Phase retrieval using radiation and matter-wave fields: Validity of Teague's method for solution of the transport-of-intensity equation

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Although 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 paraxial radiation and matter-wave fields. Such applications include using electron wave fields to quantitatively image magnetic skyrmions and spin ices, 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 using the transport-of-intensity equation, 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 paraxial radiation or matter-wave field. 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 solution. However, we also describe a counter example in the context of phase-amplitude retrieval using hard x-rays, in which the relative root-mean-square difference between the exact solution and that obtained using Teague's method is 9%. These findings clarify the foundations of one of the most widely applied methods for propagation-based phase retrieval of both paraxial matter and radiation wave fields and define a region for its applicability.

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I. INTRODUCTION

One form of the "phase problem," as posed by Wolfgang Pauli in his famous Handbuch article, asks whether it is possible to reconstruct a complex spatial wavefunction u given both its modulus $|u|$ and the modulus of its Fourier transform (momentum-space representation) $|F\{u\}|$ [1]. This motivates the related and more general phase problem of the means for determining a beamlike unbounded complex wave function given measurements of probability density over one or more two-dimensional (2D) planes [2]. Such measurements can be obtained via an ensemble of identically prepared quantum systems (e.g., in the context of electron diffraction using a modern source [3]) or via a coherent optical system (e.g., in the context of coherent visible-light optics [4] or coherent x-ray optics [5]).

The latter phase problem is sketched in Fig. 1, which depicts a coherent mono-energetic spatial wave field u_{in} incident upon an elastically scattering potential ("sample") A. For the sake of concreteness, u_{in} might correspond to a coherent electron wave field in which spin may be neglected. A transmission electron microscope may be used to obtain a focal series of two images B and C, over each plane of which the probability density of the scattered-electron wave function is registered [2,3]. This probability-density map, hereafter termed "intensity," is measured through the individual collapse of a large number of almost-identically-prepared electron wave functions emitted by a tungsten source or field emission gun [3]. If we assume that the scattering potential is varying sufficiently slowly in space, and that the incident field is a z-directed plane wave, then the elastically scattered field will be paraxial (i.e., all probability-current-density vectors, downstream of the object, will make a small angle with respect to the optical axis z) [5].

This indicative high-energy potential scattering scenario has direct analogs in the scattering of visible light or hard x-rays by a slowly spatially varying refractive-index distribution [6], scattering of coherent visible light by cold atoms [7] and Bose-Einstein condensates [8], or in the scattering of neutrons from macroscopic samples [9]. In all of the above cases, "slowly varying" refers to the scatterer varying slowly over length scales comparable to the wavelength of the incident matter- or radiation-wave field [10].

The phase-reconstruction problem, mentioned in the first paragraph, has ramifications for the problem of structure determination using the data described in the second paragraph. Specifically, one seeks to reconstruct information regarding the scattering potential A (see Fig. 1) given measurements of paraxial-wave-field moduli over planes B, C, etc. downstream of the sample A. Often, one has a transparent or weakly absorbing scatterer A, which implies that the phase but not the magnitude of the wave field over plane B is significantly affected by the sample [11]. Examples of such "phase objects" are well known in the context of imaging using visible light [4,7,8,12], electrons [3,13], neutrons [9], and hard x-rays [5].

We elaborate on three examples of this common situation regarding "phase objects":

(i) *Electrons.* Medium-resolution bright-field transmission electron microscopy of thin noncrystalline

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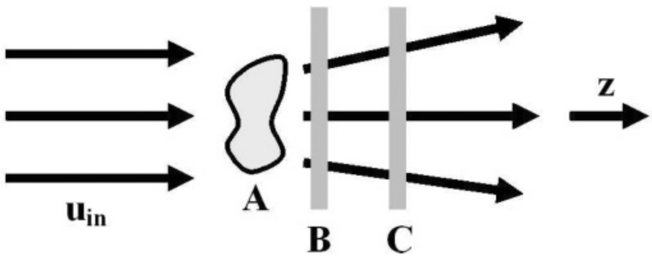

FIG. 1. Generic propagation-based phase-retrieval scenario using paraxial radiation- or matter-wave fields.

samples often yields an in-focus image with negligible contrast [13]. Under the projection approximation, the phase of the wave function over the nominally planar exit surface B (see Fig. 1) is given by the famous Aharonov-Bohm phase factor [14,15], with the probability density over this plane being approximately constant.

(ii) *X-rays.* Materials with similar x-ray attenuation coefficients (e.g., different types of soft biological tissues) are often difficult to distinguish using conventional absorption-based x-ray imaging or computed tomography (CT). In such cases, a suitable form of phase-contrast imaging (PCI) can be helpful [16–18]. For example, propagation-based phase contrast [19,20], in which the act of free-space propagation can convert transverse phase variations (over plane B in Fig. 1) into transverse intensity variations (over plane C), can help to significantly improve the contrast and signal-to-noise ratio in x-ray images of samples consisting predominantly of low-Z materials.

(iii) *Neutrons.* When performing propagation-based phase contrast imaging using neutrons [9], one often has the case where elements in the sample of interest (e.g. small organic samples, lead samples, etc.) are transparent, or the closely related case where distinct materials (e.g., titanium and steel) have very similar absorptive properties, but impart different phase shifts on the neutron beam traversing the sample.

To obtain quantitative information from phase-contrast images, as may be required, for example, in x-ray [21–28], neutron, or electron CT [15,29–32], it is usually necessary to perform an image processing operation known as "phase retrieval." Phase retrieval uses one or more images collected with a position-sensitive detector to produce a quantitative map of projected phase shifts in transverse sections of the beam transmitted through a sample [5]. Image acquisition parameters that are varied between the multiple images used for phase retrieval may include the sample-to-detector and/or source-to-sample distance, and the energy or the spectrum of the illuminating field [19]. In each case a special algorithm is required to convert the intensity distributions in the collected images into quantitative maps of the corresponding phase distribution.

