Structure Determination from Intensity Measurements in Scattering Experiments

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The problem of determining a scattering potential from measurements of the far-field intensity distribution obtained in a set of scattering experiments is addressed within the Born approximation. It is shown that this problem admits a conceptually and computationally simple approximate solution if the incident and scattered radiation are mutually coherent in the far field and if the spatial resolution at which the far-field distribution of total intensity is measured is sufficiently high. The resolution of the inversion procedure is discussed and a computer simulation illustrating the proposed method is presented.

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Introduction.— In this Letter we propose a novel reconstruction procedure for estimating a scattering potential directly from measurements of the far-field intensity pattern measured in a set of scattering experiments employing highly coherent incident plane waves. The experimental configuration is illustrated in Fig. 1 where a scattering object is illuminated by a coherent plane-wave beam whose cross-sectional area πl^2 is much larger than the geometrical cross section πa^2 of the scatterer. The intensity of the total wave field (incident plus scattered) is recorded in the far field over the region of overlap of the incident and scattered wave, forming, in effect, a Gabor-type "hologram" of the scattered wave field.[1] The scattering potential is then directly reconstructed from a set of such holograms corresponding to incident plane waves having varying directions of illumination.

The novel aspect of the inverse scattering procedure proposed here is not the use of holograms to record the scattered wave fields but is rather the manner in which the holographic data are used to actually generate the reconstruction. In the usual holographic formulation[2] of the structure determination problem the amplitude and phase of the scattering amplitude are first deduced from the holograms and then used to compute the scattering potential via the inverse Fourier transform that connects the two quantities within the Born (or "kinematic") approximation.[2,3] In the method proposed here the reconstruction is performed *directly* in an one-step procedure from the measured far-field intensity distribution recorded on the "holograms" and thus avoids entirely the so-called *phase problem.*[3] This approach has pronounced advantages over the usual approach because of the difficulty of actually deducing the phase of a scattered wave field from a recorded hologram. Although the hologram certainly contains this phase information there is no simple way of obtaining the phase in an unambiguous manner for arbitrary and unknown scattered wave fields.

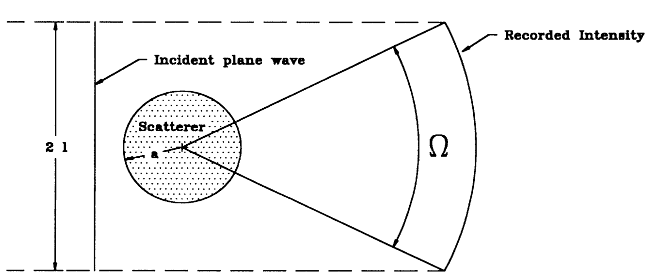


FIG. 1. Experimental configuration. The intensity of the total wave field in the far field is recorded over the region of overlap of the incident and scattered waves forming a "Gabor hologram" of the scattered wave field.

The central idea behind the reconstruction procedure is the observation that the mathematical process of inverting the Fourier-transform relation that exists between the scattering amplitude and the scattering potential can be viewed as being equivalent to superimposing the real images generated from a large number of holograms taken at different viewing angles relative to the scatterer.[4,5] Since the real and virtual images generated from a Gabor hologram are formed in different regions of space[1] it follows that an approximate reconstruction can be obtained from a superposition of the total image fields (real plus virtual plus background) generated by a set of such holograms. The reconstruction so obtained[6] will be in error due to the overlap of the virtual and background images with the real image. The superposition of the virtual and background images then forms a "noise" term whose magnitude is dependent on the distance from the scatterer at which the holograms were recorded. A major goal of the current Letter is to show that the magnitude of this noise term decreases monotonically with measurement distance and becomes negligible if the holograms are recorded in the far field. In this limit then, the reconstruction generated by the inversion process becomes identical to the theoretically optimum solution generated from both the amplitude and phase of the scattering amplitude.

The Letter includes the calculation of an upper bound for the integrated squared error between the estimate of the scattering potential generated by the procedure and the optimal estimate generated from the exact scattering amplitude, and a computer simulation illustrating the proposed approach for a spherically symmetric square-well potential.

