Fresnel diffraction by a circular aperture with off-axis illumination and its use in deconvolution of microscope images

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Received May 2, 2003; revised manuscript received September 1, 2003; accepted December 1, 2003

The Fresnel approximation for off-axis illumination of a circular aperture is reexamined. The point-spread function for an aberration-free system can be expressed in terms of redefined optical coordinates. An improved expression is given for contours of constant intensity in the focal plane. The variation in axial width of the focal spot with angle of offset is discussed. The predictions are compared with exact calculations of the Rayleigh–Sommerfeld diffraction integral. Limitations for application in deconvolution of microscope images formed with objectives of finite tube length are discussed.

OCIS codes: 050.1940, 070.2580, 080.1010, 100.1830, 110.6880, 260.1960.

1. INTRODUCTION

Surprisingly few papers have considered diffraction by a circular aperture illuminated by a focused, off-axis beam, even though this is an important basis in the imaging of extended objects. With recent improvements in computational speed, it is now straightforward to calculate the focal distribution by direct evaluation of the Rayleigh–Sommerfeld diffraction integral. However, there are a number of reasons why simplified theories based on the Fresnel approximation still are important. They are useful in understanding trends in the focusing behavior that are difficult to predict from numerical calculations. They can be used to investigate large distances from the focus where direct computational methods tend to fail. They can also be used as an accurate model of the imaging process for image restoration. So the Fresnel theories still have a place, and, moreover, comparison with results from direct computation to explore the validity of various approximations is now feasible.

Murty[1] and Zverev[2] considered resolution based on the cutoff of the angular spectrum for a focused off-axis beam in the small-angle approximation. Sheppard and Hegedus[3] extended this treatment to the highly convergent case, as can occur in lithographic lenses, for example.

Born and Wolf[4] (p. 435) analyze the on-axis focusing of light in the paraxial Debye approximation, valid for an infinite value of the Fresnel number. They develop an expression for the focal amplitude in terms of dimensionless transverse and axial optical coordinates v, u, respectively. For an aberration-free system, they go on to derive an analytic expression for the amplitude in terms of the Lommel functions of two variables (Ref. 5, pp. 537–550). The diffraction integral is cast in a form invariant with wavelength and numerical aperture. Li and Wolf[6] proposed a Fresnel theory for focusing by a lens of finite value of the Fresnel number. They gave new forms for the dimensionless optical coordinates v, u, thus allowing the diffraction integral to be expressed in a form invariant with Fresnel number. Sheppard,[7] Gibson and Lanni,[8] and Sheppard *et al.*[9] generalized this theory for off-axis illumination.

Sheppard and Hrynevych[10] described a different approach to Fresnel diffraction, including off-axis illumination, with optical coordinates defined by the aperture edge, corresponding to critical points in the asymptotic expansion.

The Gibson and Lanni theory is widely used for image restoration by deconvolution, although we show later that its validity has limitations for the usual practical implementation. The connection between the theories of Murty[1] and Gibson and Lanni[8] is also discussed.

2. FRESNEL APPROXIMATION FOR OFF-AXIS ILLUMINATION

As a starting point for the derivation of the Fresnel approximation, we take the first Rayleigh–Sommerfeld diffraction integral (RS1) in the form

$$U(P) = -\frac{i}{\lambda}\int\int A\,\frac{\exp[-ik(r-s)]}{rs}\,\frac{z_P}{s}\left(1+\frac{i}{ks}\right)\mathrm{d}S, \tag{1}$$

where $k = 2\pi/\lambda$; A is the source strength; r, s are the distances of a point in the aperture from the focus and the observation point, respectively; and the integration is performed over the plane of the aperture. The Cartesian coordinates of the focus and the observation point are x_F, y_F, z_F, and x_P, y_P, z_P, respectively, and their distances from the center of the aperture are r_F, r_P. For a point in the circular aperture, radius a, with cylindrical coordinates $(a\rho,\ \theta,\ 0)$, the distances r, s can be calculated in terms of a square root by using the Pythagorean theorem. For a focusing system of small numerical aperture (on the image side), the square root can be expanded by the binomial theorem and the distances r, s expressed as