One commonly used phase-retrieval method, generic to all of the previously cited modalities using radiation and matter-wave fields, is based on the transport-of-intensity equation (TIE). The TIE was proposed for electromagnetic radiation by Teague in 1983 [33] and later generalized to a wider class of both linear and nonlinear paraxial fields [34]. To solve this equation, Teague introduced an auxiliary function that transforms the TIE into a classical two-dimensional Poisson equation [33], which can easily be solved (e.g., by using a Fourier-transform-based method [35] or other approaches [36]). The Fourier-transform method [35] has enjoyed widespread use, with successful experimental applications to phase retrieval using visible light [4], neutrons [9], x-rays [19,20], and electrons [3,37–39], and it has been proposed for experimental applications to Bose-Einstein condensates [34,40] and atom lasers [34]. However, these and related studies have been undertaken without a detailed analysis of the validity of phase retrieval using Teague's method, usually producing phase maps that are in good agreement with *a priori* known properties of the sample or as verified by alternative analytical techniques. It is timely that the foundations upon which the method is based be thoroughly examined. Such an examination is the core topic of the present paper.

Sec. II develops the TIE for a broad general class of parabolic field equations which includes all of the physical scenarios discussed above [2,34] before outlining how Teague's auxiliary function [33] is used in the previously mentioned popular modern procedure for phase retrieval based on this equation [35]. Sec. III then demonstrates the role of the Helmholtz decomposition theorem in analyzing the validity of Teague's auxiliary-function solution to the TIE. This domain of validity is rigorously examined in Sec. IV. A core result is the development of a necessary and sufficient condition for the correctness of phase retrieval based on Teague's auxiliary function, implying the existence of a typically small error term in such phase-amplitude reconstructions. Sec. V gives an example of a phase-amplitude distribution that cannot be reconstructed via Teague's approach. We conclude with Sec. VI, which summarizes and discusses the main findings of the paper. Our work clarifies a long-unanswered question regarding the foundations of a widely applied phase-amplitude retrieval method [33,35]. We anticipate it will stimulate further research into phase-amplitude retrieval using the TIE.

II. TEAGUE'S SOLUTION FOR THE TRANSPORT-OF-INTENSITY EQUATION

Consider the following class of nonlinear (2+1)-dimensional field equations governing the spatial evolution of a stationary-state wave function u [34]:

$$[2ik\partial_z + \nabla^2 + g(|u|)]u(x,y,z) = 0. \tag{1}$$

Here, $k = 2\pi/\lambda$, λ is the wavelength or de Broglie wavelength, $\partial_z = \partial/\partial z$ denotes partial differentiation with respect to distance along the nominal optical axis z (see Fig. 1), $\nabla^2 = \partial_x^2 + \partial_y^2$ is the two-dimensional Laplacian in the plane perpendicular to z, and g is an arbitrary real function of a real variable. Note that Eq. (1) describes a paraxial wave field, which implies that all directions of propagation corresponding to non-negligible plane-wave components in the angular-spectrum decomposition make small angles with the positive z axis [5]. In particular, this allows one to neglect the second derivative of the function $u(x,y,z)$ with respect to z. We consider only such paraxial wave fields in the present paper.

Special cases of Eq. (1) 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 [41], (ii) the parabolic equation for paraxial monochromatic scalar electromagnetic waves such as coherent visible light or coherent hard x-rays [42], (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, and u is no longer a stationary-state wave function) [34], (iv) the nonlinear paraxial equation governing the propagation of intense electromagnetic fields in a nonlinear medium [43], and (v) the (2+1)-dimensional Schrödinger equation, with z again being a temporal rather than a spatial variable.

Following Madelung [44], we seek a "hydrodynamic-like" formulation of Eq. (1) by making the substitution

$$u = I^{1/2} \exp(i\varphi), \tag{2}$$

where

$$I = |u|^2 \tag{3}$$

denotes the intensity and

$$\varphi = \arg u \tag{4}$$

denotes the phase. Separating out the imaginary part yields the following continuity equation expressing the existence of a conserved current [33,34]:

$$-\mathrm{div}\,[I\,(x,y,z_0)\,\nabla\varphi\,(x,y,z_0)] = k\partial_z I\,(x,y,z_0)\,. \tag{5}$$

Note that the notation for two-dimensional vector fields and related operators (such as div, ∇, etc.), as used in Eq. (5) and elsewhere below, is outlined in Appendix A. Equation (5) is termed the transport-of-intensity equation (TIE) in the context of propagation-based phase retrieval [33]. 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 $\varphi = \arg u$ 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 [45].

Teague [33] 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. While Teague only considered the linear case where $g = 0$ in Eq. (1), Paganin & Nugent [34] pointed out that identical considerations apply to nonlinear fields with arbitrary real g—note that, in this context, the TIE is independent of g because the local conservation expressed by this equation is unchanged by the presence of any nondissipative nonlinearity.

Phase-amplitude retrieval using the TIE usually requires measurement of the intensity over at least two different planes, $z = z_0$ and $z = z_0 + \Delta$, orthogonal to the optical axis [33]. Without loss of generality we can always assume that $z_0 = 0$. Therefore, in the rest of the paper 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 nonlinear fields for which interferometric phase measurement is in general problematic on account of the interaction between object and reference waves [34].

