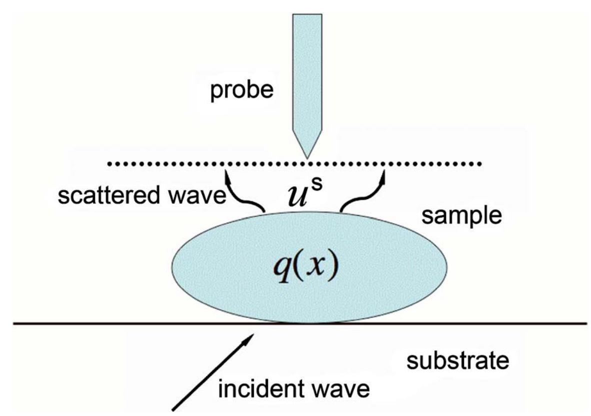

Fig. 1. (Color online) Photon scanning tunneling microscopy.

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posedness, two difficulties arise from the inhomogeneous background medium and the use of limited aperture data. The inverse problem with limited aperture is challenging, since without full aperture measurements, the ill-posedness and nonlinearity of the inverse problem become more severe. Initial results in this direction have been reported in the case of three-dimensional inhomogeneous media [8]. The basic idea is to develop an analytical solution technique for solving the linearized inverse scattering problem in the regime of the weak scattering approximation. Numerical solution of the full nonlinear inverse problem is at present completely open.

The present work is to develop a novel regularized recursive linearization method for solving the fully nonlinear inverse problem. This method requires multiple frequency scattering data, and the recursive linearization is obtained by continuation along the wavenumber k. It first solves a linear equation via the Born approximation at the lowest wavenumber. Updates are subsequently obtained by using a sequence of increasing wavenumbers. At each iteration, one forward problem and one adjoint problem of the Helmholtz equation are solved. We refer the reader to [9] for a complete description of the algorithm and related analysis. See also [10,11] for related stable and efficient recursive linearization methods for solving the two-dimensional Helmholtz equation and the three-dimensional Maxwell equations in the case of full aperture data. A homotopy continuation method with limited aperture data but in a homogeneous background medium may be found in [12].

The fundamental solution of the Helmholtz equation in a two-layered background medium in $\mathbb{R}^2$ satisfies

$$\Delta G(\mathbf{x},\mathbf{y}) + n^2(\mathbf{x})k^2 G(\mathbf{x},\mathbf{y}) = -\delta(\mathbf{x}-\mathbf{y}), \qquad (5)$$

where δ is the Dirac delta function. The solution can be obtained from the Fourier transform together with continuity conditions [6,13].

Using this fundamental solution, we obtain from Eq. (4) that the scattered field satisfies the Lippmann–Schwinger integral equation:

$$u^{\mathrm{s}}(\mathbf{x}) = k^2 \int_D G(\mathbf{x},\mathbf{y}) q(\mathbf{y})(u^{\mathrm{ref}}(\mathbf{y}) + u^{\mathrm{s}}(\mathbf{y}))\mathrm{d}\mathbf{y}. \qquad (6)$$

When the wavenumber k is small, the scattered field is weak [14]. By dropping the scattered field on the right-hand side of Eq. (6) under the weak scattering, we obtain the linearized integral equation

$$u^{\mathrm{s}}(\mathbf{x}) = k^2 \int_D G(\mathbf{x},\mathbf{y}) q(\mathbf{y}) u^{\mathrm{ref}}(\mathbf{y})\mathrm{d}\mathbf{y}, \qquad (7)$$

which is the Born approximation. In practice, the linear integral equation (7) is implemented by using the method of least squares with the Tikhonov regularization [15], which leads to a starting point for our recursive linearization method.

