Radiation, for example electrons or x rays, can be scattered from an object to determine its structure. This usually involves obtaining the wave function at the exit surface of the object, which is what is referred to as the “object” by optical researchers—a complex exit surface wave function is synonymous with a complex-valued object. Retrieving the exit surface wave function from a focal series of images (intensities or moduli squared of the propagating wave function in a series of planes with different defocus values), rather than the diffraction pattern, has two significant disadvantages. In practice, forming an image can be difficult (x rays) and the imaging system usually has aberrations which reduce resolution (electrons). Therefore imaging from a diffraction pattern, “lensless imaging,” is being vigorously pursued in both electron [1,2] and x-ray imaging [3–6].

The problem of obtaining the exit surface wave function from the diffraction pattern, or the modulus of the Fourier transform of the exit surface wave function, requires additional a priori information. As pointed out by Elser [7], at present there are no practical algorithms for solving this problem which guarantee a solution. There are, however, iterative strategies for finding a solution which can work well given suitable a priori information. Such approaches modify the exit surface wave function in each cycle until the Fourier modulus and a priori constraints are satisfied. The wave function reconstruction can be thought of as a repeated projection between two sets, one containing the wave function in the diffraction plane, which satisfies the Fourier modulus constraint, and the other containing the exit surface wave function, which satisfies the a priori constraints. Examples of such constraints are support, positivity, and atomicity [7].

The first iterative scheme based on projections was that proposed by Gerchberg and Saxton in 1972 [8]. It requires knowledge of both the diffraction pattern and the exit surface image of an object. This scheme was subsequently modified by Fienup [9] so that the constraint in the image space was the object’s support. In this context the method became known as the “error-reduction algorithm.” However, as the Fourier modulus is a nonconvex constraint the Gerchberg-Saxton and error-reduction schemes are plagued by the associated stagnation problems.

To avoid these stagnation problems, alternate schemes have been developed. Fienup devised a family of “input-output” schemes, based on ideas from control theory. Of these the hybrid input-output (HIO) method [9–12] has been the most useful over a range of applications [13–16]. This approach is formulated in the context of a support constraint, with possible additional constraints. However, Fienup stated that “In general the reconstruction of complex-valued objects is considerably more difficult than for real-valued, nonnegative objects.” and “Simple symmetric support constraints such as single ellipses (circles) or rectangles do not work well” [11]. Other researchers have concurred [17–19] and it has become the conventional wisdom that “At the theoretical level, there can . . . be problems with convergence if the object is complex” [20].

Given this perception, a common approach to the problem of exit surface wave function retrieval has been to develop experimental strategies that overcome stagnation, often resulting in an increase in experimental complexity. For example, in a recent work, Faulkner and Rodenburg [20] suggest moving an aperture to obtain a series of separate diffraction patterns from accurately located overlapping regions of the sample. Nugent et al. [21] suggest adding varying degrees of known phase curvature to the incident beam to obtain a series of “astigmatic” diffraction patterns. In this Letter we demonstrate that, given a suitable post specimen aperture (or suitably collimated beam), the exit surface wave function within the aperture can be routinely determined from a single diffraction pattern.

Elser has developed an approach to exit surface wave function retrieval based on a difference map, which ameliorates the stagnation problem [7,22–24]. This approach can accommodate a range of object constraints in a
flexible manner and it is interesting to note that Fienup’s HIO method is a special case of this formalism. Starting with an initial estimate for the exit surface wave, a sequence of iterates is generated as follows:

\[ \psi_{n+1} = \psi_n + \beta \Delta \psi_n, \quad (1) \]

where \( \beta \) is a real parameter and the difference operator \( \Delta \) is defined in terms of projection operators \( P_1 \) and \( P_2 \) as

\[ \Delta = P_1[(1 + \gamma_2)P_2 - \gamma_2] - P_2[(1 + \gamma_1)P_1 - \gamma_1], \quad (2) \]

where \( \gamma_1 \) and \( \gamma_2 \) are real parameters. The final exit surface wave function can be obtained by application of either of the two operators \( P_1 \) and \( P_2 \).

We will take the first projection operator \( P_1 \) to be the support, defined by

\[ P_{\text{sup}}[\psi(r)] = \begin{cases} \psi(r), & \text{if } r \in S, \\ 0, & \text{if } r \notin S, \end{cases} \quad (3) \]

where support \( S \) is the set of position vectors in the exit surface plane for which the wave function is not forced to take a zero value, although zero values may occur naturally within the support. The second projection operator \( P_2 \), also expressed in the object domain, is the Fourier modulus constraint and is written as

\[ P_{\text{mod}}[\psi(r)] = |\mathcal{F}^{-1} \tilde{P}_{\text{mod}} \mathcal{F}[\psi(r)]|, \quad (4) \]

where \( \mathcal{F} \) denotes a Fourier transform and \( \tilde{P}_{\text{mod}} \) is the operation of replacing the modulus of the wave function in the diffraction plane with the modulus inferred from the measured diffraction pattern.