$$r = r_F - a\rho\left(\frac{x_F}{r_F}\cos\theta + \frac{y_F}{r_F}\sin\theta\right) + \frac{a^2\rho^2}{2r_F} - \frac{a^2\rho^2}{2r_F}\left(\frac{x_F}{r_F}\cos\theta + \frac{y_F}{r_F}\sin\theta\right)^2, \quad (2)$$

$$s = r_P - a\rho\left(\frac{x_P}{r_P}\cos\theta + \frac{y_P}{r_P}\sin\theta\right) + \frac{a^2\rho^2}{2r_P} - \frac{a^2\rho^2}{2r_P}\left(\frac{x_P}{r_P}\cos\theta + \frac{y_P}{r_P}\sin\theta\right)^2, \quad (3)$$

where only terms of the second order of $a\rho/r_{F,P}$ are retained.

Following Gibson and Lanni,[8] introducing the variables

$$\xi_{F,P} = \frac{x_{F,P}}{r_{F,P}}, \qquad \eta_{F,P} = \frac{y_{F,P}}{r_{F,P}}, \qquad \zeta_{F,P} = \frac{1}{r_{F,P}} \quad (4)$$

into Eqs. (2) and (3) gives

$$\begin{aligned} r - s = {} & (r_F - r_P) - a\rho[(\xi_F - \xi_P)\cos\theta + (\eta_F - \eta_P)\sin\theta] \\ & + \frac{a^2\rho^2}{2}\left[\zeta_F\left(1 - \frac{\xi_F^2 + \eta_F^2}{2}\right) - \zeta_P\left(1 - \frac{\xi_P^2 + \eta_P^2}{2}\right)\right] \\ & - \frac{a^2\rho^2}{4}\{[\zeta_F(\xi_F^2 - \eta_F^2) - \zeta_P(\xi_P^2 - \eta_P^2)]\cos 2\theta \\ & + 2(\xi_F\eta_F\zeta_F - \xi_P\eta_P\zeta_P)\sin 2\theta\}. \end{aligned} \quad (5)$$

This expression, representing a form of the Fresnel approximation, is exact for small-enough values of the numerical aperture. Note that it was given incorrectly in Eq. (7) of Ref. 9. Harvey[11] has described how the higher-order phase terms can be regarded as equivalent to aberrations of various types. Thus the four terms in Eq. (5) represent the piston, tilt, defocus (including curvature of field), and astigmatism terms. There are no other aberration terms (e.g., coma, distortion, or spherical aberration) for this order of the expansion. If we retain only the terms to first order in $a\rho/r_{F,P}$, we obtain

$$r - s = (r_F - r_P) - a\rho[(\xi_F - \xi_P)\cos\theta + (\eta_F - \eta_P)\sin\theta]. \quad (6)$$

This represents the Fraunhofer approximation, as was assumed by Murty.[1] The only aberration terms in this case are piston and tilt, as the assumption of small numerical aperture has made the depth of field so large that defocus is negligible.

The Rayleigh–Sommerfeld diffraction integral, Eq. (1), can be simplified by assuming that A is constant, $z_P/s \approx 1$, $ks \gg 1$, and in the denominator $r = r_F$, $s = r_P$, to give, after putting $\mathrm{d}S = a^2\rho\mathrm{d}\rho\mathrm{d}\theta$,

$$U(P) = -iNA\zeta_P\int_0^{2\pi}\int_0^1 \exp[-ik(r - s)]\rho\mathrm{d}\rho\mathrm{d}\theta, \quad (7)$$

where we define the Fresnel number as

$$N = a^2/\lambda r_F. \quad (8)$$

For calculation of the focal field, various different levels of approximation can be assumed, in order of decreasing accuracy:

I. Exact. Exact computation from RS1, Eq. (1).

II. Fresnel with astigmatism. Calculation from the approximate RS1 [Eq. (7)] with full second-order approximation for $r - s$ [Eq. (5)]. In general the integral cannot be evaluated analytically.

