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PHASE RECONSTRUCTION VIA NONLINEAR LEAST-SQUARES

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PHASE RECONSTRUCTION VIA NONLINEAR LEAST-SQUARES

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Abstract. Consider the problem of reconstructing the phase ϕ of a complex-valued function $fe^{i\phi}$, given knowledge of the magnitude $|f|$ and the magnitude of the Fourier transform $|\widehat{fe^{i\phi}}|$. In this paper we consider the formulation of the problem as a least-squares minimization problem. It is shown that the problem is ill-posed. Also, suprisingly, the gradient of the least-squares objective functional is not Fréchet differentiable. A regularization is introduced which restores differentiability and also counteracts instability. It is shown how a certain implementation of Newton's method can be used to efficiently solve the regularized least-squares problem, and that the method converges locally almost quadratically. Numerical examples are given with an application to diffractive optics.

Short title *Phase reconstruction via nonlinear least-squares*

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1. Introduction. The phase reconstuction problem arises in diverse fields such as astronomy, microscopy, and optical design. With so many applications, there is naturally a large body of literature associated with this problem—too large to attempt to provide a comprehensive review here. An introduction to the problem, some applications, a description of some techniques for solution, and an extensive bibliography can be found in the recent book [14].

In this paper we study the solution of the phase reconstruction problem via nonlinear least-squares. We describe how Newton's method can be efficiently applied to solve the phase reconstruction problem, and prove that Newton's method converges locally when the problem is regularized. Newton-like methods have been previously considered infeasible for the typically large problems which arise in applications [9]; simpler steepest-descent methods and other relatives of the gradient method are currently widely used.

In applications, several versions of the phase reconstruction problem appear, depending on how much is known and what is to be determined. The version of the phase reconstruction problem we study here comes from an application in optical design which we now briefly sketch. Consider a time-harmonic electromagnetic plane wave in Euclidean space $\{(x_1, x_2, x_3)\} \subset \mathbb{R}^3$, normally incident on an opaque sheet located in the $(x_1, x_2, 0)$ plane, into which an aperature Ω has been cut. In the so-called Fraunhofer approximation (see eg. Born and Wolf [4], Chap. 8.3) the diffracted wave F in the "far-field" (a plane normal to the x_3-axis located sufficiently far from the origin in the x_3-direction) is given by the Fourier transform of the characteristic function of the aperature:

$$F(\xi) = c\int_{\mathbb{R}^2} \chi_\Omega(x) e^{-2\pi i x\cdot\xi} dx, \quad \xi = (\xi_1, \xi_2), \quad x = (x_1, x_2),$$

where $\chi_\Omega(x) = 1$ in Ω, $\chi_\Omega(x) = 0$ elsewhere, and c is some complex constant which we shall henceforth ignore. We have also omitted a scaling factor in the ξ variable which is due to the frequency of the incoming wave.

Suppose that a thin lens with thickness $\phi(x)$ is placed in the aperature Ω. Suppose also that the lens has transparency $f(x)$, that is, the lens is opaque where $f(x) = 0$, completely tranparent where $f(x) = 1$, and partially transparent where $0 < f(x) < 1$. The effect of the lens is (roughly) to change the phase and amplitude of the incoming plane wave, resulting in a wave modulated by the "transmission function" $f(x)e^{i\phi(x)}$ (see Born and Wolf [4] for a discussion). The approximate far-field wave due to a particular lens profile ϕ is then given by

$$F[\phi](\xi) = \int f(x)e^{i\phi(x)-2\pi x\cdot\xi}dx = (\widehat{fe^{i\phi}})(\xi), \tag{1}$$

where we have extended f outside of Ω by zero. The *intensity* of the far-field wave is $|F[\phi](\xi)|^2$.

The optical design problem we consider is: given the real transparency function $f(x)$ and a specified far-field intensity pattern $g(\xi)$, design a lens with thickness $\phi(x)$ such that $|F[\phi]|^2 = g$. Stated differently, given the magnitude f of the complex-valued function $fe^{i\phi}$ and the magnitude of its Fourier transform $|\widehat{fe^{i\phi}}|$, find the phase ϕ. Some interesting recent examples of applications of this problem can be found in [7,17].

Since there is no known direct method to solve this problem, iterative and indirect methods have been widely studied and implemented. A review of much of the recent work in this area can be found in the book [14]. See also [8].

The approach taken in this paper is to reformulate the problem as a least-squares minimization problem. Specifically, to solve $|F[\phi]|^2 = g$ we try to minimize the residual

$$J[\phi] = \frac{1}{2}\left\| |F[\phi]|^2 - g \right\|^2_{L^2(\mathbb{R}^2)} \tag{2}$$

over some suitable class of phase functions ϕ.

The idea of trying to minimize (2) is not new; it has been explored by other authors. The widely-used error-reduction and Gerchberg-Saxton [10] algorithms are related to simple gradient-descent schemes for minimizing the residual (2) (see [9] for a discussion). As far as we know, the present paper is the first attempt at a rigorous study of Newton's method applied to problem (2).

The paper is organized as follows. In Section 2, the phase reconstruction problem is stated and reformulated as a least-squares minimization problem. In Section 3 we briefly study the stability of the linearized problem, showing that the inverse problem is ill-posed in the sense that the linearized forward map is compact. We then introduce a regularization and describe in Section 4 how Newton's method can be efficiently applied the regularized problem. The main advantage of Newton's method over simpler gradient-descent methods is the quick convergence; we show in Section 4 that Newton's method converges locally almost quadractically on the regularized problem. To our knowledge, this is the best convergence rate of any method which has been proposed for this problem so far. The reason that the convergence rate is only *almost* quadratic is that the gradient of the least-squares objective functional is not Fréchet differentiable over L^2, violating the classical C^2 differentiability hypothesis for the quadratic convergence of Newton's method (See Dennis and Schnabel [6] Chap. 5 for a complete discussion on the convergence of Newton's method). The "nondifferentiability" is proved in the Appendix with a simple counterexample; a numerical example is also given in Section 5. The regularization introduced in Section 3 restores differentiability and also stabilizes the problem, allowing a convergence rate arbitrarily close to quadratic, depending on the choice of a parameter. The method is demonstrated in Section 5 with some numerical experiments involving an optical design problem.

2. The phase reconstruction problem. Throughout this paper, $\hat{h}$ will denote the Fourier transform of the function h: $\hat{h}(\xi) = \int h(x)e^{-2\pi i x\cdot\xi}dx$; we denote the inverse Fourier transform of h by $\check{h}(\xi) = \int h(x)e^{2\pi i \xi\cdot x}dx$. Also L^p, $1 \le p < \infty$, will denote the classical Banach space of functions integrable of order p; L^∞ denotes the space of essentially bounded functions. We will generally denote the norm on $L^p(\mathbb{R}^n)$ for $1 \le p \le \infty$ by $\|\cdot\|_p$.

Let f be a known real-valued function on $\mathbb{R}^n$, $n \ge 1$, $f \ge 0$. We will call f the *magnitude* function. For functions $\phi : \mathbb{R}^n \to \mathbb{R}$, define the map F by

$$F[\phi](\xi) = \int_{\mathbb{R}^n} f(x)e^{i\phi(x)-2\pi i\xi\cdot x}dx = (\widehat{fe^{i\phi}})(\xi), \quad \xi \in \mathbb{R}^n. \tag{3}$$

We assume that $f \in L^1 \cap L^2$ and that ϕ is measurable.

Define the map G to be the squared modulus of F:

$$G[\phi](\xi) = |F[\phi](\xi)|^2, \tag{4}$$

Thus G represents the intensity of the far-field wave.

Let $g \in L^1 \cap L^2$ be a given real-valued function, $g \ge 0$; we will call g the *target intensity.* We wish to find a phase ϕ such that $G[\phi]$ best fits g in the least-squares sense. By the Plancherel theorem (see eg. [16]) we have $\|G[\phi]\|_1 = \|f\|_2$, thus we shall assume that the magnitude f and the target g are consistent in the sense that $\|g\|_1 = \|f\|_2$.