Reconstruction procedure.— The far-field coherent intensity generated by the interaction of a monochromatic plane wave $e^{ik\mathbf{s}_0\cdot\mathbf{r}}$ with a scattering potential $V(\mathbf{r})$ is given by

$$|\psi(\rho\mathbf{s};\mathbf{s}_0)|^2 \sim 1+\frac{1}{\rho^2}\frac{d\sigma}{d\Omega} + 2\,\mathrm{Re}\left[e^{-ik\mathbf{s}_0\cdot\mathbf{s}\rho} f(\mathbf{s},\mathbf{s}_0)\frac{e^{ik\rho}}{\rho}\right], \tag{1}$$

where we have denoted the observation point in the far field by $\mathbf{r}=\rho\mathbf{s}$ and where Re stands for the real part. In this equation $f(\mathbf{s},\mathbf{s}_0)$ denotes the scattering amplitude in the direction of the unit vector $\mathbf{s}$ and $d\sigma/d\Omega = |f(\mathbf{s},\mathbf{s}_0)|^2$ is the differential scattering cross section. Within the Born approximation the scattering amplitude is related to the scattering potential via the equation[4,5]

$$f(\mathbf{s},\mathbf{s}_0) \approx -\frac{1}{4\pi}\tilde{V}(k(\mathbf{s}-\mathbf{s}_0)), \tag{2}$$

where

$$\tilde{V}(\mathbf{K}) = \int d^3r\, V(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} \tag{3}$$

is the three-dimensional spatial Fourier transform of the scattering potential.

Solving Eq. (1) for the scattering amplitude we obtain

$$f(\mathbf{s},\mathbf{s}_0) \approx D(\mathbf{s},\mathbf{s}_0) - \frac{1}{\rho}\frac{d\sigma}{d\Omega} e^{ik(\mathbf{s}_0\cdot\mathbf{s}-1)\rho} - f^*(\mathbf{s},\mathbf{s}_0) e^{2ik(\mathbf{s}_0\cdot\mathbf{s}-1)\rho}, \tag{4}$$

where

$$D(\mathbf{s},\mathbf{s}_0) = \rho e^{ik(\mathbf{s}_0\cdot\mathbf{s}-1)\rho}\{|\psi(\rho\mathbf{s};\mathbf{s}_0)|^2 - 1\}, \tag{5}$$

and where the approximation (4) requires that the total wave field $\psi(\rho\mathbf{s};\mathbf{s}_0)$ be measured in the far field $k\rho \gg 1$. The reconstruction method that we propose is to simply approximate the scattering amplitude in Eq. (2) by $D(\mathbf{s},\mathbf{s}_0)$; i.e., we compute the unknown scattering potential using the Born approximation and assuming that $f(\mathbf{s},\mathbf{s}_0) \approx D(\mathbf{s},\mathbf{s}_0)$. The reconstruction so obtained will be in error due to the absence of the last two terms on the right-hand side of Eq. (4) in the expression for f. These terms correspond to a superposition of background and virtual image fields produced by a set of Gabor holograms and will be shown to be negligible as long as the far-field condition $k\rho \gg 1$ is satisfied.[7]

One way of estimating the contribution of the last two terms on the right-hand side of Eq. (4) to the reconstruction is to employ the so-called *filtered backpropagation algorithm*[4,8] which generates the reconstruction within the Born approximation as a superposition of real images formed from the *backpropagation* of the measured scattering amplitude into the region of space occupied by the scatterer. If the scattering amplitude is approximated by $D(\mathbf{s},\mathbf{s}_0)$ in this algorithm then the resulting reconstruction will consist of two contributions: (i) The optimum reconstruction $\hat{V}$ generated from the backpropagation of f, and (ii) a noise term generated from the backpropagation of the last two terms on the right-hand side of Eq. (4). It can be readily shown that the exponentials in Eq. (4) have the effect of displacing the central location of the images formed from backpropagating the last two terms in this equation by a distance of ρ and 2ρ, respectively, from the true scatterer location.[9] Thus, if ρ is sufficiently large, the overlap of these images with the optimum reconstruction will be small, and the resulting reconstruction will be a good approximation to the optimum reconstruction within the support volume of the scatterer and will approach the optimum reconstruction in the limit where $\rho \to \infty$.

The magnitude of the contribution of the last two terms in Eq. (4) to the reconstruction can also be estimated in a straightforward manner using the Fourier inversion integral. To this end we denote the optimum reconstruction generated using $f(\mathbf{s},\mathbf{s}_0)$ by $\hat{V}$ and the approximate reconstruction generated using $D(\mathbf{s},\mathbf{s}_0)$ by $\hat{\mathcal{V}}$ and conclude from Eq. (4) that, within the Born approximation,

$$\hat{\mathcal{V}}(\mathbf{r}) = \hat{V}(\mathbf{r}) + N(\mathbf{r}), \tag{6}$$

where $N(\mathbf{r})$ is an error term whose Fourier transform is found from Eqs. (4) and (2) to be given by

$$\tilde{N}(k(\mathbf{s}-\mathbf{s}_0)) = -\frac{1}{4\pi\rho}|\tilde{V}(k(\mathbf{s}-\mathbf{s}_0))|^2 e^{-i(\rho/2k)|k(\mathbf{s}-\mathbf{s}_0)|^2} + \tilde{V}^*(k(\mathbf{s}-\mathbf{s}_0)) e^{-i(\rho/k)|k(\mathbf{s}-\mathbf{s}_0)|^2}, \tag{7}$$