III. Fresnel, improved. As II, but the astigmatism term of Eq. (5) is neglected. This is justified by the observation that because it can be positive or negative it tends to cancel out on integration over θ. For an aberration-free system the Lommel theory[4] can be applied. We then have

$$U(P) = -iNA\zeta_P\int_0^1 J_0(v\rho)\exp\left(-\frac{1}{2}iu\rho^2\right)\rho\mathrm{d}\rho, \quad (9)$$

where the optical coordinates v, u can be expressed in terms of the variables ξ, η, ζ:

$$v = ka[(\xi_P - \xi_F)^2 + (\eta_P - \eta_F)^2]^{1/2}, \quad (10)$$

$$u = ka^2(\omega_P - \omega_F), \qquad \omega_{P,F} = \zeta_{P,F}[1 - \tfrac{1}{2}(\xi_{P,F}^2 + \eta_{P,F}^2)]. \quad (11)$$

Thus the diffraction integral is expressed in a three-dimensional space-invariant form in terms of the variables ξ, η, ω.

IV. Fresnel, Gibson and Lanni. As III, but the curvature of field terms are neglected. Equations (9) and (10) still apply, but now

$$u = ka^2(\zeta_P - \zeta_F). \quad (12)$$

V. Fresnel, approximate. An approximation is made to v, given in Eq. (19).

VI. Fresnel, Murty. A further approximation is made to v, given in Eq. (20).

For any of the Fresnel theories, the Fraunhofer approximation follows when we put $u = 0$. Alternatively, calculation from the approximate RS1 [Eq. (7)] with the first-order approximation for $r - s$ [Eq. (6)] leads to $u = 0$. Then

$$U(P) = -iNA\zeta_P\int_0^1 J_0(v\rho)\rho\mathrm{d}\rho = -iNA\zeta_P\frac{J_1(v)}{v}, \quad (13)$$

with v given by Eq. (10).

3. INTENSITY IN THE FOCAL PLANE

Let us consider the case of imaging in the focal plane, when $z_F = z_P = d$, and taking, without loss of generality, $y_F = 0$. According to Eq. (5), for II there is a defocus term and an astigmatism term. The integral cannot be evaluated analytically. For III, the Lommel theory can be applied, with optical coordinates