To obtain a unique solution for the phase φ in Ω using the TIE Eq. (5), it is necessary to impose some suitable boundary conditions (e.g., Dirichlet, Neumann, or periodic boundary conditions) on the phase function (see, e.g., [46]). (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 solving Eq. (5) via the introduction of an auxiliary function ψ, which satisfies

$$\nabla\psi\,(x,y) = I\,(x,y)\,\nabla\varphi\,(x,y)\,. \tag{6}$$

Given that the right-hand side (rhs) of the above expression is proportional to the transverse component of the probability current density [44,47] (or current density [5] for classical fields), the above approximation amounts to the statement that 2D paraxial current densities [associated with fields obeying Eq. (1)] are well approximated as conservative vector fields derivable from the scalar potential ψ.

If the scalar potential ψ exists then, by substituting Eq. (6) into Eq. (5), we see that it satisfies the Poisson equation

$$-\nabla^2\psi\,(x,y) = k\partial_z I\,(x,y)\,. \tag{7}$$

After finding ψ from Eq. (7), a solution $\tilde{\varphi}$ of Eq. (5) can be determined by solving another Poisson equation:

$$\nabla^2\tilde{\varphi}\,(x,y) = \mathrm{div}[I^{-1}\,(x,y)\,\nabla\psi\,(x,y)], \tag{8}$$

which can be obtained by dividing both sides of Eq. (6) by I and taking the divergence. Therefore, this method allows one to solve Eq. (5) via two Poisson equations. One advantage of the Poisson Eqs. (7) and (8) compared to Eq. (5) is that the two former equations are amenable to a numerical solution using a fast Fourier transform (FFT). Note that we have introduced a new symbol $\tilde{\varphi}$ in Eq. (8) to distinguish the phase solution of Eq.(5) obtained by this "Teague's method."

This technique was proposed in Ref. [35] and further applied to a variety of matter- and radiation-wave fields in several other publications [2–5,9,15,29,30,37–39,48–50] (see also [36,51] and references therein for other solution methods for Eq. (5) in the context of phase retrieval). In this paper, we thoroughly examine the validity of "Teague's assumption" [i.e., the existence of the auxiliary function ψ required in Eq. (6)].

One can actually ask a more general question: regardless of the validity of "Teague's assumption" [Eq. (6)], what are the sufficient conditions under which the "Teague solution" $\tilde{\varphi}$, obtained by means of "Teague's method" [represented by Eqs. (7) and (8)] coincides exactly with or is sufficiently close to the true solution φ of the TIE [Eq. (5)]? Note that, unlike the auxiliary function ψ required in Eq. (6), a solution to Eq. (7) with appropriate boundary conditions is known to exist and to be unique [46]. Therefore, Teague's method will always deliver a solution; but the question needs to be answered about the closeness of this solution $\tilde{\varphi}$ to the true solution φ of the TIE [Eq. (5)]. In the present paper, 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 [52] that Eq. (6) represents a good approximation in most realistic cases. A different approach to the justification of the validity of Eq. (6)

based on the Helmholtz theorem [46] was given in Ref. [35]. The Helmholtz theorem is also the main tool that we use below for a detailed analysis of the problem.

III. HELMHOLTZ 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 and defined in a simply connected bounded domain $\Omega \subset \mathbf{R}^2$ 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

$$\mathbf{A}(x,y) = \nabla\psi(x,y) + \mathbf{rot}\eta(x,y) \text{ in } \Omega, \text{ and}$$
$$\nabla\psi\cdot\mathbf{n}|_{\partial\Omega} = 0 \text{ and } \eta(x,y)|_{\partial\Omega} = \text{const.} \tag{9}$$

The proof of the above special case of the Helmholtz theorem is given in Appendix B for completeness (note that, although the formulation and proof of the Helmholtz theorem in three dimensions can be found in many textbooks, such as [46], it seems much more difficult to find a corresponding formulation and proof in the literature for the 2D case).

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 and has continuous first derivatives, while φ has continuous second derivatives in Ω], where the function φ also satisfies, for example, the uniform Neumann boundary conditions $\nabla\varphi\cdot\mathbf{n}|_{\partial\Omega} = 0$, we can find a pair of unique (up to additive constants) functions (ψ,η) such that

$$I(x,y)\nabla\varphi(x,y) = \nabla\psi(x,y) + \mathbf{rot}\eta(x,y), \tag{10}$$

and the functions (ψ,η) satisfy the same boundary conditions as in Eq. (9). Then $\nabla\varphi(x,y) = I^{-1}(x,y)\nabla\psi(x,y) + I^{-1}(x,y)\,\mathbf{rot}\eta(x,y)$ and thus

$$\nabla^2\varphi(x,y) = \text{div}[I^{-1}(x,y)\nabla\psi(x,y)]$$
$$+\nabla I^{-1}(x,y)\times\nabla\eta(x,y), \tag{11}$$

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

Assuming suitable boundary conditions (e.g., Dirichlet, Neumann, or periodic boundary conditions) for the phase function in Eq. (11) that guarantee the existence of the inverse Laplacian operator in a suitable functional space over Ω, we can also obtain

$$\varphi(x,y) = \nabla^{-2}\text{div}[I^{-1}(x,y)\nabla\psi(x,y)]$$
$$+\nabla^{-2}[\nabla I^{-1}(x,y)\times\nabla\eta(x,y)]. \tag{12}$$

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., [46,53]), the inverse Laplacian can be uniquely defined; for example, 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 $\varphi(x,y)$ which is itself physically defined only up to an arbitrary additive constant.

