Chapter 8

Teague's Method for Phase Retrieval, its Validity Conditions[1]

8.1 Introduction

While originally developed for coherent paraxial scalar electromagnetic radiation in the visible-light regime, phase retrieval using the Transport of Intensity Equation has been successfully applied to a range of radiation and matter wavefields. Such applications include using electron wavefields to quantitatively image magnetic skyrmions, propagation-based phase-contrast imaging using cold neutrons and hard X-rays, and visible-light refractive imaging of the projected column density of cold-atom clouds. Teague's method for phase retrieval, which renders the phase of a paraxial complex wave indirectly measurable via the existence of a conserved current, has been applied to a broad variety of situations which include all of the experiments described above. However, these applications have been undertaken without a thorough analysis of the underlying validity of the method. Here we derive sufficient conditions for the phase-retrieval solution provided by Teague's method to coincide with the true phase of the radiation of matter wavefield. We also present a sufficient condition guaranteeing that the discrepancy between the true phase function, and that reconstructed using Teague's solution, is small. These conditions demonstrate that in most practical cases, for phase–amplitude retrieval using the Transport of Intensity Equation, the Teague solution is very close to the exact one. However, we also describe a counter-example in the context of

[1]This Chapter is based on a joint paper with David Paganin, Timur Gureyev and Konstantin Pavlov (Schmalz et al., 2011)

phase–amplitude retrieval using hard X-rays, in which the relative root-mean-square (RMS) difference, between the exact solution and that obtained using Teague's method, is equal to 9%. These findings clarify the foundations of one of the most widely-applied methods for propagation-based phase retrieval of both matter and radiation wavefields and define a region of its applicability. The proof of the 2D Helmholtz theorem, the conditions for the validity of Teague's method and a counter-example in this Chapter are obtained by the candidate under the supervision of Timur Gureyev and Konstantin Pavlov. The physical interpretation of the mathematical idea is due to David Paganin. The computer simulations were done by Timur Gureyev.

8.2 Notation

In this Chapter we use the following notations for two-dimensional linear partial differential operators:

(a) For any differentiable function of two variables, $f \equiv f(x, y)$, we use $\nabla_\perp$ for a two-dimensional gradient, i.e. $\nabla_\perp f = (\partial_x f, \partial_y f)$ is a 2D vector field. Similarly, the divergence operator for any 2D vector function $\mathbf{A}(x, y) = (A_x(x, y), A_y(x, y))$ is defined as $\mathrm{div}\mathbf{A} = \partial_x A_x + \partial_y A_y$.

(b) For a scalar function $\eta(x, y)$ we define a 2D vector field $\mathbf{rot}\eta = (\partial_y \eta, -\partial_x \eta)$. The most important property of this operation is that

$$\mathrm{div}(\mathbf{rot}\eta) = \partial_x \partial_y \eta - \partial_y \partial_x \eta = 0. \tag{8.1}$$

Note also that $\mathbf{rot}\eta \cdot \nabla_\perp \eta = (\partial_y \eta, -\partial_x \eta) \cdot (\partial_x \eta, \partial_y \eta) \equiv 0$, where we used the usual "dot" notation to denote a scalar product of two vectors.

(c) For any 2D vector function $\mathbf{A}(x, y)$ we define a scalar function $\mathrm{curl}\mathbf{A} = \partial_x A_y - \partial_y A_x$. The most important property of this operator is that

$$\mathrm{curl}(\nabla_\perp f) = \partial_x \partial_y f - \partial_y \partial_x f = 0. \tag{8.2}$$

Note that unlike the case of $\mathbb{R}^3$, we need to introduce two different variants, "rot" and "curl", of the curl operation in $\mathbb{R}^2$ as above.

(d) We shall also use the notation $\mathbf{A} \times \mathbf{B} = A_x B_y - A_y B_x$ (note that the r.h.s is a scalar function). Then $\mathrm{curl}\mathbf{A} = \nabla_\perp \times \mathbf{A}$. Note that

$$\mathrm{curl}(\mathbf{rot}\eta) \equiv \nabla_\perp \times \mathbf{rot}\eta = -\partial_x^2 \eta - \partial_y^2 \eta = -\nabla_\perp^2 \eta, \tag{8.3}$$

where $\nabla_\perp^2 = \partial_x^2 + \partial_y^2$ is the two-dimensional Laplacian. Note also that the two-dimensional functions and operators defined above in a)-d) are introduced for convenience. The conventional three-dimensional representations would be more cumbersome in our case, as we will work with functions depending on just two coordinates, (x,y), at a fixed plane $z = z_0$ in 3D space as explained in the following text.

8.3 Teague's Solution of the Transport of Intensity Equation

Consider the following class of non-linear 2+1–dimensional field equations governing the spatial evolution of a stationary-state wavefunction (Paganin and Nugent, 2002):

$$\left(2ik\partial_z + \nabla_\perp^2 + g(|u|)\right) u(x, y, z) = 0. \tag{8.4}$$

Here, $k = \frac{2\pi}{\lambda}$, λ is the wavelength or de Broglie wavelength, $\partial_z = \frac{\partial}{\partial z}$ denotes partial differentiation with respect to distance along the nominal optical axis z (see Figure 1.1), and g is an arbitrary real function of a real variable. Note that Equation (8.4) describes a paraxial wavefield, which implies that all directions of propagation corresponding to non-negligible plane-wave components in the angular-spectrum decomposition, make a small angle with the positive z axis (Paganin, 2006, Ch. 1.3). In particular, this allows one to neglect the second derivative of the function with respect to z (see Section 2.3).

Special cases of Equation (8.4) include: (i) the paraxial form of the free-space time-independent Schrödinger equation for paraxial monoenergetic electron beams in which the effects of spin may be neglected (Graef, 2003); (ii) the parabolic equation for paraxial monochromatic scalar electromagnetic waves such as coherent visible light or coherent hard X-rays (Saleh and Teich, 2007); (iii) the 2+1–dimensional Gross–Pitaevskii equation governing the complex order-parameter field of scalar Bose-Einstein condensates (here, z denotes a temporal rather than a spatial variable) (Paganin and Nugent, 2002); (iv) the non-linear paraxial equation governing the propagation of intense electromagnetic fields in a non-linear medium (Kivshar and Agrawal, 2003).

Following Madelung (Madelung, 1927), we seek a hydrodynamic-like formulation of Equation (8.4) by making the substitution

$$u = \sqrt{I}e^{i\phi}. \tag{8.5}$$

Separating out the imaginary part yields the following continuity equation expressing the existence of a conserved current (Teague, 1983; Paganin and Nugent, 2002):

$$\mathrm{div}\,(I(x, y, z_0)\nabla_{\perp}\phi(x, y, z_0)) = -k\partial_z I(x, y, z_0). \tag{8.6}$$

Equation (8.6) is termed the Transport of Intensity Equation (TIE) (Chapter 5) in the context of propagation-based phase retrieval (Teague, 1983). We restrict consideration to regimes in which the intensity is strictly positive, $I(x, y, z_0) \geqslant C > 0$, everywhere in some simply-connected domain Ω with a sufficiently smooth boundary in the plane $z = z_0$. This implies that the phase $\phi = \arg u$ is well-defined (single-valued) and continuous over the domain Ω, which excludes the existence of screw-type topological defects such as phase vortices or domain-wall defects (Nye, 1999).

