Wavefront spacing and Gouy phase in presence of primary spherical aberration

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We study the Gouy phase of a scalar wavefield that is focused by a lens suffering from primary spherical aberration. It is found that the Gouy phase has different behaviors at the two sides of the intensity maximum. This results in a systematic increase of the successive wavefront spacings around the diffraction focus. Since all lenses have some amount of spherical aberration, this observation has implications for optical calibration and metrology.

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Because of its importance in interference microscopy and optical metrology, the wavefront spacing of focused fields has been the subject of many studies. Linfoot and Wolf [1] derived that the effective wavelength of a scalar field near focus is given by the expression $\lambda_{\text{eff}} = \lambda/(1 - a^2/4f^2)$, where λ is the free-space wavelength, a is the aperture radius, and f denotes the focal length. A very qualitative explanation of this increase in wavefront spacing is given by the observation that in a focused field, the average wave vector is tilted, i.e., its component along the central axis is smaller than that of a plane wave. More recently, analyses of strongly focused, linearly polarized [2], and radially polarized beams [3] predicted a wavefront spacing that is highly irregular. Experimental observations of fringe spacings have been presented in, e.g., [4–6].

A measure of how an actual diffracted focused field differs from an ideal spherical wave is provided by the Gouy phase (sometimes called the "phase anomaly"). This is the sudden π phase shift that a focused field undergoes, compared to a nondiffracted spherical wave of the same frequency [7,8]. Its physical origin has been discussed in [9]. Recently, it has been theoretically investigated in a variety of applications, such as high-numerical aperture systems [10,11], nondiffracting beams [12,13], and partially coherent focused fields [14]. Experimental observations were reported in, e.g., [15–21]. A precise knowledge of the Gouy phase is crucial in a wide variety of metrological techniques. Examples are measurements of acceleration [22], distance [23], refractive indices [24], and volumes [25].

In an actual focusing system aberrations are always present, especially primary spherical aberration, perhaps the most common of the classical Seidel aberrations [26]. It is of interest, therefore, to examine the restrictions that a small amount of spherical aberration puts on the accuracy levels that can be achieved in optical metrology and calibration. In this Letter, we analyze the influence of primary spherical aberration on the Gouy phase and the wavefront spacing. We derive expressions for the phase behavior in terms of imaginary error functions that can easily be evaluated numerically. Our main result is that the Gouy phase at the two sides of the diffraction focus (the point of maximum intensity) is markedly different. This results in a systematic increase of the wavefront spacing around the diffraction focus. We show by numerical examples that even a small amount of spherical aberration ($\sim\lambda/4$) introduces a change in the wavefront spacing that is significantly larger than is usually assumed.

Let us then consider an aberrated, converging, monochromatic wavefield of frequency ω that emerges from a circular aperture with radius a (see Fig. 1). The geometrical focus O is taken to be the origin of the coordinate system, and f is the radius of a Gaussian reference sphere S. The field in the focal region is given by the expression [26, Section 9.1.1]

$$U(P) = -\frac{i}{\lambda}\frac{\mathcal{A}e^{-ikf}}{f}\iint_S \frac{e^{ik[\Phi+s]}}{s}\,\mathrm{d}S, \tag{1}$$

where $k = 2\pi/\lambda$ represents the wavenumber, $\mathcal{A}$ is an amplitude, Φ denotes the aberration function, and s is the distance from a point of integration Q on S to the observation point P. For a wavefront with spherical aberration [26, Section 9.3, Eq. (7)],

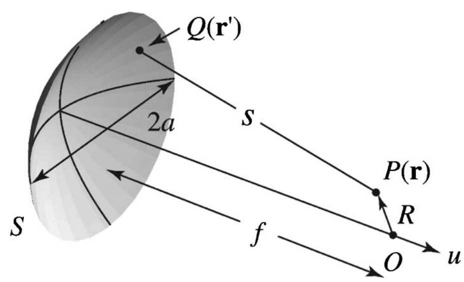

Fig. 1. Illustrating the notation.