In view of Eq. (12), "Teague's solution" $\tilde{\varphi}(x,y) = \nabla^{-2}\text{div}[I^{-1}(x,y)\nabla\psi(x,y)]$ where $\psi(x,y)$ is a solution of Eq. (7), represents a good approximation to the true solution $\varphi(x,y)$ of the TIE if and only if the error term

$$\varepsilon(x,y) = \varphi(x,y) - \nabla^{-2}\text{div}[I^{-1}(x,y)\nabla\psi(x,y)]$$
$$= \nabla^{-2}[\nabla I^{-1}(x,y)\times\nabla\eta(x,y)], \tag{13}$$

is either exactly zero or is at least sufficiently smaller 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 paper to have explicit equations for the functions ψ and η found on the rhs of Eq. (10). By taking the divergence of Eq. (10) and using Eq. (A1), it is easy to see that

$$\nabla^2\psi(x,y) = \text{div}\,[I(x,y)\nabla\varphi(x,y)],$$
$$\nabla\psi\cdot\mathbf{n}|_{\partial\Omega} = 0. \tag{14}$$

The function ψ can be found from Eq. (14) uniquely up to an arbitrary additive constant.

In order to find the function $\eta(x,y)$, take the curl of both sides of Eq. (10). Using Eqs. (A2) and (A3) and the identity $\text{curl}\,(I\nabla\varphi) = \nabla I\times\nabla\varphi$, we obtain

$$-\nabla^2\eta(x,y) = \nabla I(x,y)\times\nabla\varphi(x,y),$$
$$\eta|_{\partial\Omega} = \text{const.} \tag{15}$$

Equation (15) 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; including, conditions guaranteeing that "Teague's error term" $\varepsilon(x,y)$ defined in Eq. (13) is either exactly zero or is sufficiently small.

IV. 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 Eq. (10) above], there exists a function ψ such that $\nabla\psi(x,y) = I(x,y)\nabla\varphi(x,y)$ if and only if

$$\nabla I(x,y)\times\nabla\varphi(x,y) \equiv 0. \tag{16}$$

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

Before proceeding, we note that, for many nonabsorbing objects of interest in the context of TIE phase retrieval, we intuitively expect $\nabla\varphi$ and ∇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 $|\varphi|$) is typically associated with an increase in the actual thickness or density of a sample, and an increase in the actual thickness or density of a sample is typically associated with an increase in the absorption of the sample. Thus, while for a truly arbitrary object one would expect $\nabla\varphi$ and ∇I to be uncorrelated and therefore not necessarily parallel everywhere in Ω, for a "typical" object, $\nabla\varphi$ and ∇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 nonindependent, implying in general a nonzero 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 $\nabla\varphi$ and ∇I to be "close to parallel."

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

$$0 = \text{curl}\,[\nabla\psi\,(x,y)] = \text{curl}\,[I\,(x,y)\,\nabla\varphi\,(x,y)] = \partial_x I\,(x,y)\,\partial_y\varphi\,(x,y) - \partial_y I\,(x,y)\,\partial_x\varphi\,(x,y)\,. \quad (17)$$

On the other hand, if $\nabla I\,(x,y) \times \nabla\varphi\,(x,y) \equiv 0$, then using the Helmholtz decomposition [Eq. (10)], we obtain

$$0 = \nabla I \times \nabla\varphi = \text{curl}\,[I\,(x,y)\,\nabla\varphi\,(x,y)] = \text{curl}\,[\mathbf{rot}\eta\,(x,y)] = -\nabla^2\eta\,(x,y)\,, \quad (18)$$

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 [46,53]. Therefore, $\mathbf{rot}\eta\,(x,y) \equiv 0$ and $\nabla\psi\,(x,y) = I\,(x,y)\,\nabla\varphi\,(x,y)$.

"Teague's assumption" [i.e., the existence of a potential function ψ such that $\nabla\psi\,(x,y) = I\,(x,y)\,\nabla\varphi\,(x,y)$] implies that

$$\tilde{\varphi}\,(x,y) = \nabla^{-2}\text{div}[I^{-1}\,(x,y)\,\nabla\psi\,(x,y)] = \nabla^{-2}\text{div}\,[\nabla\varphi\,(x,y)] = \varphi\,(x,y)\,. \quad (19)$$

According to Eq. (13) this also implies that $\varepsilon\,(x,y) = 0$ (i.e., the Teague solution is exact in this case). Therefore, Eq. (16) represents a sufficient condition not only for the validity of Teague's assumption, Eq. (6), but also for the exact accuracy of Teague's solution, $\tilde{\varphi} = \varphi$.

Note, however, that the condition expressed by Eq. (16) may not be necessary for the exactness of Teague's solution. Indeed, by virtue of Eq. (13), the exactness of Teague's solution, $\varepsilon\,(x,y) = 0$, only implies that $\nabla I \times \nabla\eta = 0$ (e.g., that vectors $\nabla\eta$ and ∇I are parallel everywhere in Ω). Equation (16), on the other hand, is equivalent [by means of Eq. (15)] 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 Eq. (16). The vectors $\nabla\varphi\,(x,y)$ and $\nabla I\,(x,y)$ are parallel at all points in Ω if and only if the vectors $\nabla\varphi\,(x,y)$ and $\nabla\ln[I\,(x,y)] = I^{-1}\,(x,y)\,\nabla I\,(x,y)$ are parallel at these points. The latter means that $\nabla\varphi\,(x,y) = c\,(x,y)\,\nabla\ln[I\,(x,y)]$ for some scalar function $c\,(x,y)$. Note that this is similar, but not equivalent, to the definition of monomorphous (or homogeneous) objects [54,55], for which one has $\nabla\varphi\,(x,y) = (\gamma/2)\,\nabla\ln[I\,(x,y)]$ in the projection approximation [5,56], where γ is a constant. Therefore, the class of objects for which the "Teague assumption" [i.e., that a function ψ exists such that $\nabla\psi\,(x,y) = I\,(x,y)\,\nabla\varphi\,(x,y)$] holds may be broader than the class of all monomorphous objects. It is well known that the class of all monomorphous objects contains the subclass of all objects for which $\varphi(x,y) = (\gamma/2)\ln I\,(x,y)$ 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 [54] 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 [7]. Indeed, for such objects one obtains, assuming that the projection approximation [5,56] is valid and the incident plane wave is $\exp\,(ikz)$, that $\varphi\,(x,y) = -k\delta T\,(x,y)$ 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, $\varphi\,(x,y) = [\delta/(2\beta)]\ln[I\,(x,y)]$ (i.e., $\gamma \equiv \delta/\beta$). In the case of transmitted x-ray waves with energies between approximately 60 and 500 keV, the equality $\varphi\,(x,y) = (\gamma/2)\ln I\,(x,y)$ holds not only for objects that consist predominantly of a single material, but also for any objects consisting of chemical elements with atomic number $Z < 10$ [57]. The physical origin of this last-mentioned result is that samples composed of sufficiently light elements and illuminated at sufficiently high x-ray energy are well approximated over sufficiently large length scales by a continuous "single-material" distribution of almost-free electrons [58]. Similar considerations apply to the other forms of radiation- and matter-wave fields considered in this paper. We see that, for all of these classes of objects, Teague's assumption is valid exactly.

