Irradiance moments: their propagation and use for unique retrieval of phase

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The functional dependence of irradiance moments with distance from the pupil plane is studied within the framework of Fresnel diffraction theory. The concept of analytic pupil function is introduced, and for such pupil functions it is shown that any finite-order irradiance moment exists, even in the presence of arbitrary continuous phase aberrations. The uniqueness of the relationship between pupil-plane phase and irradiance moments, when the moments are calculated over an orthogonal plane at a fixed point along the optical axis in image space, is obscure, and the relationship between phase and moments is generally nonlinear. However, by studying the behavior of irradiance moments throughout the neighborhood of a given axial point in image space, one may determine, for a large class of pupils, the pupil-plane phase uniquely (within an arbitrary additive constant), and only a linear problem need be solved for phase retrieval. In particular, unique phase retrieval may be accomplished by measuring moments in the neighborhood of either the pupil plane or the image plane. Examples of this technique are given.

INTRODUCTION

One of the standard phase-retrieval problems (see, e.g., Ref. 1) is the following mathematical question: given two complex-valued functions

 $f(\mathbf{r}) = |f(\mathbf{r})| \exp[i\phi(\mathbf{r})], \qquad F(\rho) = |F(\rho)| \exp[i\Phi(\rho)]$ that are Fourier-transform pairs; i.e.,

$$F(\boldsymbol{\rho}) = \int d\mathbf{r} \exp(-i2\pi\boldsymbol{\rho} \cdot \mathbf{r}) f(\mathbf{r}),$$

find the phase $\phi(\mathbf{r})$ [or, equivalently, find $\Phi(\boldsymbol{\rho})$] if only the moduli $|f(\mathbf{r})|$ and $|F(\boldsymbol{\rho})|$ are known.

The case in which \mathbf{r} and $\boldsymbol{\rho}$ are two-dimensional vectors is of interest in optics [see Eq. (6)] when the question arises of determining the pupil-plane phase aberration from a knowledge of both the shape of the pupil and measurements of the image-plane irradiance distribution.

It is the viewpoint presented in this paper that giving a solution to this phase-retrieval problem means writing an explicit formula

$$\phi = \hat{o}(|f|, |F|),$$

where \hat{o} is some definite operation (e.g., differentiation, integration, exponentiation) applied to the known functions |f|and |F|. The problem is difficult because it is essentially nonlinear. Either one gets nonlinear integral equations for ϕ or, using basis functions, one gets nonlinear algebraic equations (with a large number of unknowns). In either case the equations so far have not been solved. If one finds a solution, the question of its uniqueness immediately arises. Previous papers^{1–10} have considered the uniqueness question and developed algorithms for searching a parameter space for the phase and/or estimating a phase and then iteratively improving the estimate. In addition, Refs. 8 and 9 develop closely related schemes using complex variable techniques for actually solving for the phase rather than simply searching for it. Like the present paper they require somewhat more input information than simply $|f(\mathbf{r})|$ and $|F(\mathbf{p})|$.

In this paper a mathematical solution is given to the optical phase-retrieval problem that is sufficiently general to cover many interesting cases; i.e., the phase $\phi(\mathbf{r})$ must be a finitedegree polynomial in x and y, and the pupil function must have the smoothness properties described in Section 2. (However, in Section 4 it is shown how the phase may be determined approximately for a discontinuous pupil.) In optics the Fourier transformation occurs only for special cases (Fraunhofer regions, which can be quite close to the exit pupil if a converging lens is used). In general, the transformation that occurs is the (also unitary) Fresnel transformation of Eq. (6), where the parameter z (e.g., axial distance from pupil plane) occurs. The use of irradiance data from xy planes at different z positions allows the pupil-plane phase $\phi(\mathbf{r})$ to be determined by using only linear mathematical techniques. The phase-uniqueness question does not arise, except that an additive constant term (piston) is left undetermined by the methods of this paper. In principle we will see that it is mathematically sufficient to measure irradiance data in two planes to retrieve the phase $\phi(\mathbf{r})$. In practice, signal-tonoise-ratio considerations mean that more measurement planes are needed (e.g., to retrieve the 14 aberrations up through the fourth order will generally require measurements in four planes near the image plane). This is discussed in Section 6. Hoenders⁶ came to similar conclusions in an earlier paper. His work was based on a study of analyticity properties in the complex plane but applied only to the case in which vectors \mathbf{r} , $\boldsymbol{\rho}$ were one dimensional.

It is fortuitous and unintentional that moment methods appear in this paper. However, a mathematical solution of the optical phase-retrieval problem is obvious once irradiance moments are studied as a function of axial position z. The use of moments is initially impeded by the fact that they are in general mathematically infinite. This is only a formal difficulty, which is resolved through the developments of Sections 2 and 4. The solution being presented, although straightforward, is somewhat indirect, and the procedure for

constructing ϕ from measured irradiance data is summarized in Section 7.

This paper is essentially theoretical, being an exposition of various interesting theorems in Fresnel diffraction theory. In particular, it is not intended to discuss details of system design in this paper, although an obvious immediate application is wave-front sensing, for adaptive-optics applications, based on irradiance measurements only.

1. FRESNEL DIFFRACTION THEORY

This section is included so that the basic assumptions of this paper are explicit.

The scalar-wave equation in an isotropic, homogeneous medium (thus take c = 1) is

$$(\partial_x^2 + \partial_y^2 + \partial_z^2 - \partial_t^2)\psi(x, y, z, t) = 0.$$
 (1)

An approximate solution of this equation, representing a wave traveling predominantly in the $\pm z$ direction, may be written as

$$\psi(x, y, z, t) = \exp\left[\frac{i2\pi}{\lambda}(z - t)\right] u_z(\mathbf{r}), \tag{2}$$

where $\mathbf{r} = (x, y)$ and $u_z(\mathbf{r})$ is an exact solution of the parabolic equation

$$\left[i\partial_z + \frac{\lambda}{4\pi} \left(\partial_x^2 + \partial_y^2\right)\right] u_z(\mathbf{r}) = 0. \tag{3}$$

[Here $u_z(\mathbf{r})$ depends parametrically on wavelength λ , but we suppress this label since for now we consider only the monochromatic case.] The normalization of $u_z(\mathbf{r})$ is such that the irradiance at (\mathbf{r}, z) is

$$I_z(\mathbf{r}) = |u_z(\mathbf{r})|^2. \tag{4}$$

From Eq. (3) and its complex conjugate and an application of Stokes theorem in the xy plane at z, it follows that

$$\frac{\mathrm{d}}{\mathrm{d}z}\int\mathrm{d}\mathbf{r}I_z(\mathbf{r})=0,\tag{5}$$

where the integration is over the entire xy plane. [For the right-hand side of Eq. (5) to be zero, it is sufficient for $u_z(\mathbf{r})$ to fall off at least as rapidly as any negative power of $|\mathbf{r}|$ for large $|\mathbf{r}|$.] This equation is a statement of energy conservation; it also guarantees that the relation between $u_z(\mathbf{r})$ and $u_0(\mathbf{r})$ to be given in the next sentence is a unitary transformation.

The exact solution (z > 0) of the parabolic equation may be expressed in terms of the amplitude in some initial plane where we shall take z = 0:

$$u_{z}(\mathbf{r}) = \int d\mathbf{r}' \left[\frac{\exp\left(\frac{i\pi}{\lambda z}\right)(\mathbf{r} - \mathbf{r}')^{2}}{(i\lambda z)} \right] u_{0}(\mathbf{r}')$$

$$= \left[\exp(i\pi r^{2}/\lambda z)/(i\lambda z) \right] \text{FT} \left[\exp\left(\frac{i\pi r^{2}}{\lambda z}\right) u_{0}(\mathbf{r}) \right]_{\lambda z}^{\rho=\mathbf{r}}.$$
(6)

We are using the convention

$$FT[f(\mathbf{r})]_{o} = F(\rho) = \int d\mathbf{r} \exp(-i2\pi\rho \cdot \mathbf{r})f(\mathbf{r})$$

for two-dimensional Fourier transforms and $\rho = (\xi, \eta)$. An attempt is made to conform to the definitions, notation, conventions, and normalizations of Ref. 11. This particularly applies to the special functions rect, circ, gaus, etc.

Equation (6) is the usual result for Fresnel diffraction theory (assuming that any obliquity factors have been taken to be equal to unity). The limits of applicability of the scalar-wave equation, the parabolic equation, and the Fresnel diffraction integral have been discussed extensively elsewhere. ^{11–15} In this paper Eq. (6) is taken as the basic starting point.

2. ANALYTIC PUPIL FUNCTIONS

The irradiance distribution in the xy plane at position z may be characterized by its set of two-dimensional moments. A general member of this set is

$$M_{pq}(z) = \int d\mathbf{r} I_z(\mathbf{r}) x^p y^q. \tag{7}$$

The order of a moment is p+q, and there are N+l moments of order N. The average value of x^py^q is given by $\overline{x^py^q} = M_{pq}(z)/M_{00}(0)$. [Note that $M_{00}(z) = M_{00}(0)$ by Eq. (5)].