Teague (Teague, 1983) was the first to suggest the use of the TIE for retrieval of the phase ϕ in Ω, if the distributions of intensity and its z-derivative are known there (Chapter 5). While Teague only considered the linear case where $g = 0$ in Equation (8.4), Paganin and Nugent (Paganin and Nugent, 2002) pointed out that identical considerations apply to non-linear fields with arbitrary real g - note, in this context, that the TIE is independent of g because the local conservation expressed by this equation is unchanged by the presence of any non-dissipative non-linearity.

Phase–amplitude retrieval using the TIE usually requires measurement of the intensity over at least two different planes, $z = z_0$ and $z = z_0 + d$ (see Figure 4.5), orthogonal to the optical axis (Teague, 1983). Without loss of generality we can assume that $z_0 = 0$. Therefore, in the rest of the Chapter we omit $z_0 = 0$ from the list of arguments of all functions, and only indicate dependence on the first two arguments, namely x and y. This possibility for phase retrieval, namely the determination of phase from intensity measurements without the aid of an interferometer, is of particular importance in the context of strongly non-linear fields, for which interferometric phase measurement is in general problematic on account of the interaction between object and reference waves (Paganin and Nugent, 2002).

To obtain a unique solution for the phase ϕ in Ω using the TIE Equation (8.6), it is necessary to impose some suitable boundary conditions, e.g. Dirichlet, Neumann or periodic boundary conditions, on the phase function (see e.g. (Tikhonov and Samarskii, 1990, Ch. 4)). (In the case of Neumann and periodic boundary conditions the solution will be unique only up to an arbitrary and physically meaningless additive constant).

Teague suggested to solve Equation (8.6) via the introduction of an auxiliary function ψ, which satisfies

$$\nabla_{\perp}\psi(x,y) = I(x,y)\nabla_{\perp}\phi(x,y). \tag{8.7}$$

If the scalar potential ψ exists, then substituting Equation (8.7) into Equation (8.6) we see that it satisfies the Poisson equation

$$\nabla_{\perp}^{2}\psi(x,y) = -k\partial_{z}I(x,y). \tag{8.8}$$

After finding ψ from Equation (8.8), a solution $\tilde{\phi}$ of Equation (8.6) be determined by solving another Poisson equation

$$\nabla_{\perp}^{2}\tilde{\phi}(x,y) = \nabla_{\perp}\cdot[I^{-1}(x,y)\nabla_{\perp}\psi(x,y)], \tag{8.9}$$

which can be obtained by dividing both sides of Equation (8.7) by I and taking the divergence. Therefore, this method allows one to solve Equation (8.6) via two Poisson equations. One advantage of the Poisson Equations (8.8) and (8.9) compared to Equation (8.6) is that the two former equations are amenable to a numerical solution by Fast Fourier transform (FFT). Note that we have deliberately introduced a new symbol, $\tilde{\phi}$, to distinguish the phase solution of Equation (8.6) obtained by this Teague's method.

This technique was proposed in (Paganin and Nugent, 1998a), and further applied to a variety of matter and radiation wavefields in several other publications (Yu et al., 2005; Bajt et al., 2000; Barty et al., 1998; Allman et al., 2000; Yu et al., 2011; Lade et al., 2005a,b; De Graef and Zhu, 2001; Petersen et al., 2007; Yu et al., 2010; Frank et al., 2010; Langer et al., 2008; McMahon et al., 2003), (Paganin, 2006, Ch. 4.5.2) (see also (Gureyev et al., 1999, 1995) and references therein for other solution methods for Equation (8.6) in the context of phase retrieval). However, despite its widespread use, to the best of our knowledge the validity of Teague's assumption, i.e. the existence of the auxiliary function required in Equation (8.7), has never been thoroughly examined.

One can actually ask a more general question: regardless of the validity of Teague's assumption, Equation (8.7), what are the sufficient conditions under which the Teague's solution $\tilde{\phi}$, obtained by means of Teague's method represented by Equations (8.8) and (8.9), coincides exactly with or is sufficiently close to the true solution ϕ of the TIE, Equation (8.6)? Note that unlike the auxiliary function ψ required in Equation (8.7), a solution to Equation (8.8) with appropriate boundary conditions is known to exist and be unique (Tikhonov and Samarskii, 1990, Ch. 4). Therefore, Teague's method will always deliver a solution, but the question needs to be answered about the closeness of this solution, $\tilde{\phi}$, to the true solution ϕ of the TIE, Equation (8.6). In the present Chapter, we consider both the validity of Teague's assumption and the properties of the phase solution obtained by Teague's method in general.

It has been noted by E. C. G. Sudarshan (Sudarshan, 1980) that Equation (8.7) represents a good approximation in most realistic cases. A different approach to the justification of the validity of Equation (8.7) based on the Helmholtz theorem (Tikhonov and Samarskii, 1990, Appendix to Ch. IV) was given in (Paganin and Nugent, 1998a). The Helmholtz theorem is also the main tool that we use below for a detailed analysis of the problem.

8.4 Helmholtz's Theorem in 2D and the TIE

Let us consider a special 2D case of the Helmholtz theorem. This states that for any continuous vector field $\mathbf{A}(x, y) = (A_x(x, y), A_y(x, y))$, also having continuous partial derivatives, defined in a simply-connected bounded domain $\Omega \in \mathbb{R}^2$ with a sufficiently smooth boundary $\partial\Omega$ and satisfying the boundary condition $\mathbf{A} \cdot \mathbf{n}|_{\partial\Omega} = 0$, where $\mathbf{n}$ is the external normal to $\partial\Omega$, there exists a unique (up to an additive constant) pair of scalar functions (ψ, η) in Ω such that

$$\begin{aligned} \mathbf{A}(x,y) &= \nabla_\perp\psi(x,y) + \mathbf{rot}\eta(x,y), \\ \nabla_\perp\psi\cdot\mathbf{n}|_{\partial\Omega} &= 0, \\ \eta(x,y)|_{\partial\Omega} &= \mathrm{const}. \end{aligned} \tag{8.10}$$

Here we prove this special case of the Helmholtz decomposition theorem in a bounded domain in $\mathbb{R}^2$ (note that although the formulation and proof of the Helmholtz theorem in 3D can be found in many textbooks (e.g. (Tikhonov and Samarskii, 1990, Appendix to Ch. IV)), it seems much more difficult to find a corresponding formulation and proof in the literature for the 2D case).