Consider the nonlinear least-squares problem

$$\min_{\phi} J[\phi] = \frac{1}{2}\|G[\phi] - g\|_2^2. \tag{5}$$

LEMMA 2.1. *If $f \in L^1 \cap L^2$ and $g \in L^2$, then $J[\phi]$ is well-defined and uniformly bounded over all measurable functions ϕ:*

$$J[\phi] \le C_0,$$

where $C_0 = \frac{1}{2}(\|f\|_1\|f\|_2 + \|g\|_2)^2$.

Proof. We have the estimate

$$\int |G[\phi]|^2 = \int |\widehat{fe^{i\phi}}|^4 \le \|\widehat{fe^{i\phi}}\|_\infty^2 \|\widehat{fe^{i\phi}}\|_2^2.$$

Since $|e^{i\phi}| = 1$ almost everywhere, $fe^{i\phi} \in L^1 \cap L^2$. It then follows immediately from the Plancherel theorem and the simple estimate $\|\widehat{fe^{i\phi}}\|_\infty \leq \|fe^{i\phi}\|_1$ that

$$\|G[\phi]\|_2 \leq \|f\|_1 \|f\|_2,$$

hence from (5),

$$0 \leq J[\phi] \leq \frac{1}{2}(\|f\|_1\|f\|_2 + \|g\|_2)^2.$$

□

Notice that for any phase function ϕ, there is an equivalent phase function $\tilde{\phi}$ (equivalent in the sense that $G[\tilde{\phi}] = G[\phi]$) with

$$-\pi \leq \tilde{\phi} < \pi \quad \text{a.e.},$$

obtained through the mapping

$$\phi \mapsto \phi/2\pi Z, \quad Z = \{0, \pm 1, \pm 2, \ldots\}.$$

Also, as is clear from (3), (4), if $\tilde{\phi}$ is any function such that $(\phi - \tilde{\phi})$ is constant on $\Omega = supp\ f$, then $G[\phi] = G[\tilde{\phi}]$. Thus ϕ is at best uniquely determined within a class of functions supported on Ω, modulo constant functions on Ω, whose L^∞ norm is π or less. The question of uniqueness has been addressed in slightly different contexts by other authors (for example [2,13] and the references in [14]); we will not pursue the question further here.

3. Linear instability. Holding the phase ϕ fixed, let $\delta\phi$ be a "small" perturbation to ϕ and consider formally the first variation of the map F defined in (3):

$$DF[\phi](\delta\phi) = (i\delta\phi f e^{i\phi})^{\wedge}. \tag{6}$$

Similarly, for the first variation of the complex conjugate F^* we have

$$D(F^*[\phi])(\delta\phi) = (-i\delta\phi f e^{i\phi})^{\vee} = (DF[\phi](\delta\phi))^*.$$

Since $G = F^*F$, formally we have $DG = 2Re(F^*DF)$. Thus from (6), the linearization of G at ϕ is

$$DG[\phi](\delta\phi) = 2Re[(fe^{-i\phi})^{\vee}(i\delta\phi f e^{i\phi})^{\wedge}]. \tag{7}$$

The linearized map DG is a bounded linear operator over L^2, as we now show.

LEMMA 3.1. *Let $f \in L^1 \cap L^2$, assume ϕ is measurable. Then $DG[\phi](\cdot) : L^2 \to L^2$ is bounded, independent of ϕ.*

Proof. From (7), using the Plancherel theorem and the estimate $\|(fe^{i\phi})^{\wedge}\|_\infty \leq \|f\|_1$, one easily obtains the bound

$$\|DG[\phi](\delta\phi)\|_2 \leq 2\|f\|_1\|f\|_\infty\|\delta\phi\|_2. \tag{8}$$

□

The question of whether the formal derivatives DF and DG are actually the Fréchet derivatives of F and G respectively is addressed in the Appendix. It turns out that DF *is not* the Fréchet derivative of F as a function on the space L^2, but DG *is* the Fréchet derivative of G as a function on L^2 (see Lemma A.1).

To solve the nonlinear least-squares problem (5) by any method involving linearization, it is important to understand the properties of the linearized problem

$$DG[\phi](\delta\phi) = -(G[\phi] - g). \tag{9}$$

The following theorem shows that problem (9) is ill-posed in the sense that the map $DG[\phi](\cdot)$ is compact over L^2. Thus one cannot expect to solve the normal equations corresponding to the linearization of problem (5) without imposing some kind of regularization.

THEOREM 3.2. *For all $f \in L^1 \cap L^\infty$ such that $|f| \to 0$ as $|x| \to \infty$, the map $DG[\phi](\cdot) : L^2 \to L^2$ defined by (7) is compact.*

Proof. Let B be a bounded set in L^2. We show that the set $Q = DG[\phi](B)$ is precompact in L^2. This is equivalent to showing that translates of functions in Q are sufficiently close to one another, and that functions in Q are almost supported on some compact set (see eg. Adams [1], Theorem 2.21). More precisely, we show that for every $\epsilon > 0$, there exists a number $\delta > 0$ and a subset $K \subset\subset \mathbb{R}^n$ such that for every $u \in Q$ and every $h \in \mathbb{R}^n$ with $|h| < \delta$,

$$\int_{\mathbb{R}^n} |u(\xi + h) - u(\xi)|^2 d\xi < \epsilon \tag{10}$$

and

$$\int_{\mathbb{R}^n - K} |u(\xi)|^2 d\xi < \epsilon. \tag{11}$$

Since $u \in Q$, $u = DG[\phi](b)$ for some $b \in B$. Starting from the definition (7), applying the Plancherel theorem and the estimate $\|(fe^{i\phi})\hat{}\|_\infty \leq \|f\|_1$ yields

$$\int_{\mathbb{R}^n} |u(\xi + h) - u(\xi)|^2 d\xi \leq 4\|b\|_2^2 \, \|f\|_1^2 \, \|f(e^{-2\pi i x \cdot h} - 1)\|_\infty^2.$$

Since $|f| \to 0$ as $|x| \to \infty$ and $\|b\|_2$ is bounded, we can choose $\delta > 0$ small enough that

$$\|f(e^{-2\pi i x \cdot h} - 1)\|_\infty < \frac{\epsilon}{4\|f\|_1 \|b\|_2}$$

for all $|h| < \delta$, proving (10).

With similar estimates we can bound (11):

$$\int_{\mathbb{R}^n - K} |u(\xi)|^2 d\xi \leq 4\|(fe^{i\phi})\hat{}\|_{L^\infty(\mathbb{R}^n - K)}^2 \|b\|_2^2 \, \|f\|_\infty^2.$$

Since $fe^{i\phi} \in L^1$, the Riemann-Lebesgue Theorem (see for example [16]) implies that $|(fe^{i\phi})^\wedge|(\xi) \to 0$ as $|\xi| \to \infty$. Thus the bounded set K may be chosen large enough so that

$$\|(fe^{i\phi})^\wedge\|_{L^\infty(\mathbb{R}^n - K)} < \frac{\epsilon}{2\|b\|_2 \, \|f\|_\infty}.$$

□

Although Theorem 3.2 gives no indication of the rate at which the singular values of DG decay to zero, there is reason to believe that this decay rate can be fast. Indeed, taking f as the Gaussian $f(x) = e^{-\pi|x|^2}$, the phase $\phi = 0$, and perturbations $\delta\phi_k(x) = ie^{2\pi i k \cdot x}$, one can calculate explicitly that

$$\|DG(\delta\phi_k)\|_2 = \mathcal{O}(e^{-|k|}) \quad \text{as } |k| \to \infty.$$

This example indicates that high-frequency components in the perturbation $\delta\phi$ may become damped so rapidly that there is little hope of recovering them accurately in the presence of noise.