If the integration in Eq. (7) is over the entire xy plane, a problem arises. Suppose that the plane z = 0 represents an opaque screen containing a hole with sharp edges. Then, in general, the right-hand side of Eq. (7) does not exist mathematically for finite z > 0. For example, for a round hole with sharp edges, second-order moments (z > 0) are already indeterminate, and higher-order moments are actually infinite. This is only a formal difficulty. In any practical arrangement, irradiance values will always be measured only over a finite plane—if only because, for large enough |r|, the signal would be so weak that it would be masked by the noise associated with the detection process at point (\mathbf{r}, z) . Thus signal-tonoise-ratio considerations alone force one to measure $I_z(\mathbf{r})$ only over a finite part of the xy plane, and moments calculated over such a region are necessarily finite. We do not pursue this approach here (we consider it in Section 4) because it is mathematically cumbersome; measurements over a finite xy plane for z > 0 imply mathematically that the pupil plane (z = 0) has been smoothed by a convolution operation. This is discussed in Ref. 16 and in Section 4 of the present paper. For now we take the viewpoint that it is mathematically expedient to perform directly a smoothing of the aperture.

We write the wave amplitude at the initial plane (z = 0)

$$u_0(\mathbf{r}) = \frac{\sqrt{P_0}}{w} \exp[p(\mathbf{r})] \exp[i\phi(\mathbf{r})] \exp\left(\frac{-i\pi r^2}{\lambda z_1}\right), \quad (8)$$

where P_0 is the total beam power and w is a length characterizing the transverse size of the beam at z=0. Here $p(\mathbf{r})$ and $\phi(\mathbf{r})$ are real functions. We refer to them as the pupil function and the phase-aberration function, respectively. The last factor is used to produce a paraxial focus at $z=z_1$. (For collimated light, $z_1=\infty$.)

By definition, an analytic pupil function is a $p(\mathbf{r})$ such that the initial condition [Eq. (8)] produces a diffracted irradiance field $I_z(\mathbf{r})$, which has finite moments of any finite order at any finite axial point $z \geq 0$.

For example, two classes of analytic pupil functions are

$$p_1(\mathbf{r}) = -(r/w)^{2N}, \qquad N = 1, 2, 3, \dots,$$
 (9)

$$p_{2}(\mathbf{r}) = \begin{cases} \frac{-(r/w)^{2N}}{1 - (r/w)^{2N}} \\ -\infty + r^{2} > w^{2} \end{cases} \qquad N = 1, 2, 3, \dots; \qquad r^{2} \le w^{2}.$$

$$(10)$$

For N=1, e^{p_1} is Gaussian; e^{p_2} is similar but is zero for $r\geq w$. As $N\to\infty$, both tend to $\mathrm{circ}(r/w)$, which is represented by $p_0(\mathbf{r})=0$ for r< w and by $p_0(\mathbf{r})=-\infty$ for r>w. p_0 is not an analytic pupil function. For large N (e.g., $N\gtrsim 10$), both e^{p_1} and e^{p_2} are smooth approximations to $\mathrm{circ}\,(r/w)$, with essentially all the changes in e^{p_1} and e^{p_2} occurring in the region $|(r/w)-1|\approx 1/N$. The functions $\{e^{p_1}\}$ belong to C^∞ , whereas functions $\{e^{p_2}\}$ belong to C_0^∞ . See, e.g., Ref. 17; i.e., e^{p_1} and e^{p_2} both have continuous derivatives of all orders, and in addition functions $\{e^{p_2}\}$ have bounded support.

One need not consider only apertures with circular symmetry. For example, for a square aperture, take $p(\mathbf{r}) = p_1(x) + p_1(y)$. Elliptical, rectangular, and annular analytic pupil functions can be constructed in an obvious way.

We point out that the normalization condition [Eq. (4)] generally requires that a constant be added to $p(\mathbf{r})$ in Eq. (8). The pupil functions given in Eqs. (9) and (10) are not normalized.

In Appendix A, the proof is given that functions $p_1(\mathbf{r})$ and $p_2(\mathbf{r})$ actually have the properties required by the definition of an analytic pupil function.

From now on, unless otherwise noted, we shall always assume that we have a pupil function that satisfies the definition of being analytic. We can think of it as a smoothed circ function (large N), or, if we want to obtain numerical estimates analytically, we can take the simplest case ($N=1 \Leftrightarrow$ Gaussian). We shall find that the essential results presented in this paper are largely independent of the particular form of the pupil function.

3. PROPAGATION OF IRRADIANCE MOMENTS

We wish to find the functional z dependence of irradiance moments as given by their definition in Eq. (7). It is impossible to express irradiance moments at position z in terms of irradiance moments at some initial point (unless $u_z = \text{constant}$, everywhere). However, they may be expressed in terms of the initial wave-amplitude distribution $u_0(\mathbf{r})$. From Eqs. (6) and (7) it is straightforward (details are given in Appendix A) to conclude that

$$M_{pq}(z) = \left(\frac{-i\lambda z}{2\pi}\right)^{p+q} \int d\mathbf{r} \left[\exp\left(\frac{-i\pi r^2}{\lambda z}\right) u_0^*(\mathbf{r}) \right] \\ \times \partial_x^p \partial_y^q \left[\exp\left(\frac{i\pi r^2}{\lambda z}\right) u_0(\mathbf{r}) \right], \quad (11)$$

where the asterisk denotes complex conjugation and $\partial_x^p = (\partial/\partial x)^p$. Most of the remainder of this paper is a study of the implications of Eq. (11). This equation is valid only for $u_0(\mathbf{r})$, satisfying the definition of an analytic pupil function given in Section 2. The operators $-i\partial_x$, $-i\partial_y$ are Hermitian, which guarantees the reality of $M_{pq}(z)$. [When working out Eq. (11) for special cases, the Hermitian property allows one immediately to drop certain imaginary terms, which vanish only after the integration is performed. Moreover, the differen-

tiations may act either to the right or to the left; i.e., $-i\vec{\partial}_x = +i\vec{\partial}_x$. This allows one to choose between having higher-order derivatives occur or powers of lower-order derivatives, e.g., $|\partial_x^2 u_0|^2$ versus $u_0^*(\partial_x^4 u_0)$.]

Using Eq. (8) for the form in which to express $u_0(\mathbf{r})$, we work out Eq. (11) explicitly for the low-order cases. It is convenient to define areas

$$\alpha = \frac{\lambda z}{2\pi}, \qquad \alpha_1 = \frac{\lambda z_1}{2\pi}.$$

For the zero-order moments

$$M_{00}(z) = M_{00}(0) = P_0 \int d\mathbf{r} \frac{\exp[2p(\mathbf{r})]}{w^2} = P_0.$$
 (12)

Again, this is a restatement of Eq. (5). The normalization condition in Eq. (4) is expressed in Eq. (12) as a condition on the pupil function $p(\mathbf{r})$. For the first-order moments, we have

$$\begin{bmatrix} M_{10}(z) \\ M_{01}(z) \end{bmatrix} = \left(1 - \frac{\alpha}{\alpha_1}\right) \begin{bmatrix} M_{10}(0) \\ M_{01}(0) \end{bmatrix} + \alpha \int d\mathbf{r} I_0(\mathbf{r}) \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix}, \quad (13)$$

and for the second-order moments,

$$\begin{bmatrix}
M_{20}(z) \\
M_{11}(z) \\
M_{02}(z)
\end{bmatrix} = \left(1 - \frac{\alpha}{\alpha_1}\right)^2 \begin{bmatrix}
M_{20}(0) \\
M_{11}(0) \\
M_{02}(0)
\end{bmatrix} + \left(1 - \frac{\alpha}{\alpha_1}\right) \alpha \int d\mathbf{r} I_0(\mathbf{r}) \begin{bmatrix}
2x\phi_x \\
y\phi_x + x\phi_y \\
2y\phi_y
\end{bmatrix} + \alpha^2 \int d\mathbf{r} I_0(\mathbf{r}) \begin{bmatrix}\phi_x^2 - p_x^2 - p_{xx} \\
\phi_x\phi_y - p_xp_y - p_{xy}
\end{bmatrix}, (14)$$

where here and elsewhere in this paper the x, y subscripts denote partial differentiation, e.g.,

$$\phi_x = \frac{\partial \phi}{\partial x}, \qquad p_{xy} = \frac{\partial^2 p}{\partial x \partial y}, \qquad \phi_x^2 = (\phi_x)^2.$$

Notice that the first term of Eq. (13) measures the irradiance centroid in the pupil plane ($\alpha=0$); the second term locates the centroid in the focal plane ($\alpha=\alpha_1$). For example, we get the known result that, if there are no aberrations ($\phi=0$); we consider tilt to be an aberration), the beam centroid is located at ${\bf r}=0$ at focus ($z=z_1$), no matter what the shape of the aperture at z=0. For the second-order moments, the first term in Eq. (14) gives the transverse size of the pupil; the last term gives the beam-spot size at focus.

A crude but often useful description of beam propagation/diffraction may be based on Eqs. (13) and (14), which tell directly where the beam is and how big the spot size is (and also its approximate shape) for any position z. For example, the familiar results 11 for Gaussian-beam spreading, waist location, etc. are given immediately by Eq. (14), and, in addition, the effect of arbitrary phase aberrations on the beam centroid location and beam transverse size and shape may be obtained simply and analytically from the moment equations.