where we have used the identity $|\mathbf{s}-\mathbf{s}_0|^2 = 2-2\mathbf{s}\cdot\mathbf{s}_0$. The error in the reconstruction is thus the inverse Fourier transform of the function $\tilde{N}(\mathbf{K})$ evaluated over the set of spatial frequencies $\mathbf{K}=k(\mathbf{s}-\mathbf{s}_0)$ determined from the set of scattering experiments. If we assume that the set of scattering experiments includes all incident directions $\mathbf{s}_0$ and those scattering directions $\mathbf{s}$ lying in a cone that is centered on $\mathbf{s}_0$ and which has a solid angle of Ω steradians (see Fig. 1), we find that this error is given by

$$N(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_{K\le(\Omega/\pi)^{1/2}k} d^3K\, \tilde{N}(\mathbf{K}) e^{i\mathbf{K}\cdot\mathbf{r}}, \tag{8}$$

where $\tilde{N}(\mathbf{K})$ is found from Eq. (7) to be

$$\tilde{N}(\mathbf{K}) = -(1/4\pi\rho)|\tilde{V}(\mathbf{K})|^2 e^{-i(\rho/2k)K^2} + \tilde{V}^*(\mathbf{K}) e^{-i(\rho/k)K^2}. \tag{9}$$

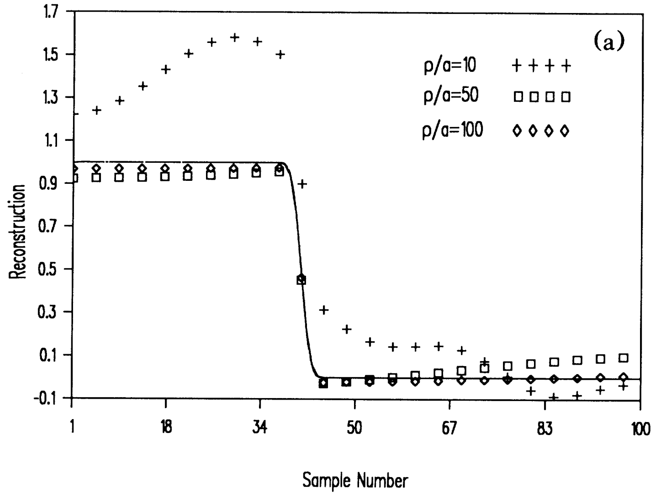
Now although the integral in Eq. (8) is taken over the interior of a sphere of radius $(\Omega/\pi)^{1/2}k$ the integrand will, in fact, be band limited to a much smaller volume due to the rapid oscillation of the two exponentials in the expression for $\tilde{N}$. In particular, a straightforward calculation shows that the effective volume of integration in Eq. (8) is the interior of a sphere of radius $K_0=2ak/\rho$, where a is the radius of the effective support volume of the scattering potential. It then follows that the integrated squared error between the approximate and optimal reconstructions $\hat{\mathcal{V}}$ and $\hat{V}$ is bounded above according to the equation

$$\epsilon=\int d^3r\,|\hat{\mathcal{V}}(\mathbf{r})-\hat{V}(\mathbf{r})|^2\le\frac{4}{3\pi^2}\left(k\frac{a}{\rho}\right)^3M^2, \quad (10)$$

where $M=\max|\tilde{N}(\mathbf{K})|$ and where we have made use of Parseval's theorem to evaluate the error bound. The error is seen to tend to zero as $\rho\to\infty$ and in this limit, then, the approximate reconstruction $\hat{\mathcal{V}}$ becomes equal to the optimal reconstruction V generated from the scattering amplitude.

In order to verify the conclusions drawn above concerning the magnitude of the error as a function of ρ, the contribution of the second term on the right-hand side of Eq. (9) to the noise $N(\mathbf{r})$ was computed for a number of ρ values for the case of a spherically symmetric square-well potential, $V(\mathbf{r})=1$ if $|\mathbf{r}|\le a$ and a zero elsewhere. Only the second term was considered since this term will yield the greatest contribution to the error for large ρ values and because, as mentioned earlier, the first term can be removed entirely by making a separate measurement of the differential scattering cross section. The transform $\tilde{N}$ and the noise term N are both spherically symmetric for this example and Eq. (8) reduces to a one-dimensional integral transform that is readily computed using a numerical integration routine. The results of the numerical integration are presented in Fig. 2 where we show the real and imaginary parts of the approximate reconstruction $\hat{\mathcal{V}}$ for a potential having a radius $a=10\lambda$, for the ratio of the measurement distance to the potential's radius ρ/a equal to 10, 50, and 100, and for a measurement solid angle $\Omega=2\pi$. It is seen from this figure that both the real and imaginary parts of the error decrease monotonically with increasing ρ/a and become negligible when ρ/a reaches a value of 100. Since the Fourier transform is linear it is clear that similar results would be obtained for any linear superposition of spherically symmetric potentials.