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

$$\|f\|_2 = \frac{\sqrt{\iint_\Omega |f(x,y)|^2 dx dy}}{\sqrt{\iint_\Omega dx dy}}. \quad (20)$$

As the inverse Laplacian is a continuous operator in suitable functional subspaces of $L_2\,(\Omega)$, then $\|\nabla^{-2} f\|_2 \leqslant L_\Omega^2\,\|f\|_2$ (see, e.g., [53]) 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 $\mathbf{R}^2$; see, e.g., [59,60]). It follows from Eq. (13) that

$$\|\varepsilon\,(x,y)\|_2 \leqslant L_\Omega^2 \|\nabla I^{-1}\,(x,y) \times \nabla\eta\|_2. \quad (21)$$

For "reasonable" functions f from $L_2\,(\Omega)$ (satisfying Dirichlet or other suitable boundary conditions) one can verify by integrating by parts that $\|\nabla f\|_2^2 \leqslant \|f\|_2\,\|\nabla^2 f\|_2$. Now we can use Eq. (15) and the continuity of the inverse Laplacian to obtain: $\|\nabla\eta\|_2 \leqslant \|\eta\|_2^{1/2}\,\|\nabla^2\eta\|_2^{1/2} \leqslant L_\Omega\,\|\nabla I \times \nabla\varphi\|_2$. Combining this with Eq. (21) we finally obtain

$$\|\varepsilon\,(x,y)\|_2 \leqslant L_\Omega^3\,\|\nabla\varphi\|_2\,\|\nabla\ln I\|_2^2\,. \quad (22)$$

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

$$|\nabla\varphi||\nabla I/I| \ll k/R, \quad (23)$$

see, for example, Ref. [10].Therefore, under the TIE validity conditions, Eq. (22) can be rewritten as

$$\|\varepsilon\,(x,y)\|_2 \ll \left(kL_\Omega^3\big/R\right)\|\nabla\ln I\|_2\,. \quad (24)$$

The rhs of Eq. (24) is a product of two factors: $N_F^{\max} \equiv kL_\Omega^2/R$; that is, the (largest) Fresnel number [42] associated with domain Ω, and $\text{var}_2\,(I) \equiv L_\Omega\,\|\nabla\ln I\|_2$ that can be interpreted as a measure of total variation of intensity across the domain. As the validity conditions of the TIE require that $N_F^{\max} \gg 1$ (see, e.g., [61]), then $\mathrm{var}_2(I) \equiv L_\Omega \|\nabla \ln I\|_2$ typically has to be very small to guarantee that Teague's solution is accurate. Recalling that Teague's solution is accurate when $\|\varepsilon(x,y)\|_2 \ll \|\varphi\|_2$, we finally obtain from Eq. (24) that a sufficient condition for the accuracy of Teague's solution is

$$N_F^{\max}\mathrm{var}_2(I) \leqslant \|\varphi\|_2 . \tag{25}$$

It follows from Eq. (25) 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 Eq. (25) 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 $\nabla I(x,y) \times \nabla\varphi(x,y) \equiv 0$ considered above, which in fact guarantees that the Teague error term $\varepsilon(x,y)$ is equal to zero, even when the variation of absorption is large. Therefore, we should emphasize that Eq. (25) is sufficient, but not necessary, for the Teague solution to be accurate.

V. TIE 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 [Eq. (5)] is significantly different from "Teague's solution"

$$\tilde{\varphi}(x,y) = \nabla^{-2}\mathrm{div}[I^{-1}(x,y)\nabla\psi(x,y)], \tag{26}$$

where ψ is a solution of Eq. (7), it is necessary, but not sufficient, to ensure that $I(x,y)\nabla\varphi(x,y)$ is not a complete potential [or, according to Sec. IV, that vectors $\nabla\varphi(x,y)$ and $\nabla I(x,y)$ are not parallel to each other at all points]. We also want to find an example where the error term $\varepsilon(x,y) = \varphi(x,y) - \tilde{\varphi}(x,y)$, is not just nonzero but is sufficiently large in an appropriate sense; for example, comparable in norm to the exact solution φ or, equivalently, comparable to the "Teague solution" $\tilde{\varphi}$. Considering Eq. (13), we may try to find a case where $\nabla I^{-1} \times \nabla\eta$ is comparable in norm to $\mathrm{div}[I^{-1}(x,y)\nabla\psi(x,y)]$. As one can see from Eq. (11), this will be the case when $\nabla^2\varphi(x,y)$ is very small, but $\nabla I^{-1}(x,y) \times \nabla\eta(x,y)$ is not.