First construct an auxiliary vector field $\mathbf{B}(x,y)$, such that $\mathrm{curl}\mathbf{B}(x,y) = 0$ and $\mathrm{div}\mathbf{B}(x,y) = \mathrm{div}\mathbf{A}(x,y)$, with the boundary property $\mathbf{B}(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$. We can always find (Tikhonov and Samarskii, 1990, Appendix to Ch. IV), (Evans, 1998) a unique (up to an additive constant) function $\psi(x,y)$ in Ω such that

$$\begin{cases} \nabla_\perp^2\psi(x,y) = \mathrm{div}\mathbf{A} \\ \nabla_\perp\psi(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0. \end{cases} \tag{8.11}$$

Then we can take $\mathbf{B}(x,y) = \nabla_\perp\psi(x,y)$, which obviously has all the required properties.

Now consider the vector field $\mathbf{C}(x,y) = \mathbf{A}(x,y) - \mathbf{B}(x,y)$. It is easy to see that $\mathbf{C}\cdot\mathbf{n}|_{\partial\Omega} = 0$, $\mathrm{div}\mathbf{C} = \mathrm{div}(\mathbf{A} - \nabla_\perp\psi) = \mathrm{div}\mathbf{A} - \nabla_\perp^2\psi = 0$ and $\mathrm{curl}\mathbf{C} = \mathrm{curl}(\mathbf{A} - \nabla_\perp\psi) = \mathrm{curl}\mathbf{A}$. As $\mathrm{div}\mathbf{C} = 0$, there exists a function $\eta(x,y)$, such that $\mathbf{rot}\eta(x,y) = \mathbf{C}(x,y)$ (see e.g., (Evans, 1998, Ch. 6)). The boundary property for such $\mathbf{rot}\eta(x,y)$ is (by construction) $\mathbf{rot}\eta\cdot\mathbf{n}|_{\partial\Omega} = 0$, which means that the vector $\mathbf{rot}\eta$ is perpendicular to the normal $\mathbf{n}$, or $\nabla_\perp\eta$ is perpendicular to the tangent of the boundary of the domain. Consequently η does not change its value along the boundary, i.e. η is a constant on the boundary. Thus, we have shown that the vector field $\mathbf{A}(x,y)$ can be represented in the form $\mathbf{A}(x,y) = \mathbf{B}(x,y) + \mathbf{C}(x,y) = \nabla_\perp\psi(x,y) + \mathbf{rot}\eta(x,y)$, where $\nabla_\perp\psi(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$, and $\eta(x,y)|_{\partial\Omega} = \mathrm{const}$.

If we have two different representations of the vector field $\mathbf{A}(x,y)$ in the form $\mathbf{A}(x,y) = \nabla_\perp\psi(x,y) + \mathbf{rot}\eta(x,y) = \nabla_\perp\psi_1(x,y) + \mathbf{rot}\eta_1(x,y)$, where

$\nabla_\perp\psi(x,y)\cdot\mathbf{n}|_{\partial\Omega} = \nabla_\perp\psi_1(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$, and $\mathbf{rot}\eta(x,y) = \mathbf{rot}\eta_1(x,y) = 0$, then $\nabla_\perp(\psi(x,y)-\psi_1(x,y)) + \mathbf{rot}\,(\eta(x,y)-\eta_1(x,y)) = 0$. Taking div and curl of this identity, we obtain, respectively, that $\bar{\psi} = \psi - \psi_1$ and $\bar{\eta} = \eta - \eta_1$ are harmonic functions in Ω satisfying uniform Neumann boundary conditions, $\nabla_\perp\bar{\psi}(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$, or Dirichlet conditions $\bar{\eta}|_{\partial\Omega} = \mathrm{const}$, respectively, and hence both these functions are constants (Tikhonov and Samarskii, 1990, Appendix to Ch. IV), (Evans, 1998, Ch. 6), which proves the required uniqueness up to additive constants of the Helmholtz decomposition.

The above 2D Helmholtz theorem implies, in particular, that for any pair of suitably well behaved functions (I, ϕ) (it is sufficient to require that $I(x,y) \geqslant C > 0$ everywhere in Ω has continuous first derivatives, while ϕ has continuous second derivatives in Ω), where the function ϕ also satisfies e.g. uniform Neumann boundary conditions $\nabla_\perp\phi\cdot\mathbf{n} = 0$, we can find a pair of unique (up to additive constants) functions (ψ,η) such that

$$I(x,y)\nabla_\perp\phi(x,y) = \nabla_\perp\psi(x,y) + \mathbf{rot}\eta(x,y), \tag{8.12}$$

and the functions (ψ,η) satisfy the same boundary conditions as in Equation (8.10). Then

$$\nabla_\perp\phi(x,y) = I^{-1}(x,y)\nabla_\perp\psi(x,y) + I^{-1}(x,y)\mathbf{rot}\eta(x,y) \tag{8.13}$$

and

$$\nabla_\perp^2\phi(x,y) = \mathrm{div}\left[I^{-1}(x,y)\nabla_\perp\psi(x,y)\right] + \nabla_\perp I^{-1}(x,y)\times\nabla_\perp\eta(x,y), \tag{8.14}$$

where we used the identity $\mathrm{div}[I^{-1}\mathbf{rot}\eta] = \nabla_\perp I^{-1}\cdot\mathbf{rot}\eta = \nabla_\perp I^{-1}\times\nabla_\perp\eta$.

Assuming suitable boundary conditions (e.g. Dirichlet, Neumann or periodic boundary conditions) for the phase function in Equation (8.14) that guarantee the existence of the inverse Laplacian operator in a suitable functional space over Ω, we can also obtain:

$$\phi(x,y) = \nabla_\perp^{-2}\mathrm{div}\left[I^{-1}(x,y)\nabla_\perp\psi(x,y)\right] + \nabla_\perp^{-2}[\nabla_\perp I^{-1}(x,y)\times\nabla_\perp\eta(x,y)]. \tag{8.15}$$

Note that because in the case of (uniform) Neumann or periodic boundary conditions the uniqueness of the solution to the boundary-value problem for the Poisson equation is guaranteed up to an arbitrary additive constant (see e.g.