By considering even and odd parts of the functions $f, \phi, \delta\phi$, it is also possible to identify cases in which DG has a nontrivial null space. The following lemma is an easy consequence of the properties of the Fourier transform on even and odd functions.

LEMMA 3.3. *If ϕ is an odd function, f is either even or odd, and $\delta\phi$ is even, then* $DG[\phi](\delta\phi) = 0$.

A key issue which we have chosen to ignore is that of determining conditions which ensure that DG is injective on L^2, aside from the special cases covered by Lemma 3.3. For the present purposes, our "remedy" for the apparent lack of injectivity of DG is simply to regularize the problem.

Given parameters $\beta > 0$ and $s > 0$ we reformulate problem (5) as the Tikhonov regularized problem

$$\min_{\phi \in L^2} J_\beta[\phi] = \frac{1}{2}\|G[\phi] - g\|_2^2 + \frac{\beta}{2}\|B_s\phi\|_2^2, \tag{12}$$

where B_s is defined by

$$(B_s\phi)(x) = \left[(1 + |\xi|^2)^{\frac{s}{2}}\hat{\phi}(\xi)\right]^\vee(x). \tag{13}$$

From the definition of B_s,

$$\|B_s\phi\|_2 = \|\phi\|_{H^s},$$

where $H^s = W^{s,2}(\mathbb{R}^n)$ is the usual Sobolev space on $\mathbb{R}^n$. See for example Adams [1] Chapter 7 for properties of the space H^s.

This regularization was chosen for two reasons. First, it stabilizes the linearized inverse problem. This will be made more precise in the next section. Second, if one can bound ϕ in H^s for $s > \frac{n}{2}$, it can be shown that the map G is sufficiently differentiable to obtain quick convergence from Newton's method. This is proved in the Appendix.

A discussion of regularization methods in the context of similar problems arising in diffractive optics can be found in [3].

The regularization provides as a "fringe benefit" a guarantee that a solution to problem (12) exists, provided that we only allow solutions which are supported on some bounded set Ω.

LEMMA 3.4. *Let $\Omega \subset \mathbb{R}^n$ be bounded. For all $f \in L^1 \cap L^\infty$, $g \in L^2$, $\beta > 0$, and integral values of $s > 0$, problem (12) has a minimizer $\phi_* \in L^2(\Omega)$.*

Proof. This is a simple consequence of the compact imbedding properties of the Sobolev space H^s (see [1], Theorem 6.2) and the continuity of G over L^2, which is proved in Lemma A.1. □

As we mentioned at the end of Section 2, solutions are at best unique only within a class of functions defined on the support of f, so in the (practical) case that $\Omega = \operatorname{supp} f$ is bounded, Lemma 3.4 gives the existence of an "actual" solution.

A pertinent question which will *not* be treated here is the accuracy of the reconstruction obtained by solving (12). Intuitively, if one can bound $\|\phi\|_{H^s}$ *a priori* then estimates of the accuracy of the regularized reconstruction should be possible. In Section 5 it will be demonstrated that it is possible in practice to obtain quite accurate reconstructions from (12) by taking β small.

4. Implementation and convergence of Newton's method. In this section, we describe an efficient implementation of Newton's method and show that the method is locally almost quadratically convergent on the regularized problem (12).

We begin with a brief derivation of Newton's method. Consider the formal derivative of the function $J[\phi]$ at ϕ in the direction $\delta\phi$:

$$\begin{aligned} DJ[\phi](\delta\phi) &= \langle DG[\phi](\delta\phi), G[\phi] - g\rangle \\ &= \langle \delta\phi, DG^t[\phi](G[\phi] - g)\rangle, \end{aligned} \tag{14}$$

where the angle brackets denote the L^2 inner product, and $DG^t[\phi](\cdot)$ is the L^2 adjoint of $DG[\phi](\cdot)$. From (14), the second derivative of J in the directions $\delta\phi_1, \delta\phi_2$ is the bilinear form

$$\begin{aligned} D^2J[\phi](\delta\phi_1, \delta\phi_2) &= \langle D^2G[\phi](\delta\phi_1, \delta\phi_2), G[\phi] - g\rangle \\ &+ \langle DG[\phi](\delta\phi_1), DG[\phi](\delta\phi_2)\rangle \\ &= \langle \delta\phi_1, D^2G^t[\phi](\delta\phi_2, G[\phi] - g) + DG^t[\phi]DG[\phi](\delta\phi_2)\rangle. \end{aligned} \tag{15}$$

Here, $D^2G^t[\phi]$ is the bilinear form on $L^2 \times L^2$ defined by

$$\langle D^2G[\phi](\delta\phi_1, \delta\phi_2), \psi\rangle = \langle \delta\phi_2, D^2G^t[\phi](\delta\phi_1, \psi)\rangle \tag{16}$$

where $\psi \in L^2$. We define the *Hessian* at ϕ acting on $\delta\phi$ by

$$H[\phi](\delta\phi) = D^2G^t[\phi](\delta\phi, G[\phi] - g) + DG^t[\phi]DG[\phi](\delta\phi). \tag{17}$$

Expanding $J[\phi]$ in a Taylor series to two terms, one obtains a *quadratic model* of J at ϕ:

$$J[\phi + \delta\phi] \approx J[\phi] + DJ[\phi](\delta\phi) + \frac{1}{2}D^2J[\phi](\delta\phi, \delta\phi). \tag{18}$$

Newton's method is an iterative algorithm which at each iteration k seeks the step $\delta\phi_k$ which minimizes the quadratic model (18). From (14),(15),(17), this is equivalent to solving the linear equation

$$H[\phi_k](\delta\phi_k) = -DG^t[\phi_k](G[\phi_k] - g). \tag{19}$$

The next iterate is then defined by $\phi_{k+1} = \phi_k + \delta\phi_k$ and the iteration continues until convergence. For the regularized functional J_β from problem (12), the Hessian H_β is

$$H_\beta[\phi](\delta\phi) = H[\phi](\delta\phi) + \beta B_s^t B_s \delta\phi. \tag{20}$$

Defining the *gradient* of J_β at ϕ

$$E_\beta[\phi] = DG^t[\phi](G[\phi] - g) + \beta B_s^t B_s \phi, \tag{21}$$

the Newton iteration for problem (12) can be written

$$\phi_{k+1} = \phi_k - H_\beta^{-1}[\phi_k]\left(E_\beta[\phi_k]\right). \tag{22}$$

Newton's method (22) cannot be expected to converge for starting points far from a solution, or in the event that $\|H_\beta^{-1}\|$ is large or unbounded. The method can be made robust with the addition of a "globalization strategy". We will make use of a particular globalization strategy called the *trust-region* approach.

In the trust-region strategy, at each iteration the linear subproblem

$$H_\beta[\phi_k](\delta\phi_k) = -E_\beta[\phi_k]$$

is constrained so that the step $\delta\phi_k$ must lie inside a ball of a certain radius (the trust-region). The radius is chosen at each step on the basis of how well the quadratic model is "trusted" as an accurate description of the behavior of J_β. This is equivalent to replacing iteration (22) with

$$\phi_{k+1} = \phi_k - (H_\beta[\phi_k] + \mu_k I)^{-1} E_\beta[\phi_k], \tag{23}$$

where $\mu_k = 0$ if the Newton step lies inside the trust-region, and $\mu_k > 0$ otherwise. (Larger μ_k corresponds to a smaller trust-region radius.) If the trust-region radius is chosen properly at each step, it can be shown under minimal assumptions that the globalized method (23) will converge to a local minimizer from any starting point. See Dennis and Schnabel [6] for a complete discussion of this strategy. The key fact we will use is that the trust-region can always be chosen so that $J_\beta(\phi_{k+1}) \leq J_\beta(\phi_k)$ at each step k. In fact, most trust-region strategies insist on much stronger decrease conditions. To retain the quick convergence of Newton's method, the trust region radius must not shrink faster than the step length: we assume that there is some constant C_1 such that $\mu_k \leq C_1\|\phi_k - \phi_*\|_2$ for all k.