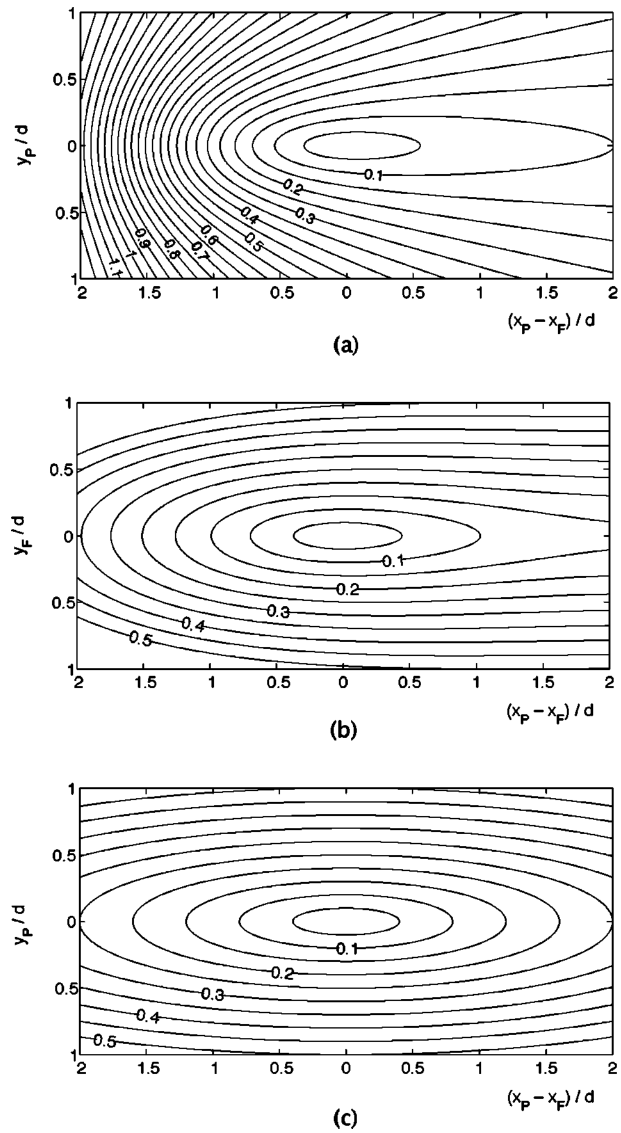

Fig. 1. Contours of constant v for $\chi = 60°$, (a) calculated from the expression of Gibson and Lanni[8] [IV, Eq. (15)], (b) calculated from Eq. (19) (V), and (c) as in the theory of Murty [VI, Eq. (20)].

$$v = ka[(\xi_P - \sin\chi)^2 + \eta_P^2]^{1/2}$$

$$= \frac{ka}{r_P}[(x_P - r_P \sin\chi)^2 + y_P^2]^{1/2}, \tag{14}$$

$$u = ka^2\left[\zeta_P\left(1 - \frac{\xi_P^2 + \eta_P^2}{2}\right) - \zeta_F\left(1 - \frac{\sin^2\chi}{2}\right)\right], \tag{15}$$

so that again there is a defocus term. Similarly, for IV there is also a defocus term given by Eq. (12) even in the focal plane, and Eq. (14) is still valid for the transverse optical coordinate.

The geometry of Eq. (14) is not readily apparent because of the r_P in the denominator of the second expression, so we now make a further approximation V to v. Introducing a shift of the origin of the coordinate system

$$x_P' = x_P - d\tan\chi, \tag{16}$$

so that

$$r_P = (x_P'^2 + 2dx_P' \tan\chi + y_P^2 + d^2\sec^2\chi)^{1/2}, \tag{17}$$

and assuming that x_P'/d, y_P/d are small so that terms up to second order are retained, we obtain

$$r_P \approx d\sec\chi + x_P' \sin\chi + \frac{x_P'^2}{2d}\cos^3\chi + \frac{y_P^2}{2d}\cos\chi. \tag{18}$$

Then, with substitution of approximation (18) into Eq. (14), the optical coordinate v is approximated by

$$v = ka\left\{\left[\frac{x_P'}{d} - \tan\chi\left(\frac{x_P'^2}{2d^2}\cos^2\chi + \frac{y_P^2}{2d^2}\right)\right]^2 \times \cos^6\chi + \left(\frac{y_P}{d}\right)^2\cos^2\chi\right\}^{1/2}. \tag{19}$$

This approximation (V) allows the geometry to be appreciated. Equation (19) shows that contours of constant v are approximately ellipses, as predicted by Murty. Thus the width of the diffraction pattern in the y direction is increased by a factor $\cos\chi$ and in the x direction by a factor $\cos^3\chi$, also as predicted by Murty.[1] However, unlike Murty, we see that the center of the ellipse moves to larger values of x_P as v increases. As an example, Fig. 1(b) shows contours of constant v for the case when $\chi = 60°$, calculated directly from Eq. (19) (V). The contours are elliptical for small v but become distorted as v increases. For comparison, Fig. 1(a) is calculated from the expression of Gibson and Lanni [IV, Eq. (15)]. Thus V gives a reasonable prediction of the shape of the contours described by IV close to the focal point.

Murty retained only the first two terms, $d\sec\chi + x_P'\sin\chi$, for r_P in approximation (18). Neglecting term of higher than second order then leads to Murty's expression (VI) for v:

$$v = \frac{ka}{d}\{x_P'^2\cos^6\chi + y_P^2\cos^2\chi\}^{1/2}, \tag{20}$$

which clearly shows that contours of constant v correspond to ellipses centered on the geometrical focal point, shown in Fig. 1(c). Figure 2 shows the intensity distribution in the focal plane about the geometrical focus calculated directly from Eq. (1) for $\lambda = 633\,\text{nm}$, $d = 160\,\text{mm}$, $\chi = 60°$, and $N = 10$, corresponding to $a = 1.423\,\text{mm}$, together with the Murty contour for the first zero in intensity that occurs when $v = 3.832$. The figure shows excellent agreement between the Murty prediction (VI) and the exact calculation (I) for this set of parameters, but it would be expected to break down as x_P'/d, y_P/d become larger.