(Tikhonov and Samarskii, 1990, Ch. IV), (Evans, 1998, Ch. 6)), the inverse Laplacian can be uniquely defined e.g. on the subset of all phase functions with zero average value over Ω. Such a restriction is consistent with the definition of the phase function $\phi(x, y)$ which is itself physically defined only up to an arbitrary additive constant. In view of Equation (8.15), Teague's solution $\tilde{\phi}(x, y) = \nabla_{\perp}^{-2}\mathrm{div}\left[I^{-1}(x, y)\nabla_{\perp}\psi(x, y)\right]$, where $\psi(x, y)$ is a solution of Equation (8.8), represents a good approximation to the true solution $\phi(x, y)$ of the TIE if and only if the following error term,

$$\epsilon(x, y) = \phi(x, y) - \nabla_{\perp}^{-2}\mathrm{div}\left[I^{-1}(x, y)\nabla_{\perp}\psi(x, y)\right] = \nabla_{\perp}^{-2}\left[\nabla_{\perp}I^{-1}(x, y) \times \nabla_{\perp}\eta(x, y)\right], \tag{8.16}$$

is either exactly zero, or is at least sufficiently small in an appropriate sense, e.g. much smaller, with respect to some suitable functional norm, than the exact solution ϕ.

It will also be useful for our analysis in subsequent sections of this Chapter to have explicit equations for the functions ψ and η found on the right-hand side of Equation (8.12). By taking the divergence of Equation (8.12) and using Equation (8.1), it is easy to see that

$$\begin{cases} \nabla_{\perp}^{2}\psi(x, y) = \mathrm{div}\left[I(x, y)\nabla_{\perp}\phi(x, y)\right] \\ \nabla_{\perp}\psi(x, y) \cdot \mathbf{n}|_{\partial\Omega} = 0. \end{cases} \tag{8.17}$$

The function ψ can be found from Equation (8.17) uniquely up to an arbitrary additive constant.

In order to find the function η, take the curl of both sides of Equation (8.12). Using Equations (8.2) and (8.3) and the identity $\mathrm{curl}(I\nabla_{\perp}\phi) = \nabla_{\perp}I \times \nabla_{\perp}\phi$, we obtain:

$$\begin{cases} -\nabla_{\perp}^{2}\eta(x, y) = \nabla_{\perp}I(x, y) \times \nabla_{\perp}\phi(x, y) \\ \eta|_{\partial\Omega} = \mathrm{const}. \end{cases} \tag{8.18}$$

Equation (8.18) allows one to obtain the function η uniquely for each constant chosen in the boundary conditions.

In the next section we will obtain some general conditions for the validity of Teague's method, i.e. conditions guaranteeing that "Teague's error term" $\epsilon(x, y)$ defined in Equation (8.16) is either exactly zero or is sufficiently small.

8.5 General Conditions for the Validity of Teague's Assumption

Let us show that for an arbitrary pair of suitably well-behaved functions (I, ϕ) in Ω (as defined before Equation (8.12) above), there exists a function ψ such that $\nabla_\perp \psi(x, y) = I(x, y)\nabla_\perp \phi(x, y)$, if and only if

$$\nabla_\perp I(x, y) \times \nabla_\perp \phi(x, y) \equiv 0. \tag{8.19}$$

That is, the function ψ exists if and only if (i) the vector fields $\nabla_\perp \phi$ and $\nabla_\perp I$ are parallel everywhere in Ω, or (ii) $\nabla_\perp I$ is zero everywhere in Ω, corresponding to a uniformly-illuminated non-absorbing object, or (iii) $\nabla_\perp \phi$ is zero, corresponding to the physically trivial case of transversely uniform wavefronts.

Before proceeding, we note that, for many non-absorbing objects of interest in the context of TIE phase retrieval, we intuitively expect $\nabla_\perp \phi$ and $\nabla_\perp I$ to be close to parallel everywhere in Ω. Loosely speaking, the physical reason for this is that a given increase in optical thickness (i.e. in $|\phi|$) is typically associated with an increase in the actual thickness or density of a sample; and an increase is the actual thickness or density of sample is typically associated with an increase in the absorption of the sample. Thus, while for a truly arbitrary object one would expect $\nabla_\perp \phi$ and $\nabla_\perp I$ to be uncorrelated and therefore not necessarily parallel everywhere in Ω, for a "typical object", $\nabla_\perp \phi$ and $\nabla_\perp I$ will be correlated. To motivate the existence of this correlation, we need only note that the phase and amplitude shifts due to each component material will be non-independent, implying in general a non-zero degree of correlation between the net phase and intensity excursions at each point on the nominally planar exit surface of a sample. Furthermore, to the extent that increases in optical thickness are accompanied by increases in absorptive thickness, one would normally expect $\nabla_\perp \phi$ and $\nabla_\perp I$ to be "close to parallel".

Returning to the main thread of the argument, we note that if ψ exists, then

$$0 = \mathrm{curl}[\nabla_\perp \psi(x, y)] = \mathrm{curl}[I(x, y)\nabla_\perp \phi(x, y)] = \partial_x I(x, y)\partial_y \phi(x, y) - \partial_y I(x, y)\partial_x \phi(x, y). \tag{8.20}$$

On the other hand, if $\nabla_\perp I(x, y) \times \nabla_\perp \phi(x, y) \equiv 0$, then using the Helmholtz decomposition Equation (8.12), we obtain

$$0 = \nabla_\perp I(x, y) \times \nabla_\perp \phi(x, y) = \mathrm{curl}[I(x, y)\nabla_\perp \phi(x, y)] = \mathrm{curl}[\mathbf{rot}\eta(x, y)] = -\nabla_\perp^2 \eta(x, y). \tag{8.21}$$

and assuming that $\eta(x, y)$ satisfies Dirichlet boundary conditions $\eta|_{\partial\Omega} = \text{const}$, we learn that $\eta(x, y)$ is a constant as a consequence of the uniqueness of solution to the Dirichlet problem for the Laplace equation (Tikhonov and Samarskii, 1990, Ch. 2), (Evans, 1998, Ch. 6). Therefore $\mathbf{rot}\eta(x, y) \equiv 0$ and $\nabla_\perp \psi(x, y) = I(x, y)\nabla_\perp \phi(x, y)$.

Teague's assumption, i.e. the existence of a potential function ψ, such that $\nabla_\perp \psi(x, y) = I(x, y)\nabla_\perp \phi(x, y)$, implies that

$$\tilde{\phi}(x, y) = \nabla_\perp^{-2} \mathrm{div}\left[I^{-1}(x, y)\nabla_\perp \psi(x, y)\right] = \nabla_\perp^{-2} \mathrm{div}\left[\nabla_\perp \phi(x, y)\right] = \phi(x, y). \tag{8.22}$$

According to Equation (8.16) this also implies that $\epsilon(x, y) = 0$, i.e. the Teague solution is exact in this case. Therefore, Equation (8.19) represents a sufficient condition not only for the validity of Teague's assumption, Equation (8.7), but also for the exact accuracy of Teague's solution, $\tilde{\phi} = \phi$.

Note, however, that the condition expressed by Equation (8.19) may not be necessary for the exactness of Teague's solution. Indeed, by virtue of Equation (8.16), the exactness of Teague's solution, $\epsilon(x, y) = 0$, only implies that $\nabla_\perp I \times \nabla_\perp \eta = 0$, e.g. that vectors $\nabla_\perp I$ and $\nabla_\perp \eta$ are parallel everywhere in Ω. Equation (8.19), on the other hand, is equivalent (by means of Equation (8.18)) to a stronger condition, namely that $\eta(x, y)$ is a constant in Ω.