Before proving the convergence of the method, we first complete our discussion by calculating the adjoint derivatives DG^t, D^2G^t and describing an efficient implementation.

From (7) and the definition of DG^t

$$\langle DG[\phi](\delta\phi), \psi\rangle = \langle \delta\phi, DG^t[\phi](\psi)\rangle,$$

a simple change in the order of integration (Fubini's theorem) yields

$$DG^t[\phi](\psi) = 2Re[ife^{i\phi}(F^*[\phi]\psi)\hat{}\,]. \tag{24}$$

From the chain rule, $D^2G = 2Re(F^*D^2F) + 2DF^*DF$. Starting from the definition (16) a simple calculation yields

$$\begin{aligned} D^2G^t[\phi](\delta\phi, \psi) &= -2Re[\delta\phi f e^{i\phi}(F^*[\phi]\psi)\hat{}\,] \\ &+ 2ife^{i\phi}[DF^*[\phi](\delta\phi)\psi)]\hat{}\,. \end{aligned} \tag{25}$$

Observe that to compute the Hessian $H[\phi](\cdot)$ acting on a function $\delta\phi$ only requires the calculation of Fourier transforms and multiplication of functions (or convolutions). In the computer implementation of Newton's method this can be exploited when solving for the step (19) or (22) if rather than discretizing and storing the operator $H[\phi](\cdot)$ as a matrix to explicitly solve the linear equation, one uses an iterative linear systems solver such as the conjugate gradient (CG) method. For a detailed description of the CG method, see for example Golub and Van Loan [12], Chapter 10. The main advantage of the CG method is that the matrix representation for the Hessian $H[\phi](\delta\phi)$ never needs to be computed; one only needs to be able to calculate the action of the Hessian on a given vector. Using the fast Fourier transform one can directly calculate the action $H[\phi](\delta\phi)$ from the formulae (24), (25) in $\mathcal{O}(N \log N)$ time, where N is the number of discretization points. The use of the CG method saves computational time and storage space since the matrix is never needed explicitly. In addition, the CG method can be incorporated into the globalization strategy. Dembo, Eisenstat, and Steihaug have established a rule for terminating the CG iteration based upon a trust-region test and shown that the quick local convergence of Newton's method can be retained [5]. The reader is referred to [5] for a more complete description of this strategy. See also [15] Sect. 2, and [11], p.153.

We next prove the local convergence of the Newton iteration (23), the main result of this paper.

THEOREM 4.1. *Assume that $f \in L^1 \cap L^\infty$, and $g \in L^1 \cap L^2$. Let $s > \frac{n}{2}$ and $\beta > 0$ be given, along with a number $M > 0$. Let ϕ_* be a solution to problem (12) and assume that at ϕ_*, the Hessian $H_\beta[\phi_*]$ is uniformly positive definite: there exists $\gamma > 0$ such that*

$$\langle H_\beta[\phi_*]\delta\phi, \delta\phi\rangle_2 \geq \gamma\|\delta\phi\|_2^2, \tag{26}$$

for all $\delta\phi \in L^2$. Then there exists an $\epsilon > 0$ such that for all starting points ϕ_0 with $\|\phi_0 - \phi_*\|_2 < \epsilon$ and $\|B_s\phi_0\|_2 \leq M$, the globalized Newton iteration (23) is well-defined, converges to ϕ_* in L^2 and satisfies

$$\|\phi_{k+1} - \phi_*\|_2 \leq C\|\phi_k - \phi_*\|_2^r, \tag{27}$$

where $r = \frac{4s-n}{2s} > 1$ *and* C *is a constant independent of* k.

By choosing s large, r can by made arbitrarily close to 2; this is what we mean by "almost quadratic" convergence. Notice also that the convergence rate r is independent of β. Thus in principle β can be taken arbitrarily small.

Proof. of Theorem 4.1.
Most of this proof is based upon Dennis and Schnabel [6], Theorem 5.2.1. Since the globalization strategy requires that $J_\beta(\phi_{k+1}) \leq J_\beta(\phi_k)$ for each iteration k, it follows from Lemma 2.1 that all iterates are uniformly bounded in the Sobolev space H^s:

$$\frac{\beta}{2}\|\phi_k\|_{H^s}^2 \leq J_\beta[\phi_k] \leq J_\beta[\phi_0] \leq C_0 + \frac{\beta}{2}M^2.$$

Let $N = [\frac{2}{\beta}C_0 + M^2]^{1/2}$, so $\|\phi_k\|_{H^s} \leq N$ for all k. It follows from Lemma A.3, that there exists a number $\epsilon_1 > 0$ such that for all ϕ with $\|\phi - \phi_*\|_2 < \epsilon_1$ and $\|\phi\|_{H^s} \leq N$ we have

$$\langle H_\beta[\phi]\delta\phi, \delta\phi\rangle_2 \geq \frac{\gamma}{2}\|\delta\phi\|_2^2.$$

Thus since $\mu_k \geq 0$, at each iterate ϕ_k we have

$$\|(H_\beta[\phi_k] + \mu_k I)^{-1}\|_{2,2} \leq \frac{2}{\gamma},$$

where $\|\cdot\|_{2,2}$ denotes the operator norm over L^2. It is easy to check that J_β is Gateaux differentiable over the domain of $B_s^t B_s$. Since ϕ_* is a minimizer it follows from the variational inequality that the gradient $E_\beta[\phi_*] = 0$. From (23),

$$\phi_1 - \phi_* = (H_\beta[\phi_0] + \mu_0 I)^{-1}\left[E_\beta[\phi_*] - E_\beta[\phi_0] - (H_\beta[\phi_0] + \mu_0 I)(\phi_* - \phi_0)\right].$$

Using Lemma A.2 and the fact that $\mu_k \leq C_1\|\phi_k - \phi_*\|_2$ yields

$$\|\phi_1 - \phi_*\|_2 \leq \frac{2}{\gamma}\left[C_4\|\phi_0 - \phi_*\|_2^{r-1} + C_1\|\phi_0 - \phi_*\|_2\right]\|\phi_0 - \phi_*\|_2. \tag{28}$$

Choosing $\epsilon = \min\left\{\epsilon_1, 1, \left[\frac{\gamma}{4(C_4+C_1)}\right]^{\frac{1}{r-1}}\right\}$ then guarantees that

$$\|\phi_1 - \phi_*\|_2 \leq \frac{1}{2}\|\phi_0 - \phi_*\|_2. \tag{29}$$

Proceeding by induction, (29) proves that the sequence $\{\phi_k\}$ converges to ϕ_* in L^2. The estimate of the convergence rate (27) follows from (28). □

The hypothesis (26) that the Hessian $H_\beta[\phi_*]$ is positive definite has some justification. First, in the case we hope for: that $G[\phi_*] - g = 0$, it is clear from (17) that the unperturbed Hessian $H[\phi_*]$ is at least positive semidefinite, then from (20), $H_\beta[\phi_*]$ satisfies (26) with $\gamma = \beta$. Second, notice that $H_\beta[\phi_*]$ must in all cases be at least positive semidefinite, otherwise ϕ_* cannot be a local minimizer. Finally, it is always possible to *force* the estimate (26): the unperturbed Hessian $H[\phi]$ has operator norm uniformly bounded over all ϕ, so one can simply choose β larger than the absolute value of the minimum negative eigenvalue of $H[\phi]$ (this effectively "convexifies" the problem).

While Theorem 4.1 only guarantees the *local* convergence of the method, in numerical experiments with the trust-region globalization, the method behaves very robustly, converging to a local minimizer from almost every starting point, and still exhibits the quick local convergence predicted by (27).