Assuming orthogonality of the two constraint subspaces, an iterative scheme to recover the exit surface wave function, which is optimized with respect to its convergence properties, is obtained for \( \gamma_1 = -\beta^{-1} \) and \( \gamma_2 = \beta^{-1} \) [7], so that the difference operator \( \Delta \) can now be written as

\[ \Delta = P_{\text{sup}}[(1 + \beta^{-1})P_{\text{mod}} - \beta^{-1}] - P_{\text{mod}}[(1 - \beta^{-1})P_{\text{sup}} + \beta^{-1}]. \quad (5) \]

Four projections are calculated for each iteration. It is also possible to tweak the algorithm to take into account nonorthogonality of the constraint subspaces [23].

The HIO method can be obtained from Eq. (2) with the choices \( \gamma_1 = -1 \) and \( \gamma_2 = \beta^{-1} \), so that the difference operator is

\[ \Delta = P_{\text{sup}}[(1 + \beta^{-1})P_{\text{mod}} - \beta^{-1}] - P_{\text{mod}}. \quad (6) \]

By applying circular supports of different radii to the complex wave function shown in Figs. 1(a) as an image and 1(b) phase we generated a set of diffraction patterns having different degrees of oversampling \( \sigma \), defined by

\[ \sigma = \frac{\text{total number of pixels in exit surface wave}}{\text{number of pixels inside the support}}, \quad (7) \]

The diffraction pattern corresponding to the test object in Figs. 1(a) and 1(b) has Euclidean norm unity. We then performed iterative reconstructions on each of the diffraction patterns obtained for a given \( \sigma \) as a function of \( \beta \), using the difference operators given in Eqs. (5) and (6). Ten thousand iterations were allowed for each reconstruction and the iterations were stopped if the Euclidean norm reached the lowest contour value indicated in Fig. 1(c). The results are displayed in Fig. 1(c), when using Eq. (5), and in 1(d) for Eq. (6). It is clear that, in both cases, there is a substantial range of \( \sigma \) and \( \beta \) values for which con-

FIG. 1 (color online). Nonperiodic test exit surface wave function, 128 × 128 pixels. Shown in (a) is the image (Erwin Schrödinger) and in (b) the phase (Prince Louis de Broglie). (c) The convergence map obtained using Eq. (5). (d) The convergence map obtained using Eq. (6), the HIO algorithm. For the retrieved complex-valued object for the case \( \sigma = 3.0 \) and \( \beta = 1.0 \) we show the recovered (e) image and (f) phase (maximum and minimum values are −2.51 and 2.46 rad within the support and concur with the corresponding range in the input phase).
vergence is obtained to the correct solution, up to the usual ambiguities associated with this problem [18]. This is contrary to customary expectations for the HIO scheme, where previous experience is based on suboptimal parameter choices. We show the retrieved complex-valued object for the case $\sigma = 3.0$ and $\beta = 1.0$ of Fig. 1(c) in Figs. 1(e), the image and 1(f), the phase.

We have carried out convergence tests for a wide range of complex-valued objects and obtain qualitatively similar results. Of particular interest is the reconstruction of a periodic object. To investigate this case an exit surface wave function was simulated for 100 keV electrons channeled through a silicon crystal of thickness 100 Å along the [001] direction. The exit surface wave function is shown in Figs. 2(a) and 2(b). Convergence maps are once again plotted for the difference maps given by Eqs. (5) and (6) and are shown in Figs. 2(c) and 2(d), respectively. While the region of best convergence is reduced, convergence is still obtained for a wide range of parameters. It is also apparent that for large values of $\sigma$ and $\beta$ convergence is problematic. However, for sufficient oversampling ($\sigma$ values larger than approximately 3.5) values of $\beta$ can always be found for which convergence can be obtained, showing the need to explore the parameter space adequately. Furthermore the transition between areas of worst and best convergence is much broader than in the nonperiodic example, shown in Fig. 1. The retrieved complex-valued object for the case $\sigma = 4.0$ and $\beta = 1.0$ of Fig. 2(c) is shown in Figs. 2(e) and 2(f).