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One can also see why the concept of analytic pupil function is required by looking at the last term in Eq. (14). If $p(\mathbf{r})$ is $p_0(\mathbf{r})$, representing a circ function, then discontinuities worse than Dirac δ functions will result in second- and higher-order moments. For example, one can get terms such as

$$\int d\mathbf{r} f(\mathbf{r}) e^{p_0} (\partial x p_0)^2$$
,

which are infinite [f(r)] is a smooth function. The infinities are not due to the peculiar way of expressing $\operatorname{circ}(r/w)$ as $e^{p(r)}$; working directly with the circ function in Eq. (8) would produce terms such as

$$\int d\mathbf{r} f(\mathbf{r}) \operatorname{circ}(r/w) \partial_x^2 \operatorname{circ}(r/w)$$

(also infinite). Elementary considerations show that the last two expressions quoted are actually divergent and not simply indeterminate or undefined.

In addition to knowing the parameters of the beam-image ellipse, 18 which are determined by the irradiance moments up through second order, it is often desirable in a crude description of diffraction to know the Strehl ratio S. This has nothing to do with irradiance moments, but we quote the result here in the notation of this paper since it will be needed later in Section 8:

$$S = \frac{I_{z_1}(0), \text{ with } \phi(\mathbf{r}) \neq 0}{I_{z_1}(0), \text{ with } \phi(\mathbf{r}) = 0}$$
$$= \overline{|\exp(i\phi)|^2} = \overline{\cos(\phi)^2} + \overline{\sin(\phi)^2}$$
$$\approx 1 - (\overline{\phi^2} - \overline{\phi}^2) \text{ for small } \phi, \tag{15}$$

where the average values are defined, e.g., by

$$\overline{\cos(\phi)} = \frac{\int d\mathbf{r} e^{p(\mathbf{r})} \cos[\phi(\mathbf{r})]}{\int d\mathbf{r} e^{p(\mathbf{r})}}.$$

[Here $p(\mathbf{r})$ need not be an analytic-pupil function for the calculation of the Strehl ratio but can be also a function such as p_0 defined in Section 3, which represents the circ function.]

Higher-order moments produce rapidly increasingly complex expressions. Appendix B presents results for third- and fourth-order moments. The essential results of this section are Eqs. (13) and (14), which explicitly give a complete low-order description of diffraction, and Eqs. (16) and (17) below, which allow a phase-retrieval scheme to be based on moment measurements.

From a study of Eqs. (11)–(14) and Appendix B, we can write the form of the general Nth-order moment (N=p+q) and show explicitly its z dependence:

$$M_{pq}(z) = \left(1 - \frac{\alpha}{\alpha_1}\right)^N M_{pq}(0) + \left(1 - \frac{\alpha}{\alpha_1}\right)^{N-1} \alpha M_{pq}^{(1)} + \left(1 - \frac{\alpha}{\alpha_1}\right)^{N-2} \times \alpha^2 M_{pq}^{(2)} + \dots + \dots \left(1 - \frac{\alpha}{\alpha_1}\right) \alpha^{N-1} M_{pq}^{(N-1)} + \alpha^N M_{pq}^{(N)}.$$
(16)

For $M_{pq}^{(1)}$, we always have the simple result that

$$M_{pq}^{(1)} = \int d\mathbf{r} I_0(\mathbf{r}) [(x^p y^q)_x \phi_x + (x^p y^q)_y \phi_y], \qquad (17)$$

while $M_{pq}^{(2)} \dots M_{pq}^{(N)}$ are of the form

$$\int d\mathbf{r} I_0(\mathbf{r})[\ldots],$$

where [...] is an expression involving derivatives of $\phi(\mathbf{r})$ and $p(\mathbf{r})$ nonlinearly (see examples in Appendix B). Equation (17) is proved by induction on N = p + q.

The principal result of this paper is that Eq. (17) involves the initial plane optical phase $\phi(\mathbf{r})$ only linearly, and the pupil function $p(\mathbf{r})$ occurs only through $I_0(\mathbf{r}) = (P_0/w^2) \exp[2p(\mathbf{r})]$ and not inside the square brackets on the right-hand side of Eq. (17). These properties make it possible to determine the pupil-plane phase (to within an additive constant) from a knowledge of $I_0(\mathbf{r})$ and $I_z(\mathbf{r})$ (for several values of z) by using inverse-moment-problem techniques.¹⁸ This is discussed in Section 5.

Finally we point out that in Eq. (8) we could absorb the focusing term $\exp(-i\pi r^2/\lambda z_1)$ into the definition of ϕ , i.e., count focus as an aberration. Then Eq. (16) would appear formally simpler as all terms $(1-\alpha/\alpha_1)^{N-n}$ would be replaced by unity. (The associated factors $M_{pq}^{(n)}$) would change since ϕ would now contain the focus term.) From the standpoint of signal-to-noise-ratio considerations, which are discussed in Section 8, this turns out not to be a good procedure. We shall use Eq. (16) as written above and set $\alpha_1 = \infty$ only if initially collimated light is being considered.

4. DISCONTINUOUS APERTURES AND GENERALIZED IRRADIANCE MOMENTS

In this section we show that all the results of this paper that are exactly valid for an analytic pupil function are approximately valid for discontinuous pupil functions if image-plane moments are calculated only over a finite area. The principal result is that, to lowest order, the discontinuous pupil function is effectively replaced by the analytic pupil function given in Eq. (26) below.

For an arbitrary pupil (analytic or not), one can force the moments to be finite by integrating only over a finite plane. This is mathematically equivalent to using a cutoff function. Define (modified) irradiance moments by

$$\mu_{pq}(z) = \int d\mathbf{r} I_z(\mathbf{r}) x^p y^q G^2(\mathbf{r}/L), \tag{18}$$

where G is a real, dimensionless cutoff function of the dimensionless variable \mathbf{r}/L and L is the cutoff length. For example, one can take

$$G_1(\mathbf{r}/L) = \text{rect}(\mathbf{r}/L)$$

or

$$G_2(\mathbf{r}/L) = \text{gaus}(\mathbf{r}/L)$$

as a suitable cutoff function. Following steps analogous to those used in Appendix A, one finds that

$$\mu_{pq}(z) = \left(\frac{-i\lambda z}{2\pi}\right)^{p+q} \int d\mathbf{r} [g'(\mathbf{r}) ** f_0*(\mathbf{r})] \times \partial_r^p \partial_q^q [g'(\mathbf{r}) ** f_0(\mathbf{r})], \quad (19)$$

where

$$g'(\mathbf{r}) = \left(\frac{L}{\lambda z}\right)^2 g\left(\frac{L\,\mathbf{r}}{\lambda z}\right) \tag{20}$$

and

$$f_0(\mathbf{r}) = \exp\left(\frac{i\pi r^2}{\lambda z}\right) u_0(\mathbf{r}),$$
 (21)

but $u_0(\mathbf{r})$ need not now describe an initial plane with an analytic pupil function. g and G are Fourier-transform pairs; both are dimensionless functions of dimensionless variables. ** denotes convolution. 11

The cutoff function G used at position z is reflected mathematically in the initial plane (z=0) by the smoothing of the pupil affected by the convolution. The effective pupil, now smoothed, is of course an analytic pupil function. [Unfortunately, the optical phase $\phi(\mathbf{r})$ appearing in Eq. (8) gets smoothed as well as $p(\mathbf{r})$.]

A broad cutoff function G implies a narrow, highly peaked function g', which is convolved with the product of initial plane-amplitude distribution and the Fresnel factor $\exp(+i\pi r^2/\lambda z)$. We now work out the lowest-order expression for this convolution.

A sharp pupil is described by its boundary, which encloses a region R in the xy plane. We describe the initial plane amplitude by writing

$$f_0(\mathbf{r}) = \frac{\sqrt{P_0}}{w} P_R(\mathbf{r}) \exp[i\phi(\mathbf{r})] \exp\left(\frac{-i\pi r^2}{\lambda z_1}\right) \exp\left(\frac{i\pi r^2}{\lambda z}\right)$$

$$\equiv \frac{\sqrt{P_0}}{w} P_R(\mathbf{r}) \exp[i\Phi(\mathbf{r})], \tag{22}$$

where P_0 is again the total power, $\phi(\mathbf{r})$ is the phase aberration, a paraxial focus is assumed at z_1 , and

$$P_R(\mathbf{r}) = \begin{cases} 1, & \mathbf{r} \in R \\ 0, & \text{otherwise} \end{cases}$$
 (23)

Here w is the size of the pupil, and the normalization is now

$$\int \frac{\mathrm{d}\mathbf{r}}{w^2} P_R(\mathbf{r}) = 1; \tag{24}$$

for example, we might have

$$P_{R_1}(\mathbf{r}) = \operatorname{circ}(\mathbf{r}/w)$$

or

$$P_{R_0}(\mathbf{r}) = \text{rect}(\mathbf{r}/w).$$

For a narrow function g', the convolution may be written as

$$g'(\mathbf{r}) ** f_0(\mathbf{r}) \simeq \frac{\sqrt{P_0}}{w} \exp[p(\mathbf{r}) + \delta p(\mathbf{r})]$$

$$\times \exp\{i[\Phi(\mathbf{r}) + \delta\Phi(\mathbf{r})]\},$$
 (25)

where

$$e^{p(\mathbf{r})} = \int d\mathbf{r}' P_R(\mathbf{r} - \mathbf{r}') g'(\mathbf{r}); \tag{26}$$

and introducing

$$\mathbf{V}(\mathbf{r}) = \frac{1}{\rho p(\mathbf{r})} \int d\mathbf{r}' P_R(\mathbf{r} - \mathbf{r}') g'(\mathbf{r}') \mathbf{r}', \tag{27}$$

$$T_{ij}(\mathbf{r}) = \frac{1}{e^{p(\mathbf{r})}} \int d\mathbf{r}' P_R(\mathbf{r} - \mathbf{r}') g'(\mathbf{r}') x'_i y'_j, \qquad (28)$$

we have

$$\delta\Phi(\mathbf{r}) \simeq -[\nabla\Phi(\mathbf{r})] \cdot \mathbf{V}(\mathbf{r}) + \frac{1}{2} [\partial_i\partial_j\Phi(\mathbf{r})] T_{ij}(\mathbf{r})$$
 (29)

and

$$\delta p(\mathbf{r}) \simeq \frac{1}{2} [\delta \Phi(\mathbf{r})]^2.$$
 (30)

[In Eqs. (28) and (29) tensor notation in xy space is used, and repeated indices are to be summed over. The vectors and gradients also are two dimensional.]