5. Numerical examples. In this section we indicate the results of some numerical experiments carried out using the method described in Section 4. In all of the following computations, Fourier transforms were performed using the Fast Fourier Transform (FFT). For simplicity, all of the examples take place in one dimension; however the method is still very computationally feasible for two dimensional problems. The domain of the functions f, ϕ, is taken to be the interval $[-1,1]$. In the following examples, functions with support outside this interval are truncated.

Before solving any problems, we wish to demonstrate with a simple example that without regularization, the gradient of the objective functional $J[\phi]$ is not differentiable over L^2. For $f(x) = e^{-4|x|^2}$, $\phi(x) = \cos 2.88x$ and $\delta\phi_{a,b} = a\chi_{[-b,b]}$, we calculated the quotient

$$q(a,b) = \frac{\|E[\phi + \delta\phi_{a,b}] - E[\phi] - H[\phi](\delta\phi_{a,b})\|_2}{\|\delta\phi_{a,b}\|_2} \tag{30}$$

in two cases:

1. the support $[-b,b]$ of $\delta\phi_{a,b}$ is fixed while the height $a \downarrow 0$;
2. the height a of $\delta\phi_{a,b}$ is fixed while $b \downarrow 0$.

In the first case, *both* $\|\delta\phi_{a,b}\|_2$ *and* $\|\delta\phi_{a,b}\|_\infty$ decrease linearly to zero with a. Figure 1 indicates that the quotient $q(a,b)$ also decreases to zero at a rate proportional to a, behavior one would expect from a differentiable function.

In the second case, $\|\delta\phi_{a,b}\|_2 \downarrow 0$ proportionally to $\sqrt{b}$, but $\|\delta\phi_{a,b}\|_\infty = a$. Figure 2 shows that in this case, the quotient $q(a,b)$ does *not* have limit zero, but rather converges to some constant $C > 0$. Thus as a function over L^∞ the gradient is Fréchet differentiable, but *not* as a function over L^2; this fact is proved in the Appendix (see Lemma A.2). This "nondifferentiable" behavior combined with the instability of the problem are responsible for the less than quadratic convergence we obtain from Newton's method.

We demonstrate the method with two simple examples from diffractive optics. We mention that since we are computing discrete Fourier transforms, all functions are implicitly periodic, and the target variable ξ is a discrete value: $\xi \in \{0, \pm 1, \pm 2, \ldots\}$.

The first example concerns the design of a simple diffraction grating. The answer is known explicitly; this provides an opportunity to check convergence. In this example, we actually achieved better performance from the method when the regularization term β was chosen to be zero. Although the convergence rate did increase with $\beta > 0$, the method converged quite quickly even with $\beta = 0$, and the reconstruction was more accurate. Thus, for this example we set $\beta = 0$. Let $f(x) = 1$, and $g(\xi) = \delta(\xi - n)$ for some integer n, where $\delta(x)$ is the Kronecker delta. Thus $g = G[\phi_*]$ where $\phi_*(x) = nx$.

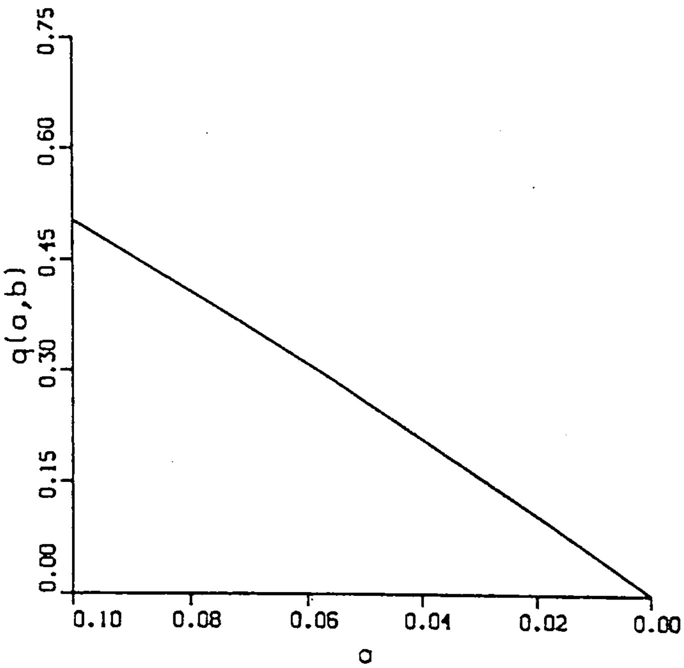

FIG. 1. *The quotient* $q(a, 0.2)$ *as* $a \downarrow 0$.

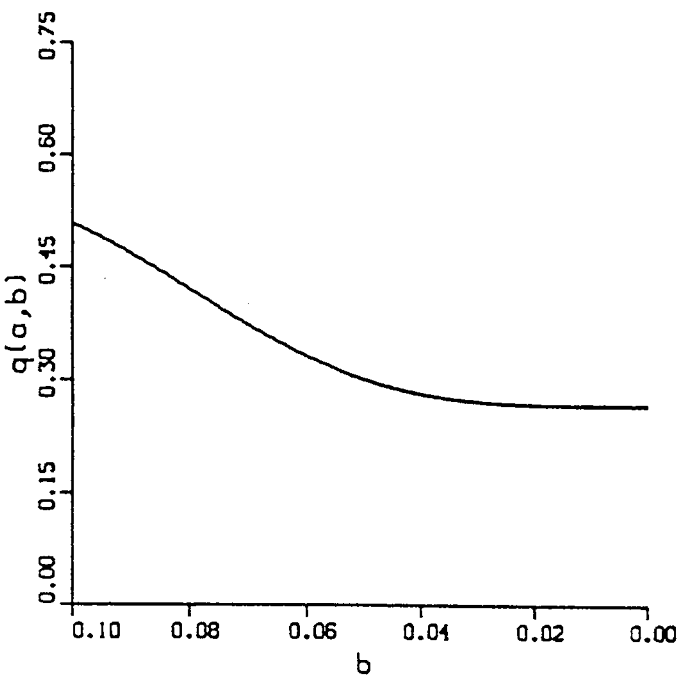

FIG. 2. *The quotient* $q(0.1, b)$ *as* $b \downarrow 0$.

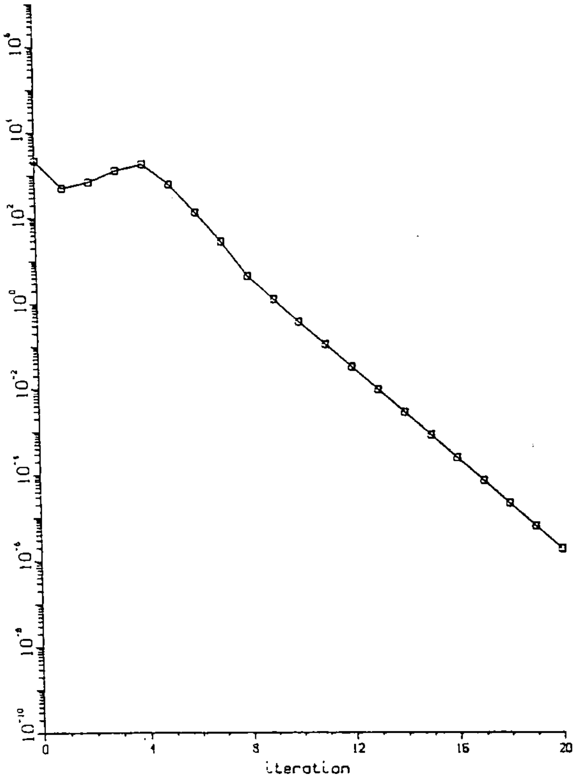

FIG. 3. L^2 *norm of gradient versus iteration number for the first example.*

We chose $n = 5$ and took as a starting guess $\phi_0(x) = \frac{1}{2}\cos 2\pi x$. The number of discretization points N is 256. Figure 3 shows the L^2 norm of the gradient of $J[\phi_k]$ versus the iteration number k. The reconstructed phase (modulo 2π) is shown in Figure 4; the reconstruction is essentially exact up to numerical roundoff error. We found that the method converged to this solution from essentially all starting points. In general, for problems with an exact solution ϕ_* such that $G[\phi_*] = g$, the method converged to a solution quickly without the regularization term.