Returning to the axial optical coordinate given by Eq. (15) for III, and using Murty's approximation for r_P, we have in the focal plane to the first order in x_P'/d

$$u = -\frac{2ka^2 x_P'}{d^2}\sin\chi\cos^2\chi(1 - \tfrac{3}{4}\sin^2\chi), \tag{21}$$

whereas for IV,

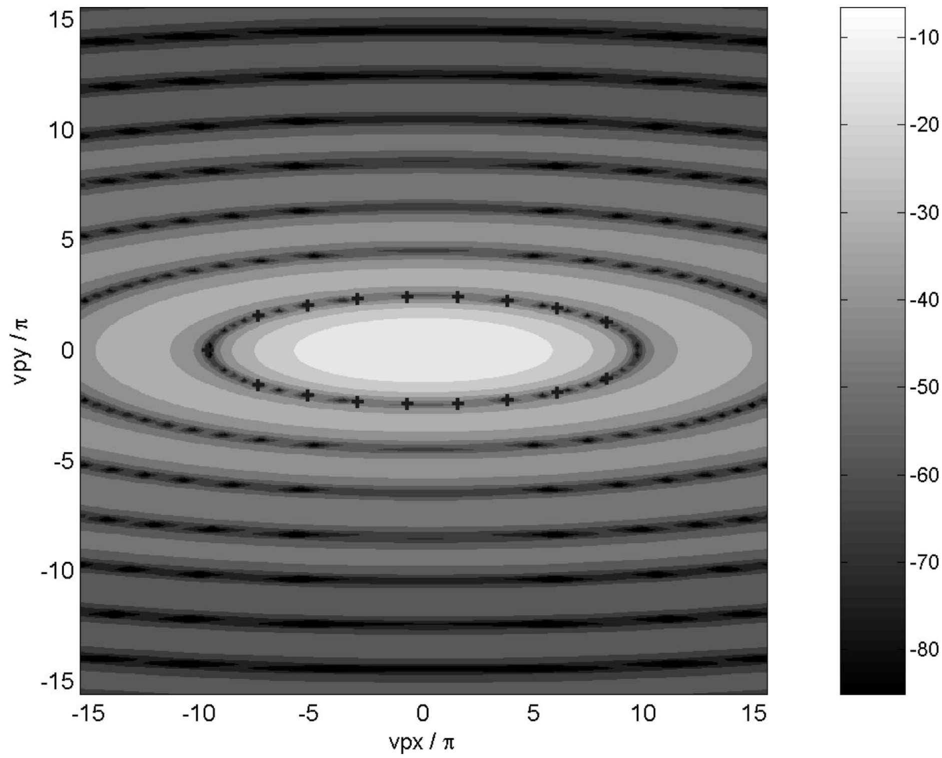

Fig. 2. Intensity distribution in the focal plane, for λ = 633 nm, $d = 160$ mm, $\chi = 60°$, and $N = 10$, corresponding to $a = 1.423$ mm, calculated by exact computation of Eq. (1) (I), and the contour for the first minimum ($v = 3.832$) from Murty's expression [VI, Eq. (20)].

$$u = -\frac{ka^2 x'_P}{d^2} \sin\chi \cos^2\chi. \tag{22}$$

Although Eqs. (21) and (22) give very different results, we find that for the parameters of Fig. 2, u is negligible in the focal plane in the region where the intensity is appreciable. This is a consequence of the tubular shape of the focal spot.[4]

4. INTENSITY ALONG A LINE FROM THE CENTER OF THE APERTURE TO THE FOCAL POINT

For an observation point on the line from the center of the aperture to the focal point and an offset angle χ,

$$\xi_P = \xi_F = \xi = \sin\chi,$$

$$\eta_P = \eta_F = 0. \tag{23}$$

We can compare the intensity predicted by three different approximate theories for $(r - s)$. For II, the integral in θ can now be performed, so that, normalizing the intensity by the value at $r_P = r_F$, we obtain

$$I_3/I_{30} = \left(\frac{r_F}{r_P}\right)^2 \left| \int_0^1 J_0\left[\frac{\pi N}{2}\left(\frac{r_F}{r_P} - 1\right)(\sin^2\chi)t\right] \times \exp\left[i\pi N\left(\frac{r_F}{r_P} - 1\right)\left(1 - \frac{\sin^2\chi}{2}\right)t\right]\mathrm{d}t\right|^2. \tag{24}$$