Consider the following example:

$$\Omega = (-10,10) \times (-10,10)(\mu m^2), \tag{27}$$

$$I(x,y) = \exp(-a_0x^2 - b_0y^2) \tag{28}$$

and

$$\varphi(x,y) = a_0x^2 - b_0y^2 - a_1x^8 + b_1y^8, \tag{29}$$

where

$a_0 = b_0 = 10^{-2}\ \mu\mathrm{m}^{-2}$ and $a_1 = b_1 = 0.25 \times 10^{-8}\ \mu\mathrm{m}^{-8}$ [Figs. 2(a) and 2(b)]. This phase function satisfies uniform Neumann boundary conditions. Physically, such a beam could be generated for the case of x-ray 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) with $\delta = 1.39 \times 10^{-6}$ and $\beta = 7.48 \times 10^{-10}$ [62]) with a saddle-like profile of projected thickness $T(x,y)$, and normally illuminating it with a focused Gaussian beam [42] such that the waist of the illuminating beam coincides with the entrance surface of the object. Note that the phase

$$\varphi(x,y) = -\frac{2\pi}{\lambda}\delta T(x,y) + \mathrm{const.}, \tag{30}$$

is defined up to a constant [5]. The maximal projected thickness $T_{\max}$ for our object required to produce the appropriate phase shift is about 17 μm. Then the maximal attenuation caused by this object is very small:

$$\exp\left(-\frac{4\pi}{\lambda}\beta T_{\max}\right) \approx 0.99, \tag{31}$$

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 entirely due 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 1 cm downstream the optical axis, $I(x,y,z=1\ \mathrm{cm})$, calculating the intensity derivative as

$$\partial_z I(x,y,z=0) \cong [I(x,y,z=1\ \mathrm{cm}) - I(x,y,z=0)]/\Delta z, \tag{32}$$

and then solving the TIE [Eq. (5)] for the phase $\varphi(x,y)$. However, if one tries to reconstruct the phase distribution in this case using "Teague's method" represented by Eqs. (7) and (8), the resultant phase distribution $\tilde{\varphi}(x,y)$ will be significantly different from the exact distribution, as explained below.

It is easy to verify that, for the scenario described above, the two vectors

$$\nabla I(x,y) = I(x,y)(-2a_0x, -2b_0y), \tag{33}$$

and

$$\nabla\varphi(x,y) = (2a_0x - 8a_1x^7, -2b_0y + 8b_1y^7), \tag{34}$$

are not parallel at most points in Ω [see Eq. (16)]. 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 $\varepsilon(x,y)$ formulated in the previous section are valid in this example. Finally, the Laplacian

$$\nabla^2\varphi(x,y) = 56a_1(y^6 - x^6) \tag{35}$$

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 $\tilde{\varphi}$ is significantly different from the exact solution φ of the TIE). We could not solve the relevant equations [e.g., Eq. (14)] analytically, so we resorted to numerical solutions using a well-tested software package for x-ray image analysis and simulation: X-TRACT [63]. We first calculated the 2D distribution $-\mathrm{div}[I(x,y)\nabla\varphi(x,y)] = k\partial_z I(x,y)$ for the above phase and intensity by computing the corresponding differential expressions on a numerical grid with 2048 × 2048 square pixels within the domain $\Omega = (-10,10) \times (-10,10)\ \mu\text{m}^2$ [see Fig. 2(c)]. Then we numerically solved the Poisson equation (using the Fourier transform method [35] as implemented in X-TRACT [63]) to obtain the distribution of $\psi(x,y) = \nabla^{-2}\text{div}[I(x,y)\,\nabla\varphi(x,y)]$ in Ω [Fig. 2(d)]. Solving the second Poisson equation according to "Teague's method," we obtained the phase distribution $\tilde{\varphi}(x,y) = \nabla^{-2}\text{div}[I^{-1}(x,y)\,\nabla\psi(x,y)]$ [Fig. 2(e)]. Finally we calculated the difference

$$\varepsilon(x,y) = \varphi(x,y) - \tilde{\varphi}(x,y) \tag{36}$$

between the exact phase and the one obtained using "Teague's method" [Fig. 2(f)]. These numerical calculations showed that

$$\|\varphi(x,y) - \tilde{\varphi}(x,y)\|_2 \cong 0.09\,\|\varphi(x,y)\|_2\,. \tag{37}$$

That is, the relative root-mean-square error is approximately 9%.

VI. CONCLUSIONS

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 nonlinear parabolic equation (1) or by its special case where $g = 0$. All such fields, both linear and nonlinear, have a spatial evolution of intensity which is governed by the associated continuity equation [Eq. (5)], which is termed the TIE in the context of phase retrieval [33]. The TIE has been used for such phase retrieval using electrons, visible light, hard x-rays, and neutrons. Notwithstanding these successes,