When the wavenumber k is small, the Born approximation allows a reconstruction of those low Fourier modes for the function $q(x)$. We now describe a procedure that recursively determines a sequence of approximations q_k at $k=k_l$ for $l=1,2,\ldots$ with increasing wavenumber. Suppose now that an approximation of the scatterer, $q_{\tilde{k}}$, has been recovered at some wavenumber $\tilde{k}$ and that the wavenumber k is slightly larger that $\tilde{k}$. We wish to determine q_k, or equivalently, to determine the perturbation

$$\delta q = q_k - q_{\tilde{k}}.$$

For the reconstructed scatterer $q_{\tilde{k}}$, we solve at the wavenumber k the forward-scattering problem

$$\Delta \tilde{u}_i^{\mathrm{s}} + n^2 k^2 (1 + q_{\tilde{k}}) \tilde{u}_i^{\mathrm{s}} = -k^2 q_{\tilde{k}} u_i^{\mathrm{ref}}, \qquad (8)$$

where u_i^{ref} is the reference field corresponding to the ith incident wave, $i=1,\ldots,p$.

For the scatterer q_k, we have

$$\Delta u_i^{\mathrm{s}} + n^2 k^2 (1 + q_k) u_i^{\mathrm{s}} = -k^2 q_k u_i^{\mathrm{ref}}. \qquad (9)$$

Subtracting Eq. (8) from (9) and omitting the second-order smallness in δq and in $\delta u_i^{\mathrm{s}} = u_i^{\mathrm{s}} - \tilde{u}_i^{\mathrm{s}}$, we obtain

$$\Delta \delta u_i^{\mathrm{s}} + n^2 k^2 (1 + q_{\tilde{k}}) \delta u_i^{\mathrm{s}} = -k^2 \delta q (u_i^{\mathrm{ref}} + \tilde{u}_i^{\mathrm{s}}). \qquad (10)$$

Given a solution u_i^{s} of Eq. (9), we define the measurements

$$M u_i^{\mathrm{s}}(\mathbf{x}) = [u_i^{\mathrm{s}}(\mathbf{x}_1), \ldots, u_i^{\mathrm{s}}(\mathbf{x}_m)]^T. \qquad (11)$$

The measurement operator M is well defined, which maps the scattered field to a vector of complex numbers in $\mathbb{C}^m$.

For the scatterer q_k and the reference field u_i^{ref}, define the forward-scattering operator

$$S_i(q_k) = M u_i^{\mathrm{s}}. \qquad (12)$$

Let $S_i'(q_{\tilde{k}})$ be the Fréchet derivative of $S_i(q_k)$ and denote the residual operator

$$R_i(q_{\tilde{k}}) = M(\delta u_i^{\mathrm{s}}). \qquad (13)$$

It follows from the linearization of the nonlinear equation (12) that

$$S_i'(q_{\tilde{k}}) \delta q = R_i(q_{\tilde{k}}). \qquad (14)$$

Applying the Landweber iteration [15] to the linearized equation (14) yields

$$\delta q = \alpha S_i'(q_{\tilde{k}})^* R_i(q_{\tilde{k}}), \qquad (15)$$

where α is a positive relaxation parameter and $S_i'(q_{\tilde{k}})^*$ is the adjoint operator of $S_i'(q_{\tilde{k}})$.

To compute the correction δq, it is crucial to compute $S_i'(q_{\tilde{k}})^* R_i(q_{\tilde{k}})$. The following adjoint state method is developed to serve this purpose [9]. Given residue $R_i(q_{\tilde{k}}) = [\zeta_{i1}, \ldots, \zeta_{im}]^T \in \mathbb{C}^m$, there is a function ψ_i satisfying the adjoint equation

$$\Delta \psi_i + n^2 k^2 (1 + q_{\tilde{k}}) \psi_i = -k^2 \sum_{j=1}^{m} \zeta_{ij} \delta(\mathbf{x} - \mathbf{x}_j) \qquad (16)$$