If we neglect the astigmatism term (III), the integral in Eq. (9) reduces to the form described by Born and Wolf for $v = 0$,[4] so that

$$I_2/I_{20} = \left(\frac{r_F}{r_P}\right)^2 \left\{\frac{\sin\left[\frac{\pi N}{2}\left(\frac{r_F}{r_P} - 1\right)\left(1 - \frac{\sin^2\chi}{2}\right)\right]}{\frac{\pi N}{2}\left(\frac{r_F}{r_P} - 1\right)\left(1 - \frac{\sin^2\chi}{2}\right)}\right\}^2, \tag{25}$$

and from the Gibson and Lanni model (IV),

$$I_1/I_{10} = \left(\frac{r_F}{r_P}\right)^2 \left\{\frac{\sin\left[\frac{\pi N}{2}\left(\frac{r_F}{r_P} - 1\right)\right]}{\frac{\pi N}{2}\left(\frac{r_F}{r_P} - 1\right)}\right\}^2. \tag{26}$$

These three predictions are compared in Fig. 3 for the cases when $\chi = 30°$ and 60° and $N = 10$. By checking comparisons with the exact theory I, we showed that II is accurate for typical values of a/f ($\leqslant 0.02$). For small offset angles, the axial width of the focus predicted by II and III increases with increasing angle of offset by a factor $[1 - (\sin^2\chi)/2]$, while IV does not predict an increase in width. Model III gives a good prediction for the behavior for χ less than ~30°, but by 60°, model III overemphasizes the decrease in resolution. The relative shape of the curves predicted by the three models is independent of Fresnel number, all becoming more asymmetric for small values of N. To investigate the breakdown of III, we studied the variation of the width of the curves at half intensity for large N, and the results are shown in Fig. 4. It is seen that III agrees well with II for χ less than $\sim 30°$ when the width has increased by a factor of 1.2, whereas IV predicts no change in width.

5. APPLICATION TO THREE-DIMENSIONAL MICROSCOPY

The expressions of Gibson and Lanni[8] have been widely used for microscope image restoration. However, here we discuss the limitations. The treatment presented above assumes an aberration-free imaging system, but it is known that for an optical system of high numerical aperture (in object space) that satisfies the sine condition, spherical aberration is introduced for a change in the effective tube length. For an object point situated distant from the focal plane of the objective, the image becomes distorted axially in image space.[12] In practice in three-dimensional microscopy, the image detector is retained in the image plane and the object is scanned axially, and a series of two-dimensional images are recorded with the detector. An arbitrary object point is imaged out of focus but with $z_P = d =$ constant, where d is the correct tube length for the objective. Thus no spherical aberration is introduced for the object in the plane of the detector when the object is in focus, but there is a spatially variant spherical aberration term that cannot be accurately modeled with the Lommel function model.

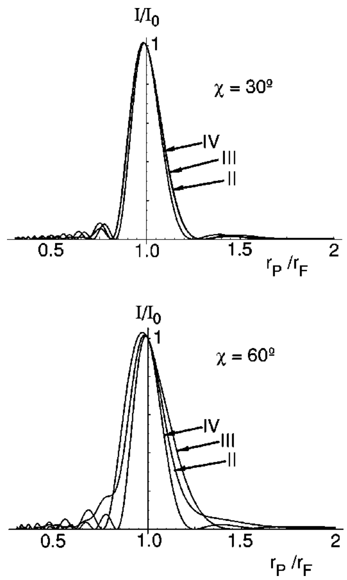

Fig. 3. Intensity along the line from the center of the aperture to the focal point for offset angles of 30° and 60° and $N = 10$: (II) retaining the astigmatism term [Eq. (24)], (III) improved theory incorporating an extra defocus term dependent on the transverse coordinates of the focus and observation points [Eq. (25)], and (IV) theory of Gibson and Lanni [Eq. (26)]. II was shown to agree with the exact expression I for typical parameters.