For the image-plane cutoff functions gaus(\mathbf{r}/L) and $\exp(-|\mathbf{r}|/L)$, the initial plane-smoothing functions are, respectively, a Gaussian and a Lorentzian function. For these cases, $e^{p(\mathbf{r})}$ is positive and nonzero so \mathbf{V} and T_{ij} are everywhere defined. For the cutoff function $\operatorname{rect}(\mathbf{r}/L)$, the smoothing is done by a sinc function. {In this case there are isolated points for $|\mathbf{r}| > w$ at which $e^{p(\mathbf{r})}$ vanishes. Near such points, Eq. 25 should be replaced by the (always valid) expression

$$g' ** f_0 \simeq \frac{\sqrt{P_0}}{w} \exp[i\Phi(\mathbf{r})][e^{p(\mathbf{r})} - ie^{p(\mathbf{r})}\mathbf{V}(\mathbf{r})$$
:

$$\cdot \nabla \Phi(\mathbf{r}) + \frac{i}{2} e^{p(\mathbf{r})} T_{ij}(\mathbf{r}) \partial_i \partial_j \Phi(\mathbf{r})]. \}$$

For a narrow function $g'(\mathbf{r})$, whose width is of order $\sigma = \lambda z/L$, the maximum magnitude of $e^{p(\mathbf{r})}$ is of order unity, whereas the maximum magnitude of both \mathbf{V} and T_{ij} is of order σ . Thus, to lower order,

$$g' ** f_0 \simeq \frac{\sqrt{P_0}}{w} e^{p(\mathbf{r})} \exp[i\Phi(\mathbf{r})],$$

which means that, even when irradiance moments are calculated only over a finite xy plane, the results of Section 3 can be used. $e^{p(\mathbf{r})}$ is now given by Eq. (26), which gives an effective pupil function that satisfies the requirements for being an analytic pupil function.

For small but nonzero widths σ , the correction to the phase $\Phi(\mathbf{r})$ caused by the convolution is of order σ/w . If one is seeking to determine Φ only to a given accuracy (e.g., $2\pi/20$), the correction term may well be negligible. If this is not the case, the phase-retrieval scheme discussed in Section 5 must be modified slightly; this will be discussed in Section 9.

5. PHASE RETRIEVAL FROM KNOWN VALUES OF $M_{na}^{(1)}$

In Section 6 we discuss how to obtain $M_{pq}^{(1)}$ [see Eq. (17)] from measured irradiance data. For now we assume that $M_{pq}^{(1)}$ is known for sufficiently many values of p and q, and we show how such data determine uniquely the initial plane phase $\phi(\mathbf{r})$ as defined in Eq. (8) or (22).

It is convenient in this section to use dimensionless variables in the initial plane. With the substitutions $x \to wx$, $y \to wy$ (w is a length), x and y become dimensionless, and Eq. (17) may be written as

$$\frac{M_{pq}^{(1)}}{P_0 w^{p+q-2}} \equiv b_{pq} = \overline{(\nabla x^p y^q) \cdot [\nabla \phi(\mathbf{r})]}, \tag{31}$$

where P_0 is the total beam power and for any function $f(\mathbf{r})$

$$\overline{f(\mathbf{r})} = \frac{\int d\mathbf{r} I_0(\mathbf{r}) f(\mathbf{r})}{\int d\mathbf{r} I_0(\mathbf{r})}.$$

Equation (31) is similar to the inverse-moment problem; it is not the same problem because of the presence of the gradient operators. However, the usual techniques 18 allow $\phi(\mathbf{r})$ to be found if the set $\{b_{pq}\}$ is given. We shall write (using the mo-

ment-matching approach)

$$\phi(\mathbf{r}) = \sum_{n=1}^{n_{\text{max}}} \sum_{m=0}^{n} \phi_{n-m,m} x^{n-m} y^{m},$$
 (32)

where $\{\phi_{pq}\}$ are dimensionless constants. [For example, if $\phi_{20} = \phi_{02} = 2\pi$, there would be one wave of defocus at position $(x^2 + y^2)^{1/2} = 1$]. Since Eq. (31) leaves undetermined a constant ϕ_{00} , we have started the summation with n=1 instead of n=0. If $n_{\max} = \infty$, an infinite number of parameters must be determined. In cases of practical interest, n_{\max} is always finite. Then expansion (32) used in Eq. (31) gives a finite set [there are $N=n_{\max}(n_{\max}+3)/2$ equations in N unknowns] of linear equations for the phase parameters $\{\phi_{pq}\}$ in terms of the measured irradiance data set $\{b_{pq}\}$. Although Eq. (31) always yields N equations, the equations need not be completely coupled. For example, for symmetric pupils [defined by

$$\overline{x^m y^n} = 0$$

for m and/or n odd nonnegative integers (this implies no symmetry properties of the phase ϕ)], we get the following equations if $n_{\text{max}} = 4$ (i.e., all aberrations up through fourth order):

$$\begin{bmatrix} 1 & 3\overline{x^2} & \overline{y^2} \\ 3\overline{x^2} & 9\overline{x^4} & 3\overline{x^2y^2} \\ \overline{y^2} & 3\overline{x^2y^2} & \overline{y^4 + 4x^2y^2} \end{bmatrix} \begin{bmatrix} \phi_{10} \\ \phi_{30} \\ \phi_{12} \end{bmatrix} = \begin{bmatrix} b_{10} \\ b_{30} \\ b_{12} \end{bmatrix}, \quad (33)$$

$$\begin{bmatrix}
\overline{x^{2} + y^{2}} & \overline{x^{4} + 3x^{2}y^{2}} & \overline{y^{4} + 3x^{2}y^{2}} \\
\overline{x^{4} + 3x^{2}y^{2}} & \overline{x^{6} + 9x^{4}y^{2}} & \overline{3x^{4}y^{2} + 3x^{2}y^{4}}
\end{bmatrix}
\begin{bmatrix}
\phi_{11} \\
\phi_{31} \\
\phi_{13}
\end{bmatrix} =
\begin{bmatrix}
b_{11} \\
b_{31} \\
b_{13}
\end{bmatrix}, (34)$$

$$\begin{bmatrix}
4\overline{x^{2}} & 0 & 8\overline{x^{4}} & 4\overline{x^{2}y^{2}} & 0 \\
0 & 4\overline{y^{2}} & 0 & 4\overline{x^{2}y^{2}} & 8\overline{y^{4}}
\end{bmatrix}
\begin{bmatrix}
\phi_{11} \\
\phi_{31} \\
\phi_{13}
\end{bmatrix} =
\begin{bmatrix}
b_{11} \\
b_{31} \\
b_{13}
\end{bmatrix}, (34)$$

$$\begin{bmatrix}
4\overline{x^{2}} & 0 & 8\overline{x^{4}} & 4\overline{x^{2}y^{2}} & 0 \\
0 & 4\overline{y^{2}} & 0 & 4\overline{x^{2}y^{2}} & 8\overline{y^{4}}
\end{bmatrix}
\begin{bmatrix}
\phi_{20} \\
\phi_{02} \\
\phi_{40} \\
\phi_{22} \\
\phi_{04}
\end{bmatrix} =
\begin{bmatrix}
b_{20} \\
b_{02} \\
b_{40} \\
b_{22} \\
\phi_{04}
\end{bmatrix}. (35)$$

The three remaining equations are obtained from Eq. (33) by interchanging x and y in the matrix and simultaneously switching the order of subscripts in both column vectors. Thus in this case one gets three 3×3 sets and one 5×5 set of equations rather than one 14×14 set. Solving Eqs. (33)–(35) is elementary; as an example, we quote the results for the case that the initial plane contains a centered, round pupil of radius w, i.e., $I_0(\mathbf{r}) = (P_0/\pi w^2)$ circ(\mathbf{r}):

$$\begin{bmatrix}
\phi_{10} \\
\phi_{30} \\
\phi_{12}
\end{bmatrix} = \begin{bmatrix}
5/2 & -3/2 & -3/2 \\
-3/2 & 11/6 & 1/2 \\
-3/2 & 1/2 & 9/2
\end{bmatrix} \begin{bmatrix}
b_{10} \\
b_{30} \\
b_{12}
\end{bmatrix}, (36)$$

$$\begin{bmatrix} \phi_{11} \\ \phi_{31} \\ \phi_{13} \end{bmatrix} = \begin{bmatrix} 10 & -8 & -8 \\ -8 & 12 & 4 \\ -8 & 4 & 12 \end{bmatrix} \qquad \begin{bmatrix} b_{11} \\ b_{31} \\ b_{13} \end{bmatrix}, \tag{37}$$

$$\begin{bmatrix} \phi_{20} \\ \phi_{02} \\ \phi_{40} \\ \phi_{22} \\ \phi_{04} \end{bmatrix} = \begin{bmatrix} 7 & 2 & -5 & -6 & -1 & b_{20} \\ 2 & 7 & -1 & -6 & -5 & b_{02} \\ -5 & -1 & 9/2 & 3 & 1/2 & b_{40} \\ -6 & -6 & 3 & 18 & 3 & b_{22} \\ -1 & -5 & 1/2 & 3 & 9/2 & b_{04} \end{bmatrix}.$$
(38)

Equation (36) also holds if the order of the subscripts on both sides of the equation is simultaneously interchanged.