Let us consider the physical meaning of the condition expressed by Equation (8.19). The vectors $\nabla_\perp \phi$ and $\nabla_\perp I$ are parallel at all points in Ω if and only if the vectors $\nabla_\perp \phi$ and $\nabla_\perp \ln I(x, y) = I^{-1}(x, y)\nabla_\perp I(x, y)$ are parallel at these points. The latter means that $\nabla_\perp \phi(x, y) = c(x, y)\nabla_\perp \ln I(x, y)$ for some scalar function. Note that this is similar, but not equivalent to the definition of monomorphous (or homogeneous) objects (Paganin et al., 2002, 2004a), for which one has $\nabla_\perp \phi(x, y) = (\gamma/2)\nabla_\perp \ln I(x, y)$ in the projection approximation (Paganin, 2006, Ch. 2.2), (De Caro et al., 2008), where γ is a constant. Therefore, the class of objects for which the Teague assumption (i.e., a function ψ exists such that $\nabla_\perp\psi(x,y) = I(x,y)\nabla_\perp\phi(x,y))$ holds may be broader than the class of all monomorphous objects. It is well known that the class of all monomorphous objects contains the sub-class of all objects for which $\phi(x,y) = (\gamma/2)\ln I(x,y)$ with some constant γ. This relationship between the phase and intensity holds, for example, in quantitative X-ray imaging of objects consisting of a single material (Paganin et al., 2002) with a complex refractive index $n = 1 - \delta + i\beta$, or in the visible-light refractive imaging of the projected column density of cold atom clouds (Turner et al., 2004). Indeed, for such objects one obtains, assuming that the projection approximation (Paganin, 2006, Ch. 2.2), (De Caro et al., 2008) is valid and the incident plane wave is e^{ikz}, that $\phi(x,y) = -k\delta T(x,y)$ and $\ln I(x,y) = -2k\beta T(x,y)$, where $T(x,y)$ is the transverse distribution of the projected thickness of the object. One can see that for such objects $\phi(x,y) = (\delta/2\beta)\ln I(x,y)$, i.e. $\gamma \equiv \delta/\beta$. In the case of transmitted X-ray waves with energies between approximately 60 keV and 500 keV, the equality $\phi(x,y) = (\gamma/2)\ln I(x,y)$ holds not only for objects that consist predominantly of a single material, but also for any objects consisting of chemical elements with $Z<10$ (Wu and Liu, 2004). The physical origin of this last-mentioned result is that samples, composed of sufficiently light elements illuminated at sufficiently high X-ray energy, are well approximated by a continuous "single material" distribution of almost-free electrons (Cloetens, 2011). Similar considerations apply to the other forms of radiation and matter wavefield considered in this Chapter. We see that for all of these classes of object, Teague's assumption is valid exactly.

We have found sufficient conditions for "Teague's error term" $\epsilon(x,y)$ to be zero. Now, we describe another type of sufficient condition guaranteeing that the error term is small. Define a normalised L_2-norm for square-integrable function in Ω as

$$\|f\|_2 = \frac{\left(\iint_\Omega |f(x,y)|^2 dxdy\right)^{\frac{1}{2}}}{\left(\iint_\Omega dxdy\right)^{\frac{1}{2}}}. \tag{8.23}$$

As the inverse Laplacian is a continuous operator in suitable functional subspaces of $L_2(\Omega)$, then $\|\nabla_\perp^{-2} f\|_2 \leqslant L_\Omega^2 \|f\|_2$ (see e.g. (Evans, 1998, Ch. 8.3)) where L_Ω is a positive constant with the dimensionality of length; L_Ω is proportional to the diameter of Ω ($L_\Omega = D/\pi$, where D is the domain diameter, in the case of a convex domain Ω in $\mathbb{R}^2$, see e.g., (Acosta and Duran, 2004; Payne and Weinberger, 1960)). It follows from Equation (8.16) that

$$\|\epsilon(x, y)\|_2 \leqslant L_\Omega^2 \|\nabla_\perp I^{-1}(x, y) \times \nabla_\perp \eta\|_2. \tag{8.24}$$

For "reasonable" functions f from $L_2(\Omega)$ (satisfying Dirichlet or other suitable boundary conditions) one can verify by integrating by parts that $\|\nabla_\perp f\|_2^2 \leqslant \|f\|_2 \|\nabla_\perp^2 f\|_2$. Now we can use Equation (8.18) and the continuity of the inverse Laplacian to obtain: $\|\nabla_\perp \eta\|_2 \leqslant \|\eta\|_2^{1/2} \|\nabla_\perp^2 \eta\|_2^{1/2} \leqslant L_\Omega \|\nabla_\perp I \times \nabla_\perp \phi\|_2$. Combining this with Equation (8.24) we finally obtain

$$\|\epsilon(x, y)\|_2 \leqslant L_\Omega^3 \|\nabla_\perp \phi\|_2 \|\nabla_\perp \ln I\|_2^2. \tag{8.25}$$

Note that the conditions of validity of the TIE generally require that

$$|\nabla_\perp \phi| \left| \frac{\nabla_\perp I}{I} \right| << \frac{k}{R}, \tag{8.26}$$

see e.g. (Gureyev and Wilkins, 1998).

Therefore, under the TIE validity conditions, Equation (8.25) can be rewritten as

$$\|\epsilon(x, y)\|_2 << \frac{k L_\Omega^3}{R} \|\nabla_\perp \ln I\|_2. \tag{8.27}$$

The right-hand side of Equation (8.27) is a product of two factors: $N_F^{max} \equiv \left(k L_\Omega^2\right)/R$, that is the (largest) Fresnel number (Saleh and Teich, 2007) associated with domain Ω, and $var_2(I) \equiv L_\Omega \|\nabla_\perp \ln I\|_2$ that can be interpreted as a measure of total variation of intensity across the domain. As the validity conditions of the TIE require that $N_F^{max} >> 1$ (see e.g. (Gureyev et al., 2004b)), then $var_2(I) \equiv L_\Omega \|\nabla_\perp \ln I\|_2$ typically has to be very small to guarantee that Teague's solution is accurate. Recalling that Teague's solution is accurate when $\|\epsilon(x, y)\|_2 << \|\phi\|_2$, we finally obtain from Equation (8.27) that a sufficient condition for the accuracy of Teague's solution is

$$N_F^{max} var_2(I) \leqslant \|\phi\|_2. \tag{8.28}$$

It follows from Equation (8.28) that when the variation of absorption in the sample is very weak, then the Teague solution is accurate. The opposite may not be true. Indeed, note that the estimate in Equation (8.28) does not take into account some geometric factors affecting the accuracy of the Teague solution. In particular, it does not take into account the condition $\nabla_\perp I(x, y) \times \nabla_\perp \phi(x, y) \equiv 0$ considered above, which in fact guarantees that the Teague error term, $\epsilon(x, y)$, is equal to zero, even when the variation of absorption is large. Therefore, we should emphasise that Equation (8.28) is sufficient, but not necessary, for the Teague solution to be accurate.