with a radiation condition, such that

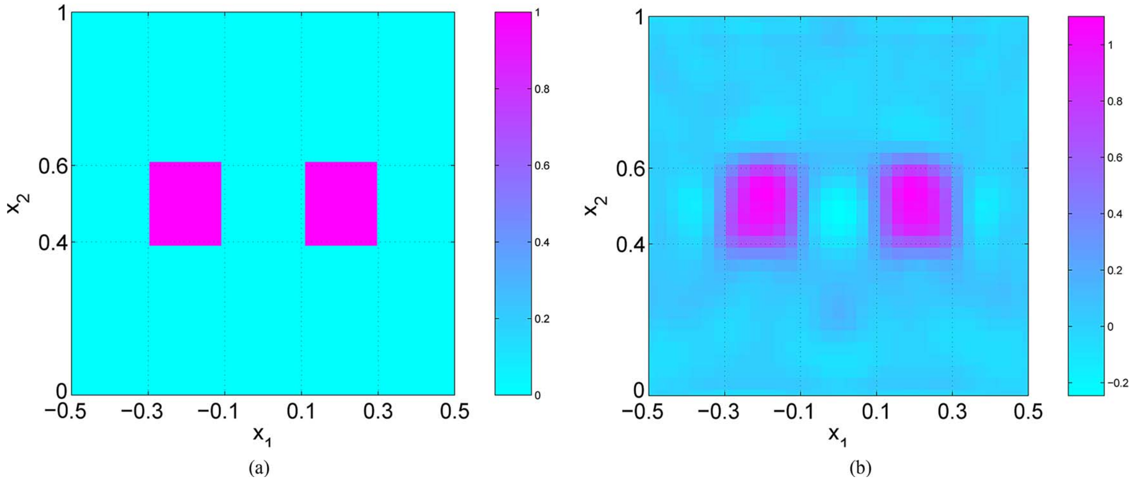

Fig. 2. (Color online) Example 1: (a) true scatterer, (b) reconstructed scatterer.

$$S_i'(q_{\tilde{k}})^* R_i(q_{\tilde{k}}) = (\overline{u_i^{\mathrm{ref}}} + \overline{\tilde{u}_i^{\mathrm{s}}})\psi_i, \quad (17)$$

where the overline denotes the complex conjugate.

Consequently, we can rewrite Eq. (15) as

$$\delta q = \alpha(\overline{u_i^{\mathrm{ref}}} + \overline{\tilde{u}_i^{\mathrm{s}}})\psi_i. \quad (18)$$

Thus, for each incident wave, we solve one forward problem (8) and one adjoint problem (16). Once δq is determined, q_k is updated by $q_{\tilde{k}} + \delta q$. After completing the pth sweep, we get the reconstructed scatterer q_k at the wavenumber k.

To illustrate the performance of our algorithm, we present a numerical example. The scattering data are obtained by numerical solution of the forward-scattering problem, which is implemented by using the finite element method with a perfectly matched layer technique [16].

The index of refraction $n_0 = 2$ in the lower half-space and the relaxation parameter α is taken to be $0.1/k^2$. The scattered fields are measured on $\mathbf{x}_j = (x_{1j}, 1.0), x_{1j} = -0.5 + j/32, j = 0, \ldots, 32$, and the incident angle $\theta_i = -2\pi/5 + i4\pi/50, i = 0, \ldots, 8$. Evidently, the incident waves consist of the evanescent plane waves and the propagating plane waves. For stability analysis, some relative random noise is added to the data, i.e., the scattered field takes the form

$$u_i^{\mathrm{s}}(\mathbf{x}_j) := (1 + \sigma\,\mathrm{rand})u_i^{s}(\mathbf{x}_j), j = 0, \ldots, 32, i = 0, \ldots, 8.$$

Here, rand gives uniformly distributed random numbers in $[-1, 1]$, and σ is a noise level parameter taken to be 0.05 in our numerical experiments. Example 1 (Fig. 2) is to reconstruct a single scatterer and two isolated scatterers inside the domain $D = [-0.5, 0.5] \times [0.0, 1.0]$, respectively. Figures 1(a) and 2(a) show the true scatterers. Figures 1(b) and 2(b) present the reconstructed scatterer at the wavenumber $k = 21$ with step size $\Delta k = 0.5$.

In summary, we have presented a regularized recursive linearization method for reconstructing the sample permittivity in the modality of PSTM. The proposed method is stable and efficient for solving the inverse medium scattering in the inhomogeneous background medium with limited aperture data.

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