The reader will notice that, if a coefficient ϕ_{pq} appears in Eq. (32), then one must know b_{pq} , which will require measurement(s) of moment M_{pq} .

As n_{max} gets larger, the dimensionality of the matrices that must be inverted to solve for the phase parameter ϕ_{pq} increases. In the usual inverse-moment problem, 18 it is known that if orthogonal moments are used, the matrixes that occur are already diagonal. [In our notation usual moments are $\{\overline{x^py^q}\}$ and orthogonal moments are $\{\overline{f_{pq}(xy)}\}$, where $\{f_{pq}(x,y)\}$ are orthogonal (with respect to some weighting function) polynomials in x and y.] For example, for a square pupil, two-dimensional Legendre polynomials would be the appropriate functions $\{f_{pq}(xy)\}\$, whereas Zernike polynomials would be used for a centered, round pupil. In the present case the use of orthogonal moments slightly reduces the complexity of the problem (e.g., for $n_{\text{max}} = 4$ and a square pupil, using Legendre moments leads to four 2×2 , three 1×1 , and one 3×3 matrix to be inverted) but does not result in a trivially diagonal matrix because of the presence of the gradient operators in Eq. (31).

Although in this paper we do not use orthogonal moments, we quote the results here: Any orthogonal polynomial in x and y may be written as

$$f_{mn}(x, y) = \sum_{p,q} C_{pq}^{mn} x^p y^q,$$
 (39)

where $C_{pq}^{\ mn}$ are constants. Then, instead of Eq. (31), we have

$$\sum_{pq} C_{pq}^{mn} b_{pq} = \overline{\left[\nabla (f_{mn}(x, y)) \cdot \left[\nabla \phi(\mathbf{r})\right]\right]}, \tag{40}$$

and instead of Eq. (32), $\phi(\mathbf{r})$ is expressed as

$$\phi(\mathbf{r}) = \sum_{m,n} \lambda_{mn} f_{mn}(x, y). \tag{41}$$

The phase-retrieval problem then reduces to solving for the phase parameters λ_{mn} . The appropriate set of polynomials is determined by $I_0(\mathbf{r})$, which furnishes the weighting function,

with respect to which the polynomials f_{mn} are orthogonal. When the objective is to minimize the wave-front phase variance $\Delta\phi_{\rm rms}$, the polynomials should be chosen to be orthonormal with respect to weight function $[I_0({\bf r})]^{1/2}$.

The reader will notice that it is crucial to this phase-retrieval scheme that matrices of the type in Eqs. (33)-(35) be invertible. For a round, uniform pupil, this has been checked up through $N_{\text{max}} = 4$, which involves solving a 14 × 14 set of linear equations, and the result is given explicitly in Eqs. (36) and (37). For a square, uniform pupil, the nonvanishing of the determinant of the relevant matrices was explicitly checked up through $N_{\text{max}} = 5$, which involves a 20×20 set of linear equations. It is conjectured that for these pupils the relevant determinants are nonvanishing for any finite N_{max} , but no general proof has been found. The only example in which a general proof of invertibility can be easily given is the aberrated Gaussian pupil with the function $e^{2p} = \exp[(x^2 + y^2)$]. Then use of Hermite polynomials $f_{mn}(x, y) =$ $H_m(x)$ $H_n(y)$ gives only a diagonal matrix, which is trivially inverted. This exceptional occurrence is so because differentiation of a Hermite polynomial changes it into a unique, other Hermite polynomial; i.e., $H_n'(x) = 2nH_{n-1}(x)$.

6. OBTAINING THE TERM $M_{pq}^{(1)}$ FROM MEASURED IRRADIANCE DATA

The form of the z dependence of any Nth-order irradiance moment is the same. Accordingly, in this section it is convenient to introduce an abbreviated notation M_N to refer to any Nth-order two-dimensional moment M_{pq} , where p+q=N. Then the results for moment propagation up through fourth order, as given in Eqs. (13) and (14) and Appendix B, may be written as

$$M_{1} = \left(1 - \frac{\alpha}{\alpha_{1}}\right) w a_{1} + \frac{\alpha}{w} b_{1},$$

$$M_{2} = \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{2} w^{2} a_{2} + \left(1 - \frac{\alpha}{\alpha_{1}}\right) \alpha b_{2} + \frac{\alpha^{2}}{w^{2}} c_{2},$$

$$M_{3} = \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{3} w^{3} a_{3} + \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{2} \alpha w b_{3}$$

$$+ \left(1 - \frac{\alpha}{\alpha_{1}}\right) \frac{\alpha^{2}}{w} c_{3} + \frac{\alpha^{3}}{w^{3}} d_{3},$$

$$M_{4} = \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{4} w^{4} a_{4} + \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{3} \alpha w^{2} b_{4}$$

$$+ \left(1 - \frac{\alpha}{\alpha_{1}}\right)^{2} \alpha^{2} c_{4}$$

$$+ \left(1 - \frac{\alpha}{\alpha_{1}}\right) \frac{\alpha^{3}}{w^{2}} d_{4} + \frac{\alpha^{4}}{w^{4}} e_{4},$$
(42)

where α and α_1 are as before [defined just before Eq. (12)], M_1 ... M_4 have been divided by $M_{00} = P_0$, and dimensionless variables have been introduced in the initial plane (z=0) by the substitutions $x \to wx$, $y \to wy$. The terms a, b, c, d, and e with subscripts are dimensionless numbers obtained by averaging derivatives of the phase $\phi(\mathbf{r})$ and the pupil function $p(\mathbf{r})$ over the initial plane. For example, if $a_2 = a_{20}$, then $a_2 = \overline{x^2}$, $b_2 = \overline{2x\phi_x}$, and $c_2 = \overline{\phi_x}^2 - p_x^2 - p_{xx}$; the other cases are obtained explicitly from Eqs. (13) and (14) and Appendix B but will not be needed.

The objective is to obtain

$$b_N = b_{[N]} = b_{pq} = \overline{(x^p y^q)_x \phi_x + (x^p y^q)_y \phi_y},$$

on which the phase-recovery procedure of Section 5 may be implemented. The terms a_N are already known (initial plane-irradiance moments), whereas c_N ... are averages involving ϕ nonlinearly and thus are not useful for our purposes.

First consider the case in which moments are obtained for an axial point near the image plane (paraxial focus at z_1). Then the useful variable is not z but the set

$$\delta = (z - z_1) / \left(\frac{2}{\pi} (f \#)^2 \lambda\right), \qquad \Lambda = \lambda f \# / \pi, \qquad \Delta = \Lambda / w,$$
(43)

and Eqs. (42) may be written as

$$M_{1} = \Lambda[b_{1} + \delta(-a_{1} + \Delta b_{1})],$$

$$M_{2} = \Lambda^{2}[c_{2} + \delta(-b_{2} + 2\Delta c_{2}) + \delta^{2}(a_{2} - \Delta b_{2} + \Delta^{2}c_{2})],$$

$$M_{3} = \Lambda^{3}[d_{3} + \delta(-c_{3} + 3\Delta d_{3}) + \delta^{2}(b_{3} - 2\Delta c_{3} + 3\Delta^{2}d_{3}) + \delta^{3}(-a_{3} + \Delta b_{3} - \Delta^{2}c_{3} + \Delta^{3}d_{3})],$$

$$M_{4} = \Lambda^{4}[e_{4} + \delta(-d_{4} + 4\Delta e_{4}) + \delta^{2}(c_{4} - 3\Delta d_{4} + 6\Delta^{2}e_{4}) + \delta^{3}(-b_{4} + 2\Delta c_{4} - 3\Delta^{2}d_{4} + 4\Delta^{3}e_{4}) + \delta^{4}(a_{4} - \Delta b_{4} + \Delta^{2}c_{4} - \Delta^{3}d_{4} + \Delta^{4}e_{4})],$$

$$(44)$$

where $f \# = z_1/2w$. Notice that each moment is expressed as a polynomial in powers of δ ; moreover, the coefficient of each power of δ is itself a polynomial in powers of Δ . [In many practical cases, Δ is of order 10^{-5} to 10^{-6} , and only the first term in each of the parentheses on the right-hand side of set (44) need be kept.] Recalling that a_N is known a priori, one sees from set (44) that, in order to determine the remaining unknowns, one needs first-order moments in one plane, second-order moments in two planes, third-order moments in three planes, fourth-order moments in four planes, etc. Moreover, the form of set (44) shows that the measurement planes should be placed typically a distance of order $\lambda(f \#)^2$ apart. From known values of the moments in several planes, obtaining b, c, \ldots is an elementary linear problem. The price that we are paying to solve exactly a nonlinear problem using only linear techniques is that multiple measurement planes are required. Although one could solve for c, d, e, ..., it is not necessary to do so; one can obtain the b values without actually solving for the other unknowns.