8.6 Solutions that Cannot Be Obtained Using Teague's Assumption

When searching for a counter-example to Teague's method for solving the TIE - i.e. for a pair of functions (I, ϕ), such that the exact solution ϕ of the TIE equation, Equation (8.6), is significantly different from Teague's solution $\tilde{\phi}(x, y) = \nabla_\perp^{-2} \mathrm{div}\left(I^{-1}(x, y)\nabla_\perp \psi(x, y)\right)$, where ψ is a solution of Equation (8.8) — it is necessary, but not sufficient, to ensure that $I(x, y)\nabla_\perp \phi(x, y)$ is not a complete potential (or, according to Section 8.5, that vectors $\nabla_\perp \phi$ and $\nabla_\perp I$ are not parallel to each other at all points). We also want to find an example where the error term, $\epsilon(x, y) = \phi(x, y) - \tilde{\phi}(x, y)$, is not just non-zero, but is sufficiently large in an appropriate sense, e.g. comparable in norm to the exact solution ϕ, or, equivalently, is comparable to the Teague solution $\tilde{\phi}(x, y)$. Considering Equation (8.16), we may try to find a case where $\nabla_\perp I^{-1} \times \nabla_\perp \eta$ is comparable in norm to $\mathrm{div}\left(I^{-1}(x, y)\nabla_\perp \psi(x, y)\right)$. As one can see from Equation (8.14), this will be the case when $\nabla_\perp^2 \phi(x, y)$ is very small, but $\nabla_\perp I^{-1}(x, y) \times \nabla_\perp \eta(x, y)$ is not.

Consider the following example: $\Omega = (-10, 10) \times (-10, 10)\,\mu m^2 \subset \mathbb{R}^2$, $I(x, y) = e^{-a_0 x^2 - b_0 y^2}$ and $\phi(x, y) = a_0 x^2 - b_0 x^2 - a_1 x^8 + b_1 y^8$, where $a_0 = b_0 = 10^{-2} \mu m^{-2}$ and $a_1 = b_1 = 0.25 \times 10^{-8} \mu m^{-8}$ (Figures 8.1 and 8.2). This phase function satisfies uniform Neumann boundary conditions. Physically, such a beam could be generated for the case of electromagnetic radiation with wavelength $\lambda = 0.1 nm$ by taking a thin single-material transparent screen (i.e. a phase object made from polypropylene $(C_3H_6)_n$ with $\delta = 1.39 \times 10^{-6}$ and $\beta = 7.48 \times 10^{-10}$ (Henke et al., 1993) with a saddle-like profile of projected thickness $T(x, y)$, and normally illuminating it with a focussed Gaussian beam (Saleh and

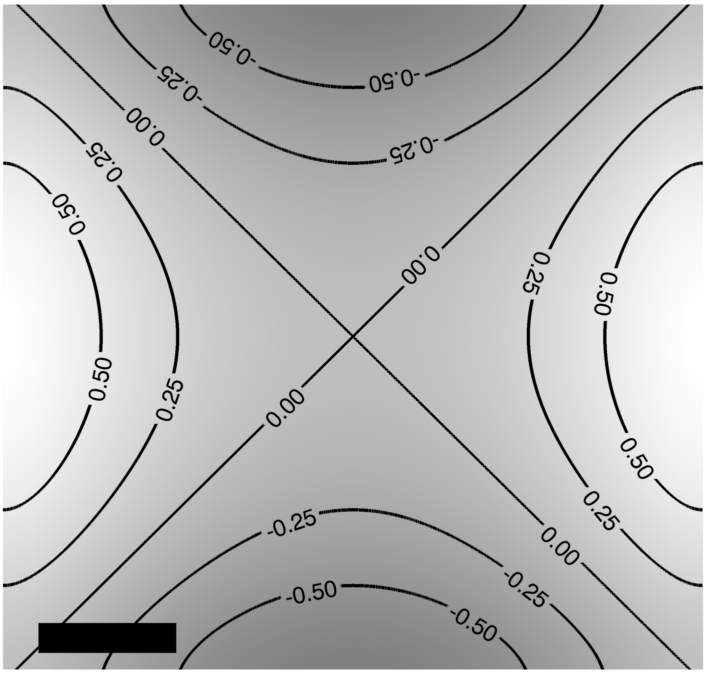

Figure 8.1: Phase distribution, $\phi(x, y)$, defined in $\Omega = (-10, 10) \times (-10, 10)(\mu m^2)$ as in the counter-example. The value range of the phase is approximately $(-0.75, 0.75)$. Scale bar $= 4\mu m$.

Teich, 2007) such that the waist of the illuminating beam coincides with the entrance surface of the object. Note that the phase, $\phi(x, y) = -k\delta T(x, y) + const$, is defined up to a constant. The maximal projected thickness, T_{max}, for our object, required to produce the appropriate phase shift, is about 17 microns. Then the maximal attenuation caused by this object is very small, $e^{-2k\beta T_{max}} \approx 0.99$, which corresponds to the case of a phase object. The disturbance, at the exit surface of the screen, would have the unusual (from the perspective of phase-amplitude imaging) property that intensity and phase would be independent of one another, insofar as the former is due entirely to the illuminating beam and the latter is entirely due to the illuminated object.

The above phase distribution can be retrieved in an experiment, for example, by measuring the transmitted intensity distribution $I(x, y, z = 0)$ immediately after the screen and at a distance of approximately $1cm$ downstream the optical axis, $I(x, y, z = 1cm)$, calculating the intensity derivative as $\partial_z I(x, y, z = 0) \approx (I(x, y, z = 1cm) - I(x, y, z = 0)) / \Delta z$ and then solving the TIE, Equation (8.6),