The second example is somewhat less trivial. In this example, a diffractive lens in illuminated by a monochromatic laser beam with Gaussian intensity profile $f(x) = e^{-4|x|^2}$. A lens profile ϕ_* is sought which results in a specified far-field intensity pattern $g(\xi)$, say the one pictured in Figure 5. As far as we know, there is no exact solution. In this example, the regularization parameter β had a substantial effect on the convergence of the method. We illustrate two runs of the method, one with the parameter $\beta = 0$, another with $\beta = 5 \times 10^{-5}$ and $s = \frac{3}{4}$. The number of discretization points is $N = 128$. Starting from the initial profile $\phi_0(x) = \pi(1 - |x|)$, the L^2 norm of the gradient versus iteration number for $\beta = 0$ is shown in Figure 6. For this run, the iteration was stopped after 60 steps even though no real convergence had taken place. With $\beta = 5 \times 10^{-5}$, Figure 7 indicates that near the minimizer (starting at about iteration 12) the convergence was almost quadratic. The final phase profiles for the runs with $\beta = 0$ and $\beta = 5 \times 10^{-5}$ are shown in Figures 8 and 9, respectively. Notice that due to the regularization, the solution in Figure 9 is slightly "smoother" than the one in Figure 8. The final far-field intensity patterns for the runs with $\beta = 0$ and $\beta = 5\times10^{-5}$ are shown in Figures 10 and 11, respectively. Comparison of Figure 5 with Figures 10 and 11 reveals that a reasonable solution was obtained with or without regularization.

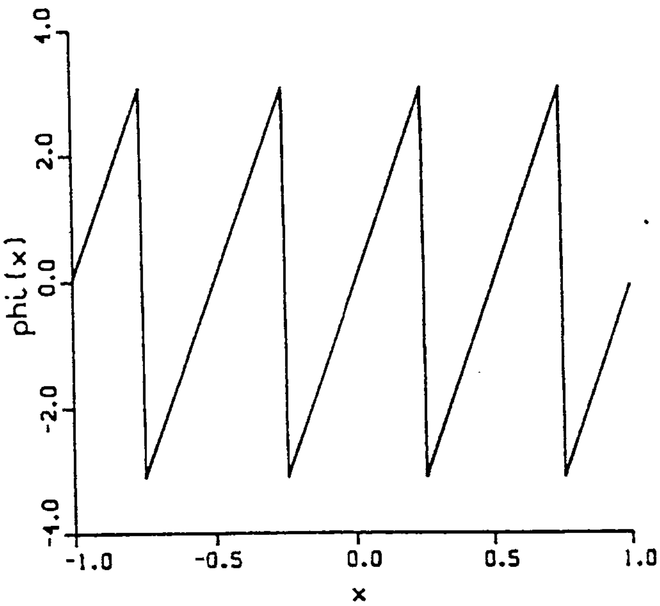

FIG. 4. *Reconstructed phase profile ϕ_* for the first example.*

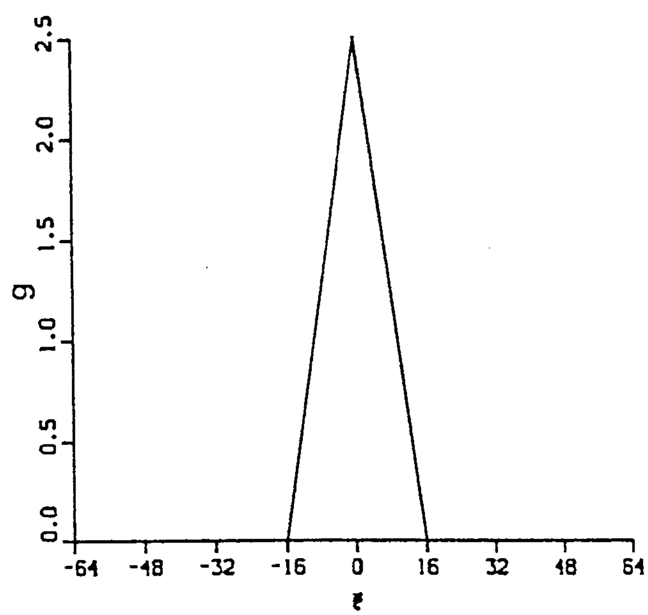

FIG. 5. *Desired far-field intensity pattern g for second example.*

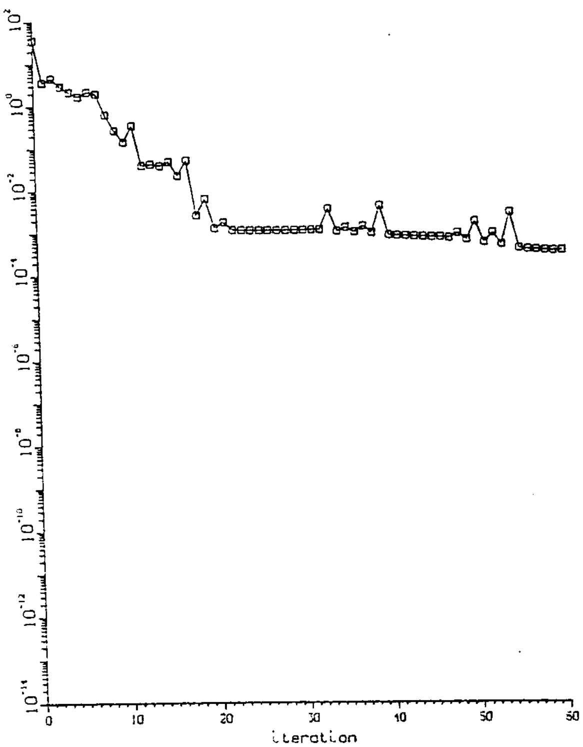

FIG. 6. L^2 *norm of gradient versus iteration number for* $\beta = 0$.

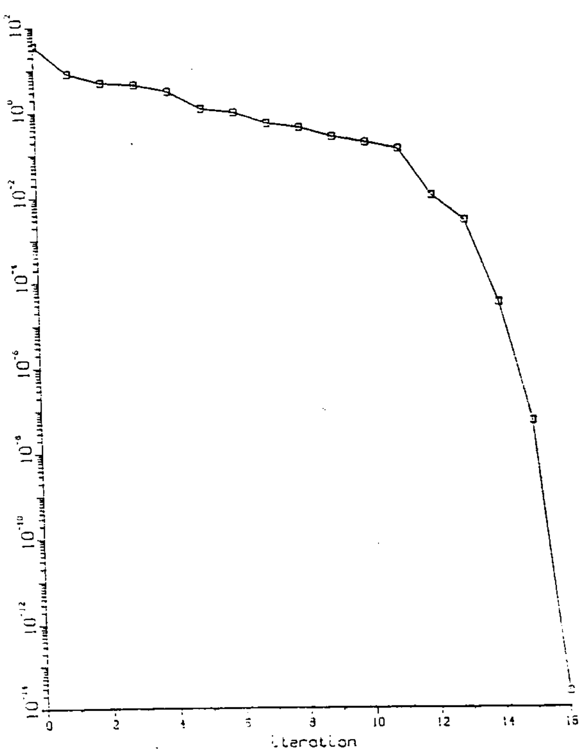

FIG. 7. L^2 *norm of gradient versus iteration number for* $\beta = 5 \times 10^{-5}$.