Once more the question of the general invertibility of the relevant linear equations arises. However, in this case the general proof is easily given. The reader will notice that (whether Δ is small or not) the basic problem is the following: Given $y = a_0 + a_1x + a_2x^2 + \dots a_nx^n$ for n+1 distinct x values, find the n+1 a_j 's. This leads immediately to Vandermonde's matrix, whose invertibility is well known. 19,20

We now show that in principle only two (closely spaced) measurement planes are needed. For now assume that Eq. (8) is valid but that $z_1 = \infty = \alpha_1$; i.e., if there is a focusing phase term, let it be included in $\phi(\mathbf{r})$. Then, from Eq. (16), we have

$$\frac{\lambda}{2\pi} M_{pq}^{(1)} = \left[\frac{dM_{pq}^{(z)}}{dz} \right]_{z=0} = \int d\mathbf{r} \left[\frac{\partial I_z(\mathbf{r})}{\partial z} \right]_{z=0} x^p y^q. \tag{45}$$

If z=0 is the pupil plane, Eq. (45) and the results of Sections 2–6 show that measurement of $[\partial I_z(\mathbf{r})/\partial z]_{z=0}$ is mathematically sufficient to allow an arbitrary (continuous) phase $\phi(\mathbf{r})$ at plane z=0 to be recovered. If z=0 is not the pupil plane but an arbitrary axial point in image space, the technique of this paper allows the phase at that point to be determined. Thus Eq. (45) and Section 5 mathematically constitute an interferometer for measuring local phase by using only irradiance data at the two points needed to obtain $(\partial I_z/\partial z)_{z=0}$. The phase at any other axial point is then obtained by using the Fresnel transform (or its inverse) given in Eq. (6). (The accuracy of the two-plane phase-retrieval scheme depends obviously on how accurately the needed derivative can be approximated by an experimentally measured difference.)

The reasons for the more complicated approach of Eqs. (42) and (44) are, first, that we may want to determine, e.g., pupil-plane phase directly from image-plane data without first finding image-plane phase and then performing an inverse Fresnel transform. The latter approach obviously requires greater computational effort and time. Second, Eq. (45) is not always favorable from the viewpoint of signal-to-noise-ratio considerations. In particular, one should not generally attempt to calculate by using

$$\frac{\lambda}{2\pi}M_{pq}^{(1)} = \frac{M_{pq}(\delta z) - M_{pq}(0)}{\delta z}$$

since the two terms on the right-hand side would typically need to be measured to a precision of, e.g., 1 part in 10⁶. Then photon statistics alone implies long integration times for the detection process, and, in addition, the moments would have to be calculated over a high-density mesh to prevent truncation errors. However, in some cases in which one is not in a photon-starved situation, e.g., laser-output-beam wave-front phase sensing, the two-plane measurement technique may be viable.

7. SUMMARY OF THE PHASE-RETRIEVAL SCHEME

Consider the case in which the initial plane phase is to be obtained from irradiance data in the neighborhood of the image plane $(z=z_1)$. The phase $\phi(\mathbf{r})$ in the initial plane (z=0) is described by the parameters ϕ_{pq} [Eq. (32)]. The set ϕ_{pq} is linearly related [Eqs. (33)–(35)] to the quantities b_{pq} [Eq. (31)], which are obtained from measurements, i.e., linearly related to irradiance moments M_{pq} in possibly several planes [Eq. (41)]. These linear relations are conveniently expressed in a matrix notation. Define row vectors $[\phi]$ and [b] whose ordered elements are, respectively, ϕ_{10} , ϕ_{01} , ϕ_{20} , ϕ_{11} , ϕ_{20} , ... ϕ_{13} , ϕ_{04} , ... and b_{10} , b_{01} , b_{20} , b_{11} , b_{02} , ... b_{13} , b_{04} , ... Then

$$[\phi] = U[b], \tag{46}$$

where U is a square matrix [e.g., 14×14 if $\phi(\mathbf{r})$ contains all unsymmetrical aberrations up through fourth order]. Its elements are determined by moments of the initial plane irradiance distribution [see Eqs. (33)–(35)] and are constants unless the irradiance there is time varying. Define a moment (row) vector M whose ordered elements are

$$M_{10}(z_1), M_{01}(z_1), M_{20}(0), M_{20}(z_1), M_{20}(z_2), M_{11}(0),$$

 $M_{11}(z_1), M_{11}(z_2), M_{30}(0), M_{30}(z_1), M_{30}(z_2), M_{30}(z_3), \ldots,$

where z_1 is the image plane and z_2, z_3, z_4, \ldots are nearby points whose separation will be discussed later. For second- and higher-order moments, the initial plane moment must also be included; these are just constants in the time-independent case, but the time-varying case may be treated quasi-statically, allowing for the variation of the initial plane moments. Then

$$[b] = V[M], \tag{47}$$

where V is a constant, nonsquare matrix obtained by solving Eq. (44) for the set b_{pq} . V depends on the distances z_1, z_2, z_3, \ldots , the system f #, and wavelength λ . In the example in which U is 14×14 , V is a 14×52 matrix. U and V are both sparse matrices because many moments M_{pq} and phase parameters ϕ_{pq} are not coupled. The solution to the phase-retrieval problem may then be written as

$$[\phi] = UV[M]. \tag{48}$$

8. PHOTON SENSITIVITY IN THE IDEAL CASE

In order to determine approximately the photon sensitivity that such a moment-interferometry technique would possess, we give an idealized treatment of the process of making irradiance measurements. Assume that the irradiance is measured by an ideal photon detector (quantum efficiency 1) and the dominant noise is photon-counting noise, i.e., also assume negligible error associated with (1) the integration needed to get moments from irradiance and (2) the measurement of different axial positions z_1, z_2, \ldots

The irradiance that we have been discussing until now was assumed to be averaged over photon statistics and should have been written as

$$I_z(x,y) = \frac{h\nu}{\Delta t} \frac{\overline{N_z(x,y)}}{\mathrm{d}x\mathrm{d}y},\tag{49}$$

where $h\nu$ is the photon energy and $N_z(x, y)$ is the actual number of photons counted in time Δt by detector element of area dxdy at position z. We assume that the detection process is described by Poisson statistics. Then²¹

$$\overline{\Delta N_z(\mathbf{r})^2} = \overline{N_z(\mathbf{r})} \tag{50}$$

and

$$\overline{\Delta N_z(\mathbf{r})\Delta N_{z'}(\mathbf{r}')} = 0 \tag{51}$$

for \mathbf{r} , \mathbf{r}' not in the same element $\mathrm{d}x\mathrm{d}y$ and z,z' not in the same measurement plane. [If the interferometer measurements are used to modify the initial plane phase distribution, the right-hand side of Eq. (51) is nonzero; this case has been treated by Dyson.²¹] Then, from Eqs. (49)–(51) and (7), we find the photon noise in irradiance moments characterized by

$$\overline{\Delta M_{pq}(z)\Delta M_{p'q'}(z)} = \frac{h\nu}{\Delta t} M_{p+p',q+q'}(z)$$
 (52)

[for example, $\Delta \overline{M_{20}}^2 = (h\nu/\Delta t)M_{40}$]. Moments in the different measurement planes we consider are statistically independent. [We have reverted to previous notation by omitting the bar over the right-hand side of Eq. (52), which would explicitly indicate an average over photon statistics].

For a specified accuracy with which the initial plane phase $\phi(\mathbf{r})$ must be measured (e.g., so that any aberrations may be compensated for by means of adaptive-optics techniques to the same accuracy), Eq. (52) imposes nontrivial restrictions on the minimum number of photons that must be counted in each measurement plane to determine the irradiance there to sufficient accuracy.

To estimate the size of these numbers, we take the Gaussian pupil (Gaussian beam). Then all integrations that we need can be done analytically. The aberration-free irradiance distribution is given everywhere by

$$I_z(\mathbf{r}) = \frac{P_0}{2\pi\sigma_z^2} \exp(-\mathbf{r}^2/2\sigma_z^2),$$
 (53)

where

$$\sigma_z^2 = w^2 \left(1 - \frac{z}{z_1} \right)^2 + \left(\frac{\lambda}{4\pi w} \right)^2 z^2 \tag{54}$$

[for this distribution, the average value of x^n is $(n-l)!!\sigma_z^n$ for n even].