$$\Phi(\rho) = A_0\rho^4, \tag{2}$$

with A_0 the wave aberration at the edge of the exit pupil and $0 \le \rho \le 1$ a scaled transverse distance. We notice that the focused field is rotationally symmetric about the optical axis. The position of an observation point P is indicated by the dimensionless Lommel variables u and v, i.e.,

$$u = kz\left(\frac{a}{f}\right)^2, \tag{3}$$

$$v = k(x^2 + y^2)^{1/2}\frac{a}{f}. \tag{4}$$

After approximating the factor $1/s$ in Eq. (1) by $1/f$, and applying the usual Debye approximation $s - f \approx -\mathbf{q}\cdot\mathbf{R}$, where $\mathbf{q}$ denotes a unit vector in the direction OQ [26, Section 8.8.1], [27, Section 12.1.2], we find that

$$U(u, v; A_0) = C\int_0^1 J_0(\rho v)e^{i(-u\rho^2/2 + kA_0\rho^4)}\rho\,\mathrm{d}\rho, \tag{5}$$

where $C = -ik\mathcal{A}(a/f)^2e^{i(f/a)^2u}$ and J_0 denotes the Bessel function of the first kind of order 0. It follows from Eq. (5) that

$$U^*(u, v; A_0) = -U(-u, v; -A_0), \tag{6}$$

which means that the axial intensity distribution obeys the symmetry relation

$$|U(u, 0; A_0)|^2 = |U(-u, 0; -A_0)|^2, \tag{7}$$

and that the phase of the field, $\arg[U(u, v; A_0)]$, satisfies the formula

$$\arg[U(u, v; A_0)] + \arg[U(-u, v; -A_0)] = -\pi.\ (\mathrm{mod}\ 2\pi). \tag{8}$$

Equation (8) is a generalization of the expression

$$\arg[U(u, v)] + \arg[U(-u, v)] = -\pi, \tag{9}$$

for a focused field without spherical aberration [26, Section 8.8.4].

For axial points ($v = 0$), Eq. (5) can be written (omitting the v dependence from now on) as

$$U(u; A_0) = -C\frac{(-1)^{3/4}\sqrt{\pi}}{4\sqrt{kA_0}}e^{-iu^2/16kA_0} \times\left\{\mathrm{erfi}\left[\frac{(-1)^{1/4}(4kA_0 - u)}{4\sqrt{kA_0}}\right] + \mathrm{erfi}\left[\frac{(-1)^{1/4}u}{4\sqrt{kA_0}}\right]\right\}, \tag{10}$$

where erfi denotes the imaginary error function. It is seen from Eq. (10) that the axial intensity distribution is symmetric about the position $u = 2kA_0$ [26, Section 9.3]. When $|A_0| \lesssim \lambda$, this point is also the intensity maximum

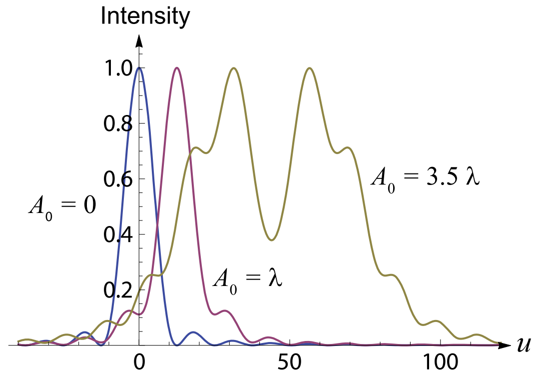

Fig. 2. Axial intensity distribution for different values of the spherical aberration parameter, $A_0 = 0$ (blue curve), $A_0 = \lambda$ (red curve), and $A_0 = 3.5\lambda$ (olive curve). Here, and in all the following examples, a/f is taken to be 1/2.