Further discussion in this Letter is based on choosing $\beta = 1.0$, where the difference maps given by Eqs. (5) and (6) coincide. The first issue we explore is whether discontinuities in the phase such as vortices, in either the object or diffraction plane (which may occur when the intensity goes to zero) cause convergence problems. In the object plane we are interested in discontinuities in the support region. For the wave function shown in Figs. 3(a) and 3(b) this is indeed the case. For $\sigma = 4.0$ robust retrieval of the wave function within the support region is shown in Figs. 3(c) and 3(d).

It has recently been demonstrated by Faulkner and Rodenberg [20] that stagnation in the “error-reduction algorithm” for a complex-valued object can be overcome using a series of diffraction patterns. The proposed technique requires the use of an aperture which must be scanned to two or more overlapping positions. From a technical point of view this requires a method for moving the aperture a known distance across the sample, for example, using piezoelectric devices. We apply the difference map approach to the test object used by Faulkner and Rodenberg [20], reproduced in Figs. 3(e) and 3(f). Assuming an aperture located as in their Figs. 3(e) and 3(f) ($\sigma = 6.0$) an accurate reconstruction is obtained, unlike their result, as shown in Figs. 3(g) and 3(h). There is no need for accurately known overlapping regions of interest.

![Fig. 2](color online). Periodic test exit surface wave function, 128 x 128 pixels. Shown in (a) is the image and in (b) the phase. (c) The convergence map obtained using Eq. (5). (d) The convergence map obtained using Eq. (6), the HIO algorithm. For the retrieved complex-valued object for the case $\sigma = 4.0$ and $\beta = 1.0$ we show the recovered (e) image and (f) phase (maximum and minimum values are $-1.18$ and $1.73$ rad within the support and concur with the corresponding range in the input phase).

We tested the difference map approach using “loose” supports, supports which are larger than those used to form the diffraction patterns. Once again Scrödinger Fig. 1(a) and de Broglie 1(b) were used to form a complex-valued object. We tested this for $\sigma = 4.0$ to 8.0, with success. For example, for $\sigma = 8.0$ we formed a diffraction pattern. From this diffraction pattern a phase retrieval was then performed using a support $\sigma = 7.2$, 10% larger than the actual support. The result obtained is shown in Fig. 3(i), the image and 3(j), the phase.

As a further test, simulations were performed in which noise was added to the diffraction patterns. This was done...
and nanodiffraction imaging modalities of transmission complex-valued objects. The selected area diffraction distribution [25]. Satisfactory retrievals were achieved in calculated using a random deviate drawn from a Poisson distribution with correspondingly larger amounts by adding 0.1% noise to the largest pixel value in the diffraction pattern, with correspondingly larger amounts of noise on less intense pixels, where the number of counts is lower. The statistical error for each intensity value was limited by the aberrations in an objective lens, for both nonperiodic and periodic objects. There are also important ramifications for imaging based on x rays and nuclear particles.

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FIG. 3. A variety of test exit surface wave functions, all 128 × 128 pixels. (a) The image and (b) the phase of a test object containing vortices. [For example, pairs of vortices joined by branch cuts are present in the “eye” and “eyebrow” in (b)]. (c) The image and (d) the phase reconstructed using the difference map scheme with \( \sigma = 4.0 \) and \( \beta = 1.0 \) (maximum and minimum are \(-3.00 \) and \(3.00 \) rad). (e) The image and (f) the phase of a test object from Ref. [20]. (g) The image and (h) the phase reconstructed using the difference map approach with \( \sigma = 6.0 \) and \( \beta = 1.0 \) (maximum and minimum are \(0.71 \) and \(2.11 \) rad). (i) The image and (j) the phase retrieved using a loose support, \( \sigma = 7.2 \), that was 10% bigger than the actual support (maximum and minimum are \(-2.08 \) and \(2.08 \) rad). All maximum and minimum phase values refer only to the area within the support and concur with the corresponding ranges in the input phases.

by adding 0.1% noise to the largest pixel value in the diffraction pattern, with correspondingly larger amounts of noise on less intense pixels, where the number of counts is lower. The statistical error for each intensity value was calculated using a random deviate drawn from a Poisson distribution [25]. Satisfactory retrievals were achieved in all cases.

The results of this Letter have immediate and far reaching consequences for atomic scale retrieval of complex-valued objects. The selected area diffraction and nanodiffraction imaging modalities of transmission electron microscopy are ready-made environments which can be used to obtain pertinent data. It is possible to achieve “lensless imaging” at subatomic resolution, not limited by the aberrations in an objective lens, for both nonperiodic and periodic objects. There are also important ramifications for imaging based on x rays and nuclear particles.