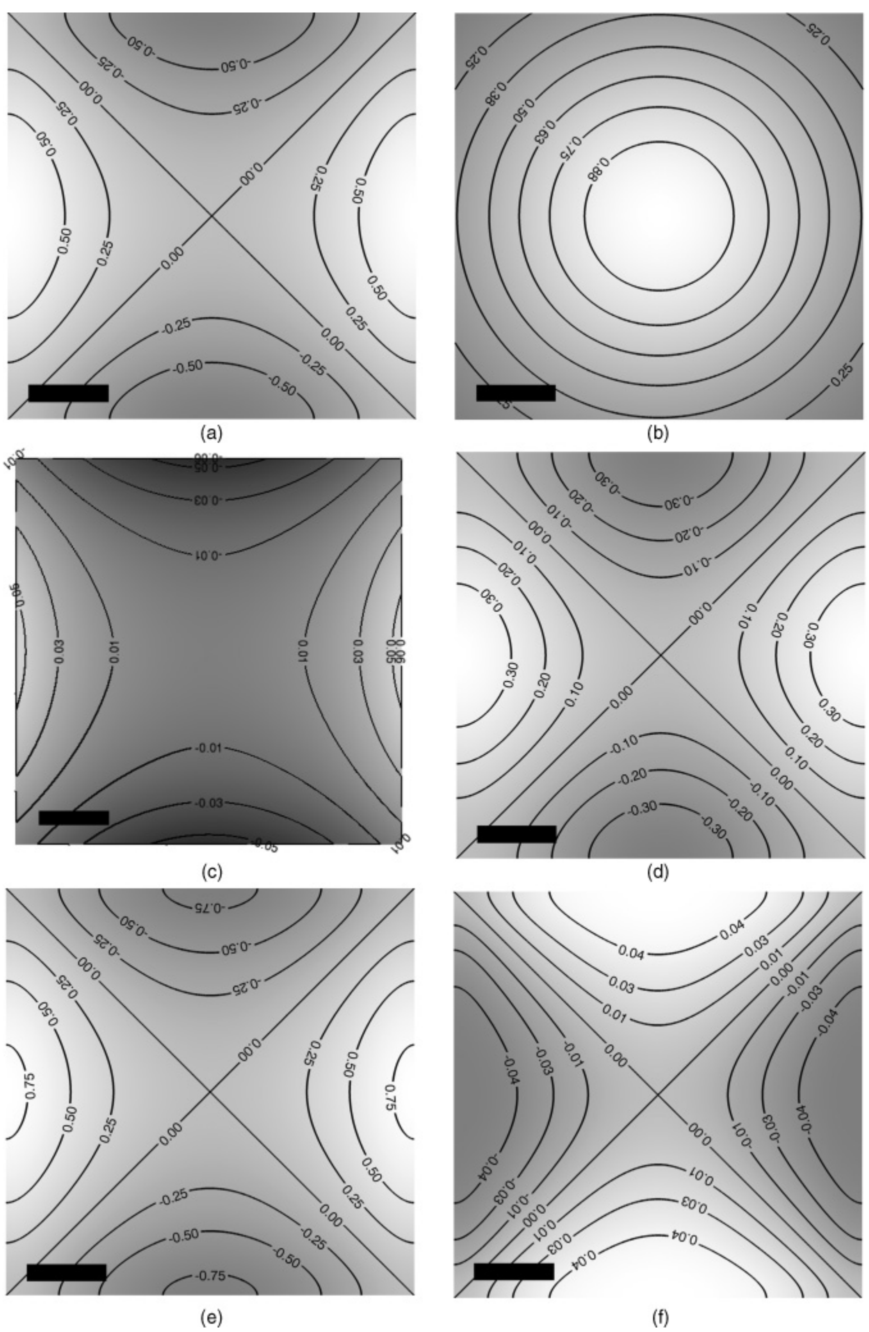

FIG. 2. Simulations corresponding to the counter example in Sec. V (see main text for details). (a) Phase distribution, $\varphi(x,y) = a_0x^2 - b_0y^2 - a_1x^8 + b_1y^8$ defined in $\Omega = (-10,10) \times (-10,10)\ \mu\text{m}^2$. The value range of the phase is approximately $(-0.75,\ 0.75)$ radians. (b) Intensity distribution $I(x,y) = \exp(-a_0x^2 - b_0y^2)$ defined in Ω. The value range of the intensity is approximately (0.14, 1.0) arbitrary units. (c) Distribution of the function $-\text{div}[I(x,y)\,\nabla\varphi(x,y)]$ in Ω. The value range of this function is approximately $(-0.073,\ 0.073)$. (d) Distribution of the function $\psi(x,y) = \nabla^{-2}\text{div}[I(x,y)\,\nabla\varphi(x,y)]$ in Ω. The value range of this function is approximately $(-0.39,\ 0.39)$ radians. (e) Distribution of the function $\tilde{\varphi}(x,y) = \nabla^{-2}\text{div}[I^{-1}(x,y)\,\nabla\psi(x,y)]$ in Ω. The value range of this function is approximately $(-0.80,\ 0.80)$ radians. (f) Distribution of error function $\varepsilon(x,y) = \varphi(x,y) - \tilde{\varphi}(x,y)$ in Ω. The value range of this function is approximately $(-0.054,\ 0.054)$ radians. Scale bar = 4 μm, in Figs 2(a)–2(f).

the validity of Teague's assumption [33]—which amounts to the assumption that the transverse component of the current density is a two-dimensional potential field and which is key to the most widely applied TIE-based phase-retrieval algorithm [35]—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 and cold atom clouds to magnetic skyrmions and spin ices [2–5,19,37–39,48–50,64]), there are some situations where the error can be relatively large. Therefore, care should be taken when using Teague's 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 proven in Sec. IV of the present paper is satisfied. This would guarantee the accuracy of the Teague-based TIE solution. Alternatively, one may prefer to solve the TIE, Eq. (5), by other methods that do not involve the use of Teague's assumption (see, e.g., [36]).

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APPENDIX A: NOTATION

In this paper we use the following notations for 2D linear partial differential operators:

(a) For any differentiable function of two variables, $f \equiv f(x,y)$, we use ∇ for a 2D gradient [i.e., $\nabla f = (\partial_x f, \partial_y f)$ 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 $\text{div}\mathbf{A} = \partial_x A_x + \partial_y A_y$.