("the diffraction focus"). For large values of A_0, there may be two peaks, as is illustrated in Fig. 2. It is also seen that the distribution becomes wider with increasing A_0.

The Gouy phase is defined as the difference between the actual phase (or "argument") of the field and that of a nondiffracted spherical wave that converges to the geometrical focus in the half-space $z < 0$ and diverges from it in the half-space $z > 0$ [26, Section 8.8.4], i.e.,

$$\delta(u; A_0) = \arg[U(u; A_0)] - \mathrm{sign}(u)kR, \tag{11}$$

with R the distance from the observation point to the geometrical focus, i.e.,

$$kR = k|z| = \left(\frac{f}{a}\right)^2|u|, \tag{12}$$

and sign(x) denotes the sign function

$$\mathrm{sign}(x) = \begin{cases} -1 & \text{if } x < 0, \\ 1 & \text{if } x > 0. \end{cases} \tag{13}$$

From Eqs. (8) and (11), we find that the Gouy phase satisfies the relation

$$\delta(u; A_0) + \delta(-u; -A_0) = -\pi\ (\mathrm{mod}\ 2\pi). \tag{14}$$

The dependence of the Gouy phase on the amount of spherical aberration is shown in Fig. 3. It is seen that the oscillations of the Gouy phase in front of the diffraction focus decrease when the parameter A_0 increases. Notice that the three curves are parallel at the respective diffraction foci ($u = 1.3, 3.1, 12.6$). This follows from Eq. (10), from which we derive $\partial \arg[U(2kA_0; A_0)]/\partial u = (f/a)^2 - 1/4$, which is indeed independent of the value the aberration parameter.

The field at geometrical focus can be calculated from Eq. (10), which gives

$$U(0; A_0) = ik\mathcal{A}\left(\frac{a}{f}\right)^2\frac{(-1)^{3/4}\sqrt{\pi}}{4\sqrt{kA_0}}\mathrm{erfi}[(-1)^{1/4}\sqrt{kA_0}]. \tag{15}$$

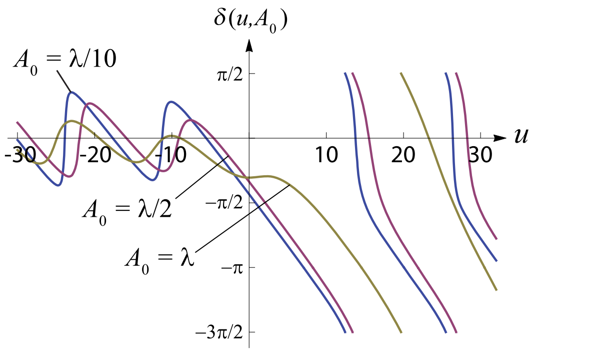

Fig. 3. Gouy phase of the field along the axis for different values of the aberration parameter A_0.

This expression implies that the phase, and equivalently, the Gouy phase, at $(u, v) = (0, 0)$ depends on the aberration parameter A_0. However, for practical purposes, the diffraction focus (the position of maximum intensity, when $|A_0| \lesssim \lambda$) is more important than the geometrical focus. It is therefore of interest to examine the Gouy phase at $u = 2kA_0$. The field there can be written as

$$U(2kA_0; A_0) = ik\mathcal{A}\left(\frac{a}{f}\right)^2 \frac{(-1)^{3/4}\sqrt{\pi}}{2\sqrt{kA_0}} e^{i2kA_0(f/a)^2} \times e^{-ikA_0/4}\,\mathrm{erfi}\left(\sqrt{ikA_0}/2\right), \tag{16}$$

which shows that the phase of the field depends on A_0 and also on a/f. The Gouy phase at the geometrical focus and at the diffraction focus are both shown in Fig. 4 as functions of the aberration parameter A_0. We note that (a) the symmetry relation Eq. (14) is satisfied by the Gouy phase at the geometrical focus, and (b) the Gouy phase at the diffraction focus can attain any value.