Resolution and sample spacing requirement.—The reconstruction procedure proposed in this paper requires that the intensity measurements be performed sufficiently far removed from the scatterer that the integrated squared error ϵ given in Eq. (10) be small. The requirement that the measurement distance ρ be large places a restriction on the resolution of the reconstruction procedure due to the fact that the incident plane wave must physically overlap the scattered wave in order for the method to be applicable. Assuming, as above, that the set of scattering experiments includes all incident directions $\mathbf{s}_0$ and those scattering directions $\mathbf{s}$ lying in a cone that is centered on $\mathbf{s}_0$ and which has a solid angle of Ω steradians, then the optimal reconstruction $\hat{V}$ is a low-pass filtered version of V, band limited to within a sphere of radius $\kappa=(\Omega/\pi)^{1/2}k$ in Fourier space.[2,3] A rough measure of the "resolution" of the reconstruction procedure is then provided by the minimum resolvable spatial wavelength of the scattering potential $\Lambda=2\pi/\kappa$ $=\lambda/(\Omega/\pi)^{1/2}$, where $\lambda=2\pi/k$ is the wavelength of the



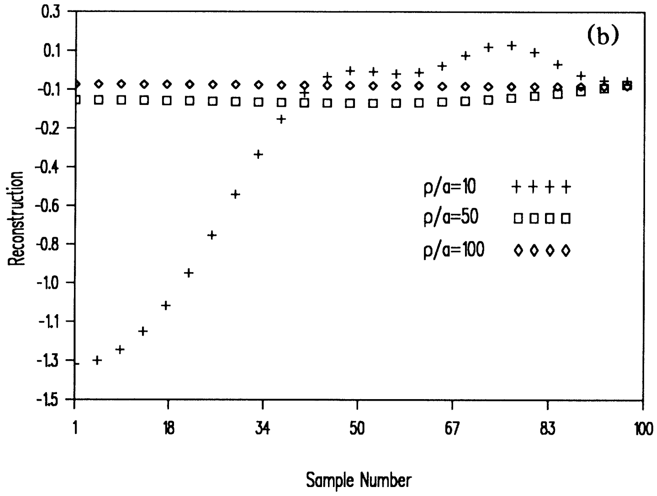


FIG. 2. The (a) real and (b) imaginary parts of the approximate reconstruction $\hat{\mathcal{V}}(r)$ of a spherically symmetric square-well potential of radius $a=10\lambda$ plotted as a function of the radius $r=|\mathbf{r}|$ using quarter-wavelength sample spacing. In the simulation $\Omega=2\pi$, corresponding to a spatial-frequency cutoff of $\sqrt{2}k$. The solid curve corresponds to the optimum reconstruction generated from the complex-valued scattering amplitude.

scattered wave field. Referring to Fig. 1 we find that if $\rho \gg l$ then $\Omega \approx \pi(l/\rho)^2$, leading to a value of $\Lambda = (\rho/l)\lambda$, wnere l is the radius of the circular cross section of the incident plane wave.

The cross-sectional area of the probing plane wave also determines the minimum sample spacing Δ required to measure the far-field intensity without introducing aliasing. This minimum sample spacing is equal to one-half of the minimum fringe spacing in the far-field intensity distribution $|\psi(\rho\mathbf{s};\mathbf{s}_0)|^2$ across the incident wave beam diameter $2l$ (see Fig. 1) and is readily found to be equal to Λ in the limit where $\rho \gg l$.

We mention finally that the resolution of the inversion procedure can be improved by employing a coherent off-axis reference beam rather than the direct (incident) wave in the measurement process. By this means the interference pattern (hologram) between the reference and scattered wave can be measured well outside the region of overlap of the incident and scattered wave and, in principle, the procedure can be extended to include the backscattered wave and thus yield the theoretical limit of resolution of a half wavelength.

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[6]The actual reconstruction need not be performed using holographic imaging algorithms and can be generated directly from the measured intensity distribution using a Fourier-based reconstruction algorithm (see Ref. 3).

[7]It should be noted that the contribution to the error from the differential scattering cross section (the background image field from the holograms) can be eliminated entirely by separately measuring $d\sigma/d\Omega$ and redefining D to be equal to $\rho e^{ik(\mathbf{s}_0\cdot\mathbf{s}-1)\rho}\{|\psi|^2 - 1 - \rho^{-2} d\sigma/\Omega\}$.

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[9]Physically this displacement corresponds to the displacement of the real and virtual images formed by a Gabor hologram.