(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

$$\text{div}(\mathbf{rot}\eta) = \partial_x \partial_y \eta - \partial_y \partial_x \eta = 0. \tag{A1}$$

Note also that $\mathbf{rot}\eta \cdot \nabla\eta = \left(\partial_y\eta, -\partial_x\eta\right) \cdot \left(\partial_x\eta, \partial_y\eta\right) \equiv 0$, 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 $\text{curl}\mathbf{A} = \partial_x A_y - \partial_y A_x$. The most important property of this operator is that

$$\text{curl}(\nabla f) = \partial_x \partial_y f - \partial_y \partial_x f = 0. \tag{A2}$$

Note that, unlike the case of $\mathbf{R}^3$, we need to introduce two different variants, "rot" and "curl", of the curl operation in $\mathbf{R}^2$ 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 rhs is a scalar function). Then $\text{curl}\mathbf{A} = \nabla \times \mathbf{A}$. Note that

$$\text{curl}(\mathbf{rot}\eta) \equiv \nabla \times \mathbf{rot}\eta = -\partial_x^2\eta - \partial_y^2\eta = -\nabla^2\eta. \tag{A3}$$

Note also that the 2D functions and operators defined above in (a)–(d) are introduced for convenience. The conventional three-dimensional (3D) 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 main text.

APPENDIX B: HELMHOLTZ THEOREM IN 2D

Here we prove a special case of the Helmholtz decomposition theorem in a bounded domain in $\mathbf{R}^2$. Given is a continuous vector field

$$\mathbf{A}(x,y) = (A_x(x,y), A_y(x,y)), \tag{B1}$$

having continuous partial derivatives, defined in a simply-connected bounded domain $\Omega \subset \mathbf{R}^2$ with a piece-wise smooth boundary $\partial\Omega$. The vector field satisfies the boundary property

$$\mathbf{A} \cdot \mathbf{n}|_{\partial\Omega} = 0, \tag{B2}$$

where $\mathbf{n}$ is the external normal to $\partial\Omega$.

Let us prove that there exists a unique (up to additive constants) pair of scalar functions (ψ, η) such that

$$\mathbf{A}(x,y) = \nabla\psi(x,y) + \mathbf{rot}\eta(x,y) \tag{B3}$$

in Ω, with the following boundary conditions:

$$\nabla\psi(x,y) \cdot \mathbf{n}|_{\partial\Omega} = 0 \text{ and } \eta(x,y)|_{\partial\Omega} = \text{const}. \tag{B4}$$

First construct an auxiliary vector field $\mathbf{B}(x,y)$, such that $\text{curl}\mathbf{B}(x,y) = 0$ and $\text{div}\mathbf{B}(x,y) = \text{div}\mathbf{A}(x,y)$, with the boundary property $\mathbf{B}(x,y) \cdot \mathbf{n}|_{\partial\Omega} = 0$. We can always find [46,53] a unique (up to an additive constant) function $\psi(x,y)$ in Ω such that

$$\nabla^2\psi(x,y) = \text{div}\mathbf{A},$$
$$\nabla\psi \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{B5}$$

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

Now consider the vector field

$$\mathbf{C}(x,y) = \mathbf{A}(x,y) - \mathbf{B}(x,y). \tag{B6}$$

It is easy to see that

$$\mathbf{C} \cdot \mathbf{n}|_{\partial\Omega} = 0, \tag{B7}$$

$$\text{div}\mathbf{C} = \text{div}(\mathbf{A} - \nabla\psi) = \text{div}\mathbf{A} - \nabla^2\psi = 0 \tag{B8}$$

and

$$\text{curl}\mathbf{C} = \text{curl}(\mathbf{A} - \nabla\psi) = \text{curl}\mathbf{A}. \tag{B9}$$

Because $\text{div}\mathbf{C} = 0$, there exists a function $\eta(x,y)$, such that $\mathbf{rot}\eta(x,y) = \mathbf{C}(x,y)$ (see, e.g., [65]). The boundary property for such $\mathbf{rot}\eta$ 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 $\nabla\eta$ is perpendicular to the tangent of the boundary of the domain. Consequently η does not change its value along the boundary; that is, 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 $\mathbf{A}(x,y) = \mathbf{B}(x,y) + \mathbf{C}(x,y) = \nabla\psi(x,y) + \mathbf{rot}\eta(x,y)$, where $\nabla\psi(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$, and $\eta(x,y)|_{\partial\Omega} = \text{const.}$

If we have two different representations of the vector field $\mathbf{A}(x,y)$ in the form

$$\begin{aligned}\mathbf{A}(x,y) &= \nabla\psi(x,y) + \mathbf{rot}\eta(x,y)\\ &= \nabla\psi_1(x,y) + \mathbf{rot}\eta_1(x,y),\end{aligned} \tag{B10}$$

where

$$\nabla\psi(x,y)\cdot\mathbf{n}|_{\partial\Omega} = \nabla\psi_1(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0, \tag{B11}$$

and

$$\mathbf{rot}\eta(x,y)\cdot\mathrm{n}|_{\partial\Omega} = \mathbf{rot}\eta_1(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0, \tag{B12}$$

then

$\nabla[\psi(x,y)-\psi_1(x,y)]+\mathbf{rot}[\eta(x,y)-\eta_1(x,y)]=0$. 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, $\nabla\bar{\psi}(x,y)\cdot\mathbf{n}|_{\partial\Omega} = 0$, or Dirichlet conditions $\bar{\eta}(x,y)|_{\partial\Omega} = \text{const.}$, respectively, and thus both these functions are constants [46,53], which proves the required uniqueness of the Helmholtz decomposition up to additive constants.

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