As mentioned above, all these results are derived while making use of the Debye approximation. However, if one requires a high level of accuracy, as in metrology, this may introduce a slight error in the calculated wavefront spacings [28]. We therefore evaluate Eq. (1) for on-axis points, without making use of the Debye approximation. This yields the expression

$$U(u; A_0) = -ik\mathcal{A}\left(\frac{a}{f}\right)^2 e^{-ikf} \int_0^1 e^{ik(s+A_0\rho^4)}\rho\,\mathrm{d}\rho, \tag{17}$$

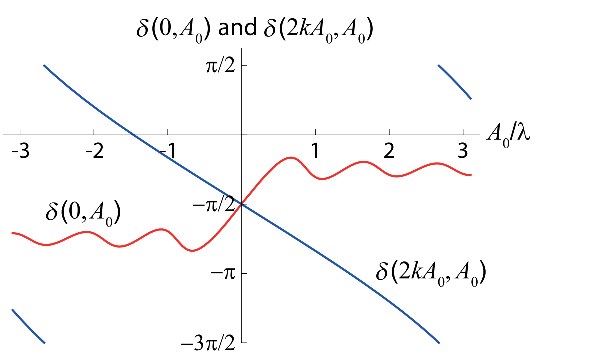

Fig. 4. Gouy phase $\delta(0, A_0)$ at the geometrical focus (red curve) and the Gouy phase $\delta(2kA_0, A_0)$ at the diffraction focus (blue curve) as functions of the aberration parameter A_0.

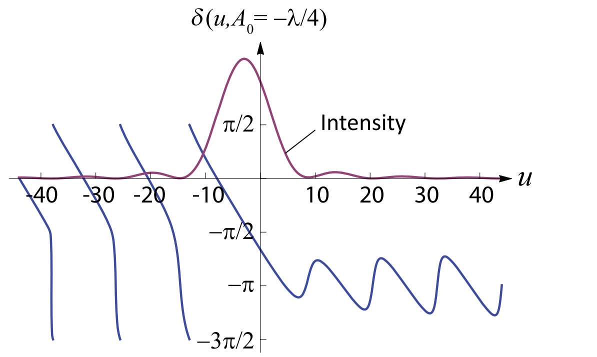

Fig. 5. Gouy phase and the intensity distribution of the field along the axis for the case $A_0 = -\lambda/4$.

with

$$s = f\left[1 + \left(\frac{uf}{ka^2}\right)^2 + \frac{2u}{ka^2}\sqrt{f^2 - a^2\rho^2}\right]^{1/2}. \tag{18}$$

The Gouy phase and the intensity distribution of the field along axis calculated from Eq. (17) are shown in Figs. 5 and 6 for two opposite values of the aberration parameter A_0. These two figures illustrate the symmetry relation (14). But more importantly, they show that the Gouy phase is highly asymmetric with respect to the diffraction focus. From this observation we may expect that the wavefront spacing before and after the diffraction focus will be different.

We define the wavefront spacings as the distance between the successive roots of the expression $\Re[U(u; A_0)] = 0$. The axial wavefront spacings for three cases ($A_0 = 0$, $A_0 = \lambda/4$ and $A_0 = -\lambda/4$) are listed in Table 1. The spacings are labeled by the index N, with $N = 1$ indicating the distance between the first zero for which $u > 2kA_0$, and the nearest zero at a smaller value of u. From the table, several trends can be deduced:

- For the case of an aberration-free lens ($A_0 = 0$), the wavefront spacings are somewhat irregular, but consistently larger than the effective wavelength $\lambda_{\mathrm{eff}} = \lambda/(1 - a^2/4f^2) = 1.0667\lambda$ derived in [1] on the basis of the Debye approximation.
- For a small amount of spherical aberration ($A_0 = \lambda/4$), the wavefront spacings increase with