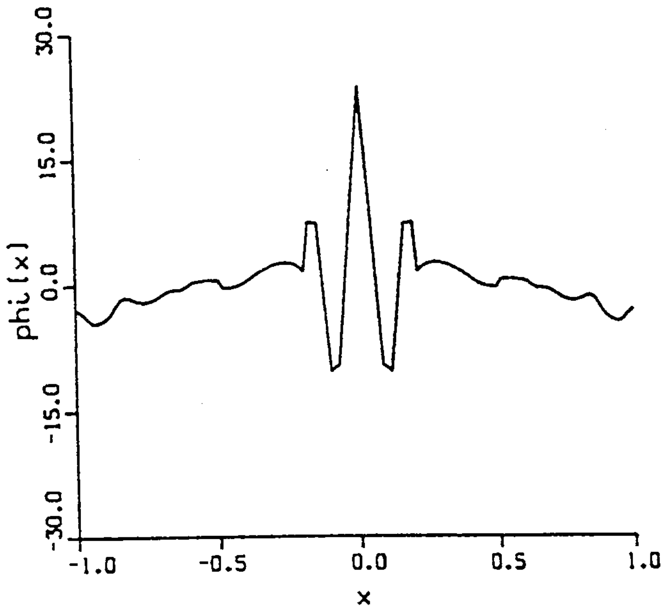

FIG. 8. *Final phase profile* ϕ_* *for* $\beta = 0$.

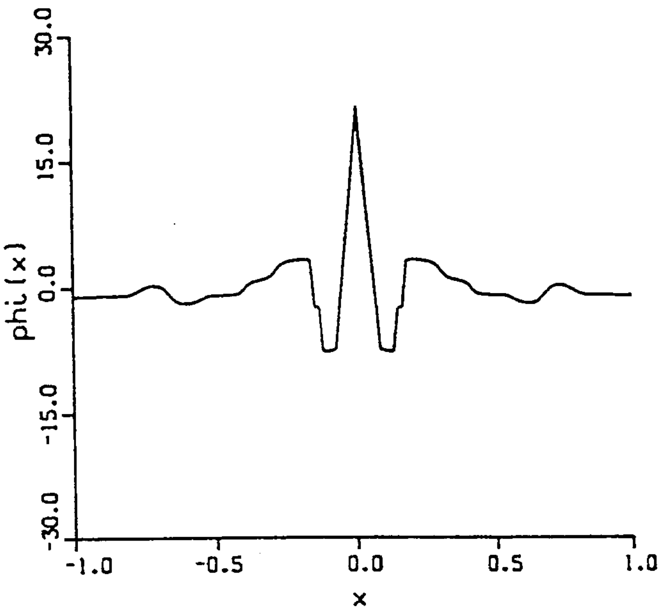

FIG. 9. *Final phase profile* ϕ_* *for* $\beta = 5 \times 10^{-5}$.

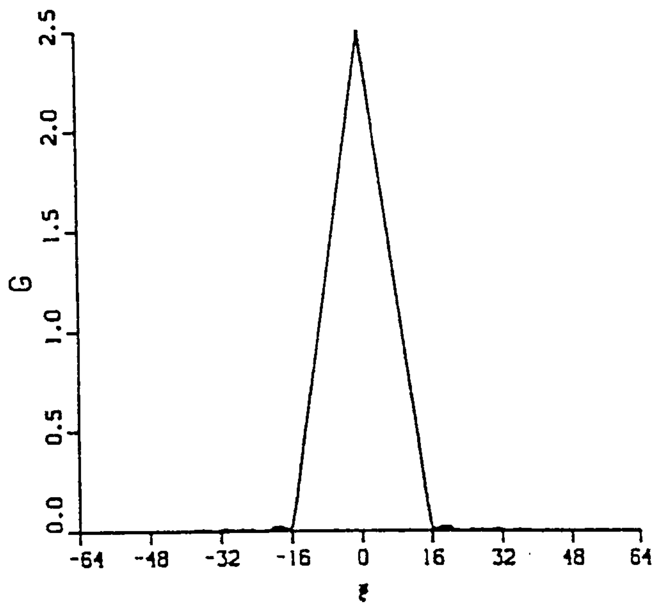

FIG. 10. *Final far-field intensity pattern* $G[\phi_*]$ *for* $\beta = 0$.

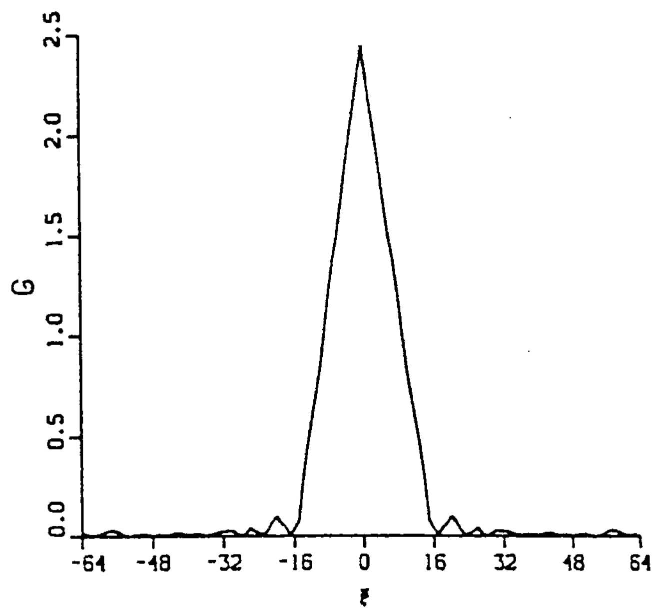

FIG. 11. *Final far-field intensity pattern* $G[\phi_*]$ *for* $\beta = 5 \times 10^{-5}$.

However, the method converged much faster with the regularization, as predicted by Theorem 4.1. From almost every starting point, the method seemed to converge to a phase profile which resulted in a close match with the target; however, different starting points often resulted in very different "solutions".

A. Appendix: regularity estimates. In this section we establish the regularity estimates necessary to prove Theorem 4.1. As mentioned earlier, it turns out that for this problem the gradient $DG^t(G-g)$ is not Fréchet differentiable over L^2. A proof of this fact will be given near the end of this section; numerical results with the same conclusion are given in Section 5.

It is interesting that the function F from which G is constructed is not even once Fréchet differentiable as a function over L^2. This fact is demonstrated with the following simple example. Let $\chi_{[0,b]}$ denote the characteristic function of the interval $[0,b]$. Define $f=\chi_{[0,1]}$, $\phi=0$, and $\delta\phi_b = a\chi_{[0,b]}$ for some fixed real number $a \neq 0$. It follows from Plancherel's theorem that

$$\|F[\phi+\delta\phi_b]-F[\phi]-DF[\phi](\delta\phi_b)\|_2 = (\int_0^b |e^{ia}-1-ia|^2)^{1/2} = |c|b^{1/2},$$

where c is the value of the constant expression under the integral sign. Then since $\|\delta\phi_b\|_2 = |a|b^{1/2}$, we have

$$\lim_{b\downarrow 0}\frac{\|F[\phi+\delta\phi_b]-F[\phi]-DF[\phi](\delta\phi_b)\|_2}{\|\delta\phi_b\|_2} = \frac{|c|}{|a|} > 0.$$

Thus DF is not the Fréchet derivative of F over L^2. It is perhaps reassuring that DF *is* the Fréchet derivative of F as a function from L^2 into L^∞; this fact facilitates the proof that G is regular (once Fréchet differentiable) over L^2, as will be established in the following lemma.

LEMMA A.1. *Assume $f\in L^1\cap L^\infty$. Then there exist constants C_2, C_3 depending only on f such that the following inequalities hold:*

$$\|G[\phi+\delta\phi]-G[\phi]\|_2 \le C_2\|\delta\phi\|_2, \tag{31}$$

$$\|G[\phi+\delta\phi]-G[\phi]-DG[\phi](\delta\phi)\|_2 \le C_3\|\delta\phi\|_2^2. \tag{32}$$

Proof. In this and the proofs that follow, C will denote a "generic" constant which depends only on f; the value of C may change from line to line.