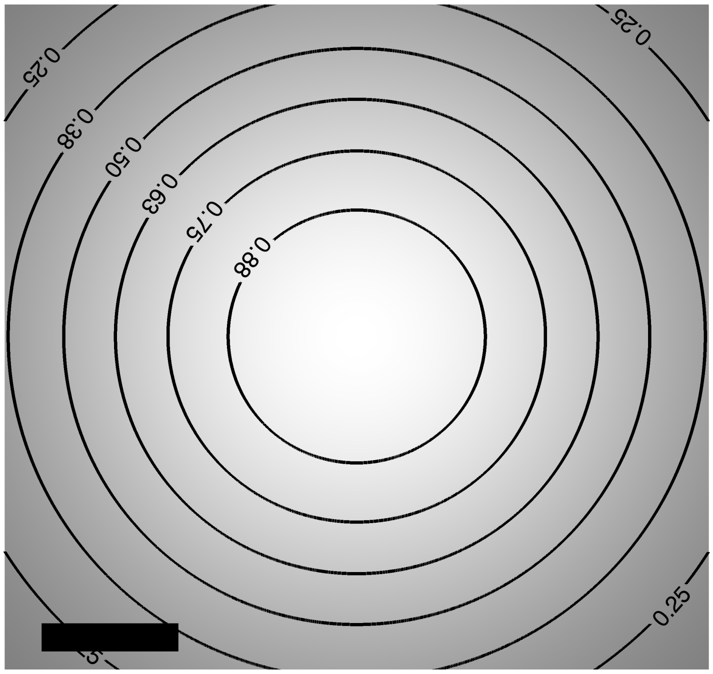

Figure 8.2: Intensity distribution, $I(x, y)$, defined in $\Omega = (-10, 10) \times (-10, 10)(\mu m^2)$ as in the counter-example. The value range of the intensity is approximately $(0.14, 1.0)$. Scale bar $= 4\mu m$.

for the phase $\phi(x, y)$. However, if one tries to reconstruct the phase distribution in this case using the Teague's method represented by Equations (8.8) and (8.9)), the resultant phase distribution $\tilde{\phi}(x, y)$ will be significantly different from the exact one, as explained below. It is easy to verify that, for the scenario described above, the two vectors, $\nabla_\perp I(x, y) = I(x, y)(-2a_0 x, -2b_0 y)$ and $\nabla_\perp \phi(x, y) = (2a_0 x - 8a_1 x^7, -2b_0 y + 8b_1 y^7)$, are not parallel at most points in Ω. Also, the variation of intensity is not small in Ω (it is comparable to the phase), which means that none of the sufficient conditions for the smallness of the error term $\epsilon(x, y)$ formulated in the previous section are valid in this example. Finally, the Laplacian $\nabla_\perp^2 \phi(x, y) = 56a_1(y^6 - x^6)$ is small at most points in Ω. Therefore, this is indeed a good candidate for a "counter-example", i.e. a case where Teague's solution $\tilde{\phi}(x, y)$ is significantly different from the exact solution $\phi(x, y)$ of the TIE. We could not solve the relevant equations (e.g. Equation (8.17)) analytically, so we resorted to numerical solutions using a well-tested software package for X-ray image analysis

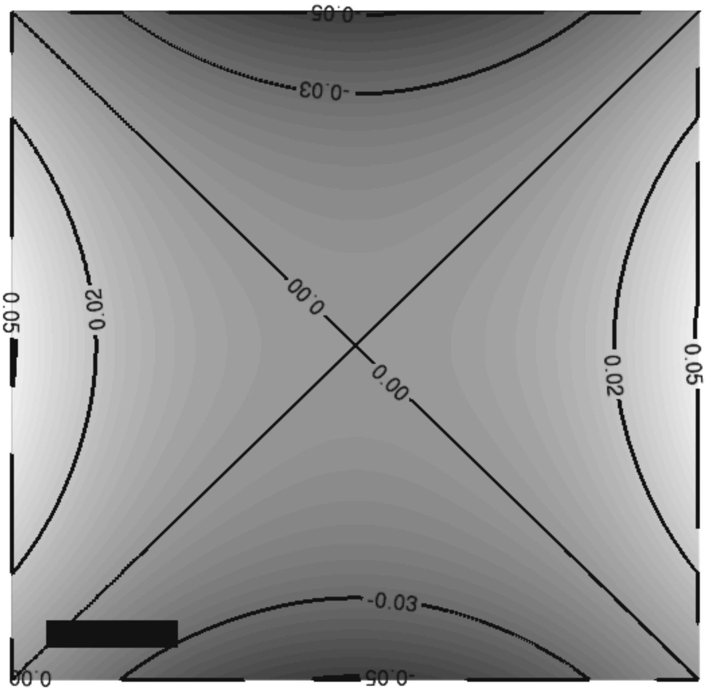

Figure 8.3: Distribution of the function $-\mathrm{div}(I(x,y)\nabla_\perp\phi(x,y))$ in Ω as in the counter-example. The value range of this function is approximately $(-0.073, 0.073)$. Scale bar $= 4\mu m$.

and simulation, X-TRACT (X-TRACT, 2010, Site accessed Nov. 2010). We first calculated the 2D distribution $-\mathrm{div}\,(I(x,y)\nabla_\perp\phi(x,y) \equiv k\partial I(x,y))$ for the above phase and intensity by computing the corresponding differential expressions on a numerical grid with 2048×2048 square pixels within the domain $\Omega = (-10, 10) \times (-10, 10)(\mu m^2)$ (see Figure 8.3). Then we numerically solved the Poisson equation (using the Fourier Transform method as implemented in (X-TRACT, 2010, Site acceced Nov. 2010) to obtain the distribution of $\psi(x,y) = \nabla_\perp^{-2}\mathrm{div}[I(x,y)\nabla_\perp\phi(x,y)]$ in Ω (Figure 8.4). Solving the second Poisson equation according to Teague's method, we obtained the phase distribution $\tilde{\phi}(x,y) = \nabla_\perp^{-2}\mathrm{div}(I^{-1}(x,y)\nabla_\perp\psi(x,y))$ (Figure 8.5). Finally we calculated the difference

$$\epsilon(x,y) = \phi(x,y) - \tilde{\phi}(x,y) \tag{8.29}$$

between the exact phase and the one obtained using the Teague's method

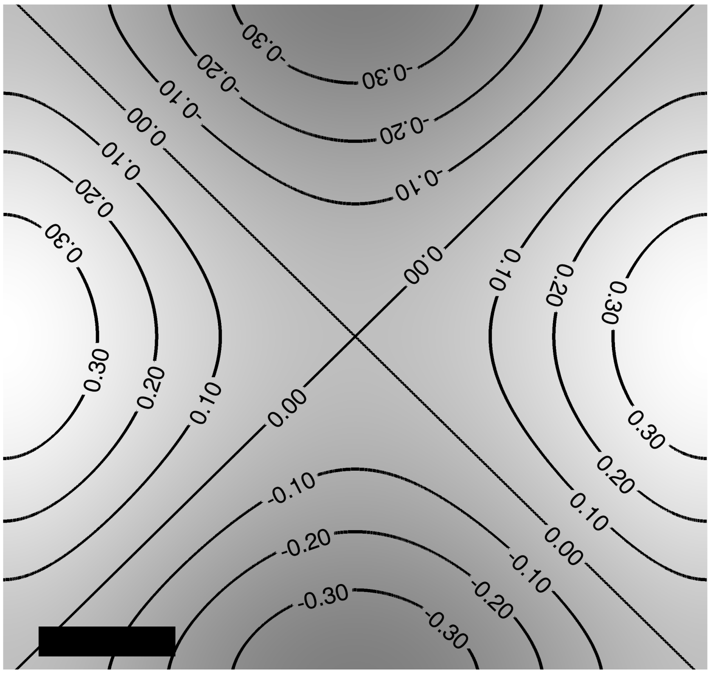

Figure 8.4: Distribution of the function $\psi(x, y) = \nabla_\perp^{-2} \mathrm{div}(I(x, y)\nabla_\perp \phi(x, y))$ in Ω as in the counter-example. The value range of this function is approximately $(-0.39, 0.39)$. Scale bar $= 4\mu m$.