The beam is focused at z_1 , and the waist occurs at

$$z_{\text{waist}} = \frac{z_1}{1 + \left(\frac{\lambda z_1}{4\pi w^2}\right)^2}.$$

Now consider the following situation. Let the beam be aberration free, i.e., $\phi = 0$ in the pupil plane. If irradiance measurements are made in the vicinity of the image plane (z $= z_1$), and these measured data are used to determine the pupil-plane phase according to the methods previously described in this paper, one will find that the average value of the phase $\overline{\phi}$ is zero, but the variance of the phase measurements is $\overline{\Delta \phi^2} = \overline{\phi^2} \propto 1/N$, where N is the total number of photons collected. Now suppose, in an adaptive-optical system, that the phase ϕ as measured in the image plane(s) is used to compensate the pupil-plane phase aberration, and suppose (arbitrarily) that we wish to have the average value of the Strehl ratio always greater than 90%. Then the measurement time must be long enough that the measured $\Delta \phi^2$ < 1/10. We wish to see how many photons N must be collected in this case, as this number determines the photon sensitivity of the phase-retrieval procedure in the best possible case (i.e., small or no phase aberrations present). For simplicity, consider the case that all ϕ_{pq} are zero except one. Then the square root of the initial plane-phase variance must be less than $2\pi/20$, i.e., average Strehl ratio > 0.9. For these four separate cases, using Eqs. (15) and (31) we find for rms values:

$$b_{10} < 0.224$$
,
 $b_{20} < 0.447$,
 $b_{30} < 0.779$,
 $b_{40} < 1.936$,

if the criterion on the Strehl ratio is to be met. In actuality, these quantities are obtained from moment measurements [see Eq. (47)]. In order that the above requirements may be met, we find by using Eqs. (47) and (52) that the minimum total number of photons $N=P_0\Delta t/h\nu$ that must be detected is, for the four cases,

$$N_{
m tilt} > 5,$$
 $N_{
m defocus} > 26,$ $N_{
m coma} > 301,$ $N_{
m spherical} > 2700.$

In getting these numbers, we have taken the separation between measurement planes to be $(1/3)(2/\pi)(f\#)^2\lambda$, thereby ensuring that $M_{pq}(z)$ varies enough from one z plane to another relative to the measurement accuracy sought. We stress that the above numbers assume that only one aberration at a time is present. For the general case of many aberrations present, i.e., Eq. (32) with some $N_{\rm max}$, the minimum number of photons that must be detected to guarantee that the initial plane wave front can be corrected to a phase variance of $(2\pi/20)^2$ will be larger than the above numbers. The convenient way to treat this problem is to expand the phase $\phi(\mathbf{r})$ in terms of function $f_{mn}(\mathbf{r})$, orthonormal with respect to the distribution $[I_0(\mathbf{r})]^{1/2}$ as a weight function. Then the phase variance $\overline{\Delta \phi^2}$ (used in finding the Strehl ratio) is just

$$\overline{\Delta \phi^2} = \sum_{m,n} \lambda_{mn}^2. \tag{55}$$

From Eqs. (32), (42), and (44) we find that

$$\phi_{pq} = C_{pq}{}^{mn}\lambda_{mn},\tag{56}$$

and, if row vectors $[\phi]$ and $[\lambda]$ are defined as before, we get

$$[\lambda] = C^{-1}UV[M] \tag{57}$$

as a solution of the phase-retrieval problem in terms of an expansion of the phase in functions orthonormal over the pupil. Only with this approach it is easy to specify how large each λ_{mn} can be for a given Strehl criterion. For example, in order to correct all 14 aberrations up through fourth order, such that the average Strehl ratio >90%, we expect to have to collect a total number of photons of order

$$N_{\text{TOT}} \approx [(2 \times 5) + (3 \times 26) + (4 \times 301) + (5 \times 2700)] \approx 15,000$$

in up to four measurement planes near the image plane. In the visible part of the spectrum this corresponds to $\approx 5\times 10^{-15}$ J or light levels of the order of 5×10^{-12} W if a millisecond measurement time is allowed in each of the four measurement planes.

9. CONCLUDING REMARKS ON PHASE RETRIEVAL USING MOMENT TECHNIQUES

To prevent any possible confusion, we remind the reader that we are using an overbar to indicate three different types of averages: (1) average with respect to the distribution $[I_0(\mathbf{r})]^{1/2}$ that occurs in Strehl ratio [Eq. (15)], (2) average with respect to distribution $I_0(\mathbf{r})$ that occurs in phase retrieval [Eq. (31)], and (3) average over photon statistics [Eq. (49)]. It is always clear from the context which average is intended.

Also, although the matrix notation compactly summarizes the solution of the phase-retrieval problem, it is not necessarily the best way to implement a determination of phase from irradiance measurements. For example in Eq. (48), U and V are constant matrices that can be multiplied to yield another constant matrix. Then when all the moments are obtained one gets $[\phi]$. Far fewer space integrals will have to

be calculated if Eq. (47) is used, e.g.,

$$b_{pq} = V_1 M_{pq}(z_1) + V_2 M_{pq}(z_2) + \dots$$

= $\int d\mathbf{r} \, x^p y^q [V_1 I_{z_1} + V_2 I_{z_2} + \dots].$

(The V_1 , V_2 are constant matrix elements.) With this approach for our typical example, one has 15 two-dimensional integrals to calculate instead of 52. The moments will usually be obtained from irradiance measured over a finite-element array. The integrations should be approximated by an algorithm at least as good as the two-dimensional Simpson rule (weights are given in Ref. 22).

We have discussed in detail determination of initial plane phase from measurements near image plane. Measurements in only two planes near the image plane will suffice to find the phase at the image plane. Pupil-plane phase must then be found by inverse Fresnel transformation. If the image plane contains an aberrated image of a point object, the photonnoise sensitivity of the measurements in the two planes will be comparable with that in the case discussed previously. However, many moments will usually be needed with only a two-plane measurement to characterize the local phase well enough to get an accurate pupil-plane phase by inverse Fresnel transformation.

If irradiance moments are measured in two planes near the pupil plane, one has to measure moments to an accuracy of order 1 part in $(w/\lambda) \sim 10^6$ for many cases. This would imply that at least an order of 10^{12} photons must be detected in each of the two planes.

The part of the phase-retrieval problem that is solved in Section 5 is not the same as, but is related to, the previously studied problem of determining phase from phase-gradient measurements. The associated literature for the latter problem may be traced from Ref. 23

At the end of Section 4 we noted that the procedure used in this paper must be modified slightly if the effect of using a finite-image plane was not negligible. The error may be removed by calculating moments over two different areas at the same z plane using methods analogous to those in Section 6

The reader will notice that the basic parameter appearing in Eq. (16) is $\lambda z/2\pi$. This suggests that initial plane phase $\phi(\mathbf{r})$ can be determined by irradiance measurements at one fixed (z>0) plane if data are collected for several λ values and if $\phi(\mathbf{r})$ is known a priori to have a given λ dependence.

Finally, it should be stated that the methods of this paper apply to extended objects, as well as to point objects, within an isoplanatic patch of the optical system.

10. PHASE RETRIEVAL IN OTHER PHYSICAL PROBLEMS

The methods of this paper apply to other physical problems. The scalar-wave equation describes acoustic-wave propagation. The parabolic equation has the form of the free-particle Schrödinger equation. The methods of this paper immediately apply to three cases: (1) Consider a constant energy-scattering problem; let the time-independent potential for z < 0 be arbitrary but weak, and let it be zero for z > 0. Then the initial plane-wave function can be determined uniquely (to within a constant overall phase) from particle-counting experiments at several z planes (z > 0). (2) Replace z in this

paper with t, and $\lambda/4\pi$ with 1/2m. Then the parabolic equation is the time-dependent Schrödinger equation for a free particle moving in two dimensions. From measurements of the probability density at several later times, the wave function at the initial time may be determined. (3) Finally, let the time-dependent parabolic Schrödinger equation just described have three space dimensions, xyz. The moment-propagation theorem generalizes immediately to three dimensions. Then, from measurements of the three-dimensional moments of the probability density at later times, the wave function at t=0 may be determined.

It is beyond the scope of this paper to consider whether having an explicit solution to these problems is physically interesting.

APPENDIX A. MOMENT-PROPAGATION THEOREM: EXISTENCE OF MOMENTS FOR ANALYTIC PUPIL FUNCTIONS

We write $f_0(\mathbf{r}) = \exp[(i\pi r^2/\lambda z)]u_0(\mathbf{r})$, where $u_0(\mathbf{r})$ is given by Eq. (8). Then Eq. (6) becomes

$$u_z(\mathbf{r}) = \frac{\exp\left(\frac{i\pi r^2}{\lambda z}\right)}{i\lambda z} F_0(\mathbf{r}/\lambda z),$$

where $F_0(\rho)$ is the Fourier transform of $f_0(\mathbf{r})$. Then

$$\begin{split} M_{pq}(z) &\equiv \int \mathrm{d}\mathbf{r} I_z(\mathbf{r}) x^p y^q \\ &= \int \mathrm{d}\mathbf{r} u_z^*(\mathbf{r}) x^p y^q u_z(\mathbf{r}) \\ &= \int \frac{\mathrm{d}\mathbf{r}}{(\lambda z)^2} F_0^*(\mathbf{r}/\lambda z) x^p y^q F_0(\mathbf{r}/\lambda z) \\ &= (\lambda z)^{p+q} \int \mathrm{d}\rho F_0^*(\rho) \xi^p \eta^q F_0(\rho) \\ &= \left(\frac{-i\lambda z}{2\pi}\right)^{p+q} \int \mathrm{d}\mathbf{r} f_0^*(\mathbf{r}) \partial_x^p \partial_y^q f_0(\mathbf{r}). \end{split}$$

The crucial step is the passage from the next-to-last to the last line. Its validity involves the same mathematical issue²⁴ that arises in quantum mechanics (take $\hbar=1$) in defining the Hilbert space of functions $\{f_0(\mathbf{r})\}$ such that the momentum operator is equal to $-i \nabla$ in (Schrödinger) position representation. For the purpose of this paper, it is sufficient to note that the last step of the proof is valid if the moments are finite, and this is guaranteed by our use of analytic pupil functions.