Plancherel's theorem yields the estimate

$$\|F[\phi+\delta\phi]-F[\phi]\|_2 \le 2\|f\|_\infty\|\delta\phi\|_2. \tag{33}$$

Expressing $G=F^*F$, and using the fact that $\|F^*[\phi+\delta\phi]+F^*[\phi]\|_\infty \le 2\|f\|_1$, (31) then holds with $C_2 = 4\|f\|_1\|f\|_\infty$.

It is easy to estimate

$$\|F[\phi+\delta\phi]-F[\phi]-DF[\phi](\delta\phi)\|_\infty \le 2\|f\|_\infty\|\delta\phi\|_2^2. \tag{34}$$

It is also easy to check that

$$\|DF^*[\phi](\delta\phi)\|_\infty, \|DF[\phi](\delta\phi)\|_2 \leq C\|\delta\phi\|_2. \tag{35}$$

Using these facts, one can estimate the left hand side of (32), expanding $G = F^*F$ and using L^∞ estimates and the triangle inequality to obtain the inequality (32). □

We will now show that with the smoothness constraint on ϕ imposed by the regularization, the gradient of $J[\phi]$ is differentiable in the sense needed to prove Theorem 4.1. The lemma will be followed by an example which shows that without the regularization, the gradient of $J[\phi]$ is not Fréchet differentiable over L^2.

LEMMA A.2. *Let $f \in L^1 \cap L^\infty$, $g \in L^1 \cap L^2$, let ϕ be measurable and assume $\|\delta\phi\|_{H^s} \leq K$ for some $s \geq n/4$. Then there exists a constant C_4 depending only on f, K, and s such that*

$$\|DG^t[\phi+\delta\phi](G[\phi+\delta\phi]-g) - DG^t[\phi](G[\phi]-g) - H[\phi](\delta\phi)\|_2 \leq C_4\|\delta\phi\|_2^r, \tag{36}$$

where $r = \frac{4s-n}{2s}$.

Proof. As this is a straightforward argument, we omit some details. Let $R = fe^{i\phi}(e^{i\delta\phi} - 1 - i\delta\phi)$, so $F[\phi+\delta\phi] = F[\phi] + DF[\phi](\delta\phi) + \hat{R}$. To simplify notation, we shall henceforth drop the argument from all functions which depend only on ϕ. Using the formulas (7),(24),(25), and rearranging terms, one can write the left hand side of (36) as

$$\begin{aligned} &\|Re\{ife^{i\phi}[F^*(G[\phi+\delta\phi] - G - DG(\delta\phi))]^\frown + ife^{i\phi}[DF^*(\delta\phi)(G[\phi+\delta\phi] - G)]^\frown \\ &+\delta\phi f e^{i\phi}[F^*(G[\phi+\delta\phi] - G)]^\frown + \delta\phi f e^{i\phi}[DF^*(\delta\phi)G[\phi+\delta\phi]^\frown \\ &+(ife^{i\phi} + \delta\phi f e^{i\phi})[\hat{R}^* G[\phi+\delta\phi]]^\frown + R[(F^*[\phi+\delta\phi])G[\phi+\delta\phi]]^\frown\}\|_2. \end{aligned} \tag{37}$$

Applying Lemma A.1, (35), and Plancherel's theorem, one can bound the L^2 norms of the first five terms in the sum above by $C\|\delta\phi\|_2^2$. The remaining term

$$\|Re\{R[F^*[\phi+\delta\phi]G[\phi+\delta\phi]]^\frown\}\|_2 \tag{38}$$

cannot by bounded by $C\|\delta\phi\|_2^2$. However, it is easy to see that

$$\|R\|_2 \leq C\|\delta\phi\|_4^2. \tag{39}$$

Estimates similar to those above then yield

$$\|R[F^*[\phi+\delta\phi]G[\phi+\delta\phi]]^\frown\|_2 \leq C\|\delta\phi\|_4^2. \tag{40}$$

(We note in passing that it follows immediately from (40) that one can also bound (38) by $C\|\delta\phi\|_2\|\delta\phi\|_\infty$; with a slightly different estimate, (38) can be bounded by $C\|\delta\phi\|_\infty^2$ as well. This explains the behavior observed numerically in Section 5 when calculating the quotient $q(a,b)$ defined in (30).)

From the Sobolev Imbedding Theorem and the interpolation properties of the Sobolev norms (see Adams [1], Theorems 7.58 and 4.17) we have

$$\begin{aligned} \|\delta\phi\|_4^2 &\leq C\|\delta\phi\|_{H^s}^{\frac{n}{2s}}\|\delta\phi\|_{L^2}^{\frac{4s-n}{2s}} \\ &= CK^{\frac{n}{2s}}\|\delta\phi\|_2^r, \end{aligned}$$

hence (36) follows from (40). □

We now show that the gradient of $J[\phi]$ is not Fréchet differentiable over L^2. Setting $f = \chi_{[-1,1]}$, $\phi = 0$, $\delta\phi_b = a\chi_{[-b,b]}$, we have $\|\delta\phi_b\|_2 = a\sqrt{2b}$. One can compute directly that for b sufficiently small,

$$\inf_{\xi\in[-b,b]} |[F^*[\phi + \delta\phi_b]G[\phi + \delta\phi_b]]^\wedge(\xi)| \geq c_0 > 0.$$

We then have

$$\|Re\{R[F^*[\phi + \delta\phi_b]G[\phi + \delta\phi_b]]^\wedge\}\|_2 \geq c_0 M\sqrt{2b},$$

where $M = |Re\{i(e^{ia} - 1 - ia)\}|$. Since the remaining terms in the expression (37) are $\mathcal{O}(\|\delta\phi_b\|_2^2) = \mathcal{O}(b)$, we can conclude that for b sufficiently small,

$$\|DG^t[\phi + \delta\phi_b](G[\phi + \delta\phi_b] - g) - DG^t(G - g) - H(\delta\phi_b)\|_2 \geq c\sqrt{b}.$$

Thus

$$\lim_{b\downarrow 0} \frac{\|DG^t[\phi + \delta\phi_b](G[\phi + \delta\phi_b] - g) - DG^t(G - g) - H(\delta\phi_b)\|_2}{\|\delta\phi_b\|_2} \geq c > 0. \tag{41}$$

It is worth noticing that for any sequence $\{\delta\phi_k\}$ for which *both* $\|\delta\phi_k\|_2 \to 0$ and $\|\delta\phi_k\|_\infty \to 0$, the limit (41) is zero (this follows from estimate (40)).

Finally, we prove the following continuity estimate for the Hessian operator $H[\phi]$ defined in (17). This lemma is used in the proof of Theorem 4.1.

LEMMA A.3. *Let f, g satisfy the hypotheses of Lemma A.2. Let $s > n/2$ and $N > 0$ be given. Then there exist constants $C > 0$ and $\delta > 0$ such that for all ϕ_1, ϕ_0 satisfying $\|\phi_1 - \phi_0\|_{H^s} \leq N$ and all $\delta\phi \in L^2$,*

$$\|(H[\phi_1] - H[\phi_0])(\delta\phi)\|_2 \leq C\|\delta\phi\|_2\|\phi_1 - \phi_0\|_2^\delta. \tag{42}$$

Proof. Using the same straightforward techniques as in the previous lemmas, one can establish that

$$\|(H[\phi_1] - H[\phi_0])\delta\phi\|_2 \leq C\|\delta\phi\|_2\|\phi_1 - \phi_0\|_\infty.$$

Choose some s_0 such that $s > s_0 > n/2$. Using the Sobolev Imbedding Theorem and interpolating yields

$$\begin{aligned} \|\phi_1 - \phi_0\|_\infty &\leq \|\phi_1 - \phi_0\|_{H^{s_0}} \\ &\leq CN^{\frac{s_0}{s}}\|\phi_1 - \phi_0\|_{L^2}^\delta, \end{aligned}$$

where $\delta = \frac{s-s_0}{s}$. □

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