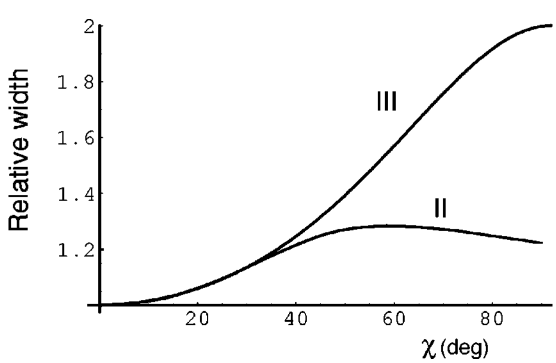

Fig. 4. Relative width of the intensity variation along the line from the center of the aperture to the focal point. The behavior for II and III is shown. The Fresnel number is assumed large. For comparison, IV predicts a constant value of unity.

Even when the aberration effect is neglected, because the aperture stop of the objective lens is positioned in the back focal plane of the lens, rays from a point distant x_o, y_o from the axis are deflected at a constant angle χ to the detector as the object is scanned axially. The center of the image of the point x_o, y_o remains at a point $x_P = Mx_o$, $y_P = My_o$, $z_P = d$ on the detector, where M is the magnification from object to detector. The coordinates of a general point on the detector are

$$\xi_P = \frac{x_P}{(d^2 + x_P^2 + y_P^2)^{1/2}}, \quad \eta_P = \frac{y_P}{(d^2 + x_P^2 + y_P^2)^{1/2}},$$

$$\zeta_P = \frac{1}{(d^2 + x_P^2 + y_P^2)^{1/2}}. \tag{27}$$

We also have for the focus at an axial scan position z_s

$$\xi_F = \frac{Mx_o}{(d^2 + M^2(x_o^2 + y_o^2)^{1/2}},$$

$$\eta_F = \frac{My_o}{(d^2 + M^2(x_o^2 + y_o^2)^{1/2}},$$

$$\zeta_F = \frac{d - M^2(z_o - z_s)}{d(d^2 + M^2(x_o^2 + y_o^2)^{1/2}}, \tag{28}$$

where z_o is the axial coordinate of the object point, so that ξ_F, η_F are constant during an axial scan. We notice that although the coordinates x_P, y_P appear in Eq. (27), z_s occurs in Eq. (28). Thus the image is not given by a spatially invariant point-spread function. However, it is possible to make the system approximately spatially invariant by assuming $x_P \approx Mx_o$, $y_P \approx My_o$ to give

$$\zeta_P - \zeta_F \approx \frac{M^2 z_o}{d(d^2 + M^2(x_o^2 + y_o^2)^{1/2}} - \frac{M^2 z_s}{d(d^2 + x_P^2 + y_P^2)^{1/2}}. \tag{29}$$

Nevertheless, it seems that more accurate restoration can be achieved by considering the imaging process in the object space rather than in the image space, by using the principle of reciprocity.

6. DISCUSSION

The Fresnel approximation for off-axis illumination of a circular aperture in the scalar paraxial domain has been reexamined. Various degrees of approximation have been investigated. A new approximate expression [V, Eq. (19)] for the shape of contours of equal intensity in the focal plane has been presented. This expression describes a distortion of the contours in comparison with those of elliptical shape predicted by Murty [VI, Eq. (20)].[1] The Murty expression is accurate for large values of the Fresnel number, when the intensity is appreciable only in the region of focus. An expression for the defocus optical coordinate [III, Eq. (11)] has been shown to be more accurate than that of Gibson and Lanni[8] [IV, Eq. (12)] for points not in the focal plane. The approximation is accurate for offset angles up to $\sim 30°$ but breaks down for larger angles. These results are useful in appreciating general trends in the off-axis illumination of a circular aperture by a focused beam. Limitations in three-dimensional microscopy and deconvolution of microscope images with a finite-tube-length objective have been discussed.

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