We now present an alternative derivation of the momentpropagation theorem, which will show directly what mathematical conditions an analytic pupil function must satisfy. Consider the Fourier transform of the irradiance distribution at z. It may be written as

$$FT[|u_z(\mathbf{r})|^2]_{\rho} = \int d\mathbf{r} f_0 *(\mathbf{r}) f_0(\mathbf{r} - \lambda z \rho).$$

Assume that f_0 has a power-series expansion in the neighborhood of **r**. Then

$$\begin{aligned} \text{FT}[|u_z(\mathbf{r})|^2]_{\rho} &= \sum_{p,q} \frac{\xi^p \eta^q}{p'q'} \left(\frac{2\pi}{i}\right)^{p+q} \\ &\times \left[\left(\frac{-i\lambda z}{2\pi}\right)^{p+q} \int d\mathbf{r} f_0 *(\mathbf{r}) \partial_x {}^p \partial_y {}^q f_0(\mathbf{r}) \right]. \end{aligned}$$

From the well-known properties of the moment-characteristic

function, 11,25 the expression in the square brackets on the right-hand side of this equation is just $M_{pq}(z)$. In order that these equations be valid, (1) $f_0(\mathbf{r}) = \exp(i\pi r^2/\lambda z)u_0(\mathbf{r})$ must have a Fourier transform, and (2) $f_0(\mathbf{r})$ must have a powerseries expansion in the neighborhood of any r, i.e., f_0 and all its derivatives must exist for all r; these are the conditions that an analytic pupil function must satisfy to guarantee finite irradiance moments. The interchange of order of the summation and integration in the last equation above is permissible because of the uniform convergence of the power series. which is guaranteed by condition (2).1

Notice that conditions (1) and (2) imply restrictions on the phase of $u_0(\mathbf{r})$ as well as on its modulus.

APPENDIX B. EXPLICIT z DEPENDENCE OF THIRD- AND FOURTH-ORDER IRRADIANCE **MOMENTS**

$$\begin{split} M_{30}(z) &= M_{30}(0) + \left(\frac{\lambda z}{2\pi}\right) \int \mathrm{d}\mathbf{r} I_0[3x^2\phi_x] \\ &+ \left(\frac{\lambda z}{2\pi}\right)^2 \int \mathrm{d}\mathbf{r} I_0 \left[3x\phi_x^2 - 3x\left(p_x^2 + p_{xx} + \frac{p_x}{x}\right)\right] \\ &+ \left(\frac{\lambda z}{2\pi}\right)^3 \int \mathrm{d}\mathbf{r} I_0[\phi_x^3 \\ &- 3\phi_x(p_x^2 + p_{xx}) - 3\phi_{xx}p_x - \phi_{xxx}], \\ M_{21}(z) &= M_{21}(0) + \left(\frac{\lambda z}{2\pi}\right) \int \mathrm{d}\mathbf{r} I_0[2xy\phi_x + x^2\phi_y] \\ &+ \left(\frac{\lambda z}{2\pi}\right)^2 \int \mathrm{d}\mathbf{r} I_0 \left[y\phi_x^2 + 2x\phi_x\phi_y - p_y - yp_x^2 - 2xp_{xy} - yp_{xx}\right] + \left(\frac{\lambda z}{2\pi}\right)^3 \int \mathrm{d}\mathbf{r} i_0[\phi_x^2\phi_y - \phi_{xxy} - (p_x^2 + p_{xx})\phi_y - 2p_x\phi_x - p_y\phi_{xx} - 2p_x\phi_{xy}], \\ M_{40}(z) &= M_{40}(0) + \left(\frac{\lambda z}{2\pi}\right) \int \mathrm{d}\mathbf{r} I_04x^3\phi_x \\ &+ \left(\frac{\lambda z}{2\pi}\right)^2 \int \mathrm{d}\mathbf{r} I_0[6x^2\phi_x^2 - 12xp_x - 6x^2(p_x^2 + p_{xx}) - 3] + \left(\frac{\lambda z}{2\pi}\right)^3 \int \mathrm{d}\mathbf{r} I_0[4x\phi_x^3 - 6\phi_{xx} - 4x\phi_{xxx} - 12\phi_x(p_x + xp_x^2 + xp_{xx}) - 12xp_x\phi_{xx}] \\ &+ \left(\frac{\lambda z}{2\pi}\right)^4 \int \mathrm{d}\mathbf{r} I_0[\phi_x^4 - 3\phi_{xx}^2 - 6(p_x^2 + p_{xx})\phi_x^2 - 4p_xp_{xxx} - 12p_x\phi_x\phi_{xx} + p_x^4 + 3p_{xx}^2 + 6p_x^2p_{xx} + p_{xxxx} - 4\phi_x\phi_{xxx}]. \end{split}$$

For simplicity in this appendix, we have set $\alpha_1 = (\lambda z_1/2\pi)$ $= \infty$. The result for finite α_1 is easily obtained by referring to Eq. (16) in Section 3. M_{03} and M_{12} may be obtained from the given results by an obvious symmetry operation. The expressions for M_{31} and M_{22} are twice as long as that for M_{40} and thus are not quoted.

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REFERENCES

- 1. R. A. Gonsalves, "Phase retrieval from modulus data," J. Opt. Soc. Am. 66, 961-964 (1976).
- 2. A. J. Devaney and R. Chidlaw, "On the uniqueness question in the problem of phase retrieval from intensity measurements,' J. Opt. Soc. Am. 68, 1352-1354 (1978).
- 3. S. R. Robinson, "On the problem of phase from intensity measurements," J. Opt. Soc. Am. 68, 87-92 (1978).
- W. H. Southwell, N. A. Massie, and J. S. Hartlove, "Wavefront sensor using far-field irradiance measurements," J. Opt. Soc. Am. 69, 1468 (A) (1979).
- H. P. Baltes, ed., Inverse Source Problems in Optics (Springer-Verlag, New York, 1978). See also Inverse Scattering Problems in Optics, H. P. Baltes, ed. (Springer-Verlag, New York, 1980).
- 6. B. J. Hoenders, "On the solution of the phase retrieval problem," J. Math. Phys. 16, 1719-1725 (1975).
- 7. J. R. Fienup, "Reconstruction of an object from the modulus of its Fourier transform," Opt. Lett. 3, 27-29 (1978).
- 8. J. G. Walker, "The phase retrieval problem; a solution based on zero location by exponential apodization," Opt. Acta 28, 735-738 (1981).
- 9. J. M. Wood, M. A. Fiddy, and R. E. Burge, "Phase retrieval using two intensity measurements in the complex plane," Opt. Lett. 6, 514-516 (1981).
- J. T. Foley and R. B. Butts, "Uniqueness of phase retrieval from intensity measurements," J. Opt. Soc. Am. 71, 1008-1014
- 11. J. D. Gaskill, Linear Systems, Fourier Transforms, and Optics (Wiley, New York, 1978).
- 12. M. Born and E. Wolf, Principles of Optics, 5th ed. (Pergamon, Oxford, 1975).
- 13. A. Papoulis, Systems and Transforms with Applications in Optics (McGraw-Hill, New York, 1968).
- 14. J. W. Goodman, Introduction to Fourier Optics (McGraw-Hill, New York, 1968).
- 15. W. H. Southwell, "Validity of the Fresnel approximation in the near field," J. Opt. Soc. Am. 71, 7-14 (1981).
- 16. N. Bareket, "Second moment of the diffraction point spread function as an image quality criterion," J. Opt. Soc. Am. 69, 1311-1312 (1979).
- 17. R. D. Richtmyer, Principles of Advanced Mathematical Physics (Springer-Verlag, New York, 1978), Vol. I. 18. M. B. Teague, "Image analysis via the general theory of mo-
- ments," J. Opt. Soc. Am. 70, 9204-930 (1980).
- 19. G. Strang, Linear Algebra and its Applications (Academic, New York, 1980).
- 20. E. U. Condon and H. Odishaw, Handbook of Physics, 2nd ed. (McGraw-Hill, New York, 1967).
- 21. F. J. Dyson, "Photon noise and atmospheric noise in active optical systems," J. Opt. Soc. Am. 65, 551-558 (1975).
- 22. P. J. Davis and P. Rabinowitz, Methods of Numerical Integration (Academic, New York, 1975).
- 23. J. Herrmann, "Cross coupling and aliasing in modal wave-front estimation," J. Opt. Soc. Am. 71, 989-992 (1981).
- 24. J. von Neumann, Mathematical Foundations of Quantum Mechanics (Princeton U. Press, Princeton, N.J., 1975), Chap. II.
- 25. A. Papoulis, Probability, Random Variables, and Stochastic Processes (McGraw-Hill, New York, 1965).