(Figure 8.6). These numerical calculations showed that $\|\phi(x, y) - \tilde{\phi}(x, y)\|_2 \approx 0.09\|\phi(x, y)\|_2$, i.e. the relative root-mean-square error is approximately 9%.

8.7 Summary

Phase–amplitude retrieval, based on the Transport of Intensity Equation, has been applied to a wide variety of paraxial radiation and matter wave-fields that are either governed by the non-linear parabolic equation (8.4), or by its special case where $g = 0$. All such fields, both linear and non-linear, have a spatial evolution of intensity which is governed by the associated continuity equation, Equation (8.6), which is termed the TIE in the context of phase retrieval. The TIE has been used for such phase retrieval using electrons, visible light, hard X-rays and neutrons. Notwithstanding these successes, the validity of Teague's assumption – which amounts to the assumption that the transverse current density is a two-dimensional potential field, and which is key to the

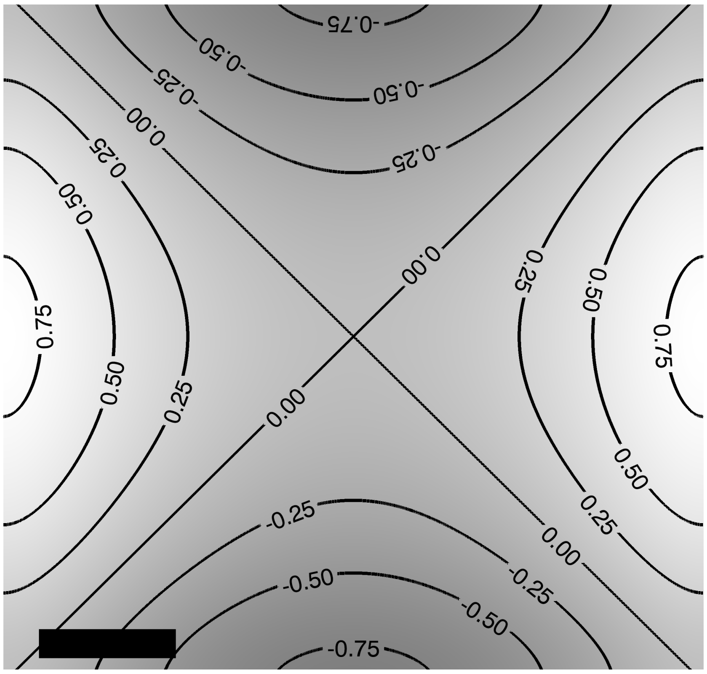

Figure 8.5: Distribution of the function $\tilde{\phi}(x, y) = \nabla_{\perp}^{-2} \mathrm{div}(I^{-1}(x, y)\nabla_{\perp}\psi(x, y))$ in Ω as in the counter-example. The value range of this function is approximately $(-0.80, 0.80)$. Scale bar $= 4\mu m$.

most widely applied TIE-based phase-retrieval algorithm – has never been rigorously examined. We have clarified this by obtaining sufficient conditions for the correctness of the solution provided by Teague's method. We have also developed a sufficiency condition, which guarantees the smallness of the error term generated by Teague's assumption in the context of TIE phase retrieval. Not all wave-fields will fulfill this condition. To explicitly demonstrate this latter finding, we developed a counter-example which shows that although in most realistic cases Teague's solution provides a very good approximation for the exact solution to the TIE (as demonstrated in many published papers studying a variety of objects which range from biomedical samples to cold atom clouds and magnetic skyrmions (Yu et al., 2005; Bajt et al., 2000; Barty et al., 1998; Allman et al., 2000; De Graef and Zhu, 2001; Petersen et al., 2007; Yu et al., 2010; Frank et al., 2010; Langer et al., 2008; McMahon et al., 2003)), (Paganin, 2006, Ch. 4.5.2), there are some situations where the error can be relatively large. Therefore, care should be taken when using Teague's

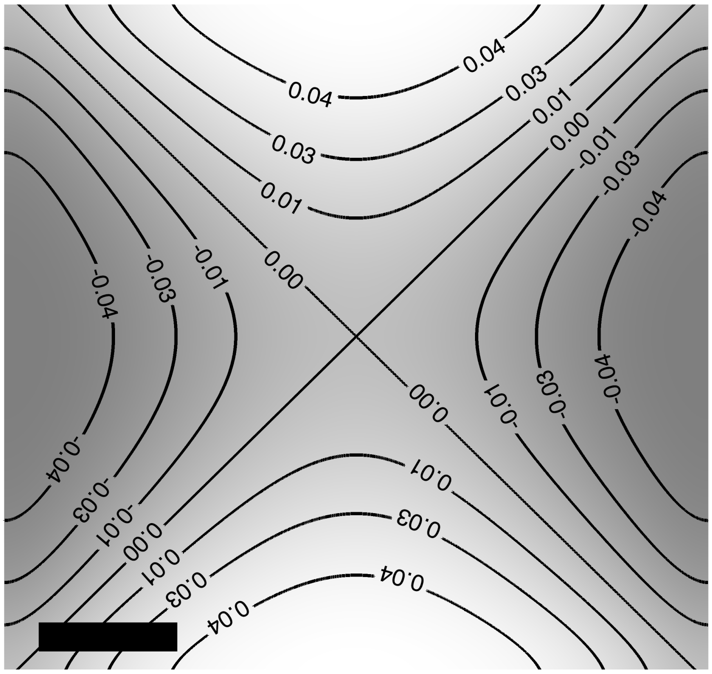

Figure 8.6: Distribution of the error function $\epsilon(x, y) = \phi(x, y) - \tilde{\phi}(x, y)$ in Ω as in the counter-example. The value range of this function is approximately $(-0.054, 0.054)$. Scale bar $= 4\mu m$.

method for solution of the TIE. In particular, it may be useful to verify if any of the conditions for the validity of Teague's method proved in Section 8.5 is satisfied. This would guarantee the accuracy of the Teague-based TIE solution. Alternatively, one may prefer to solve the TIE, Equation (8.6), by other methods that do not involve the use of Teague's assumption (see e.g. (Gureyev et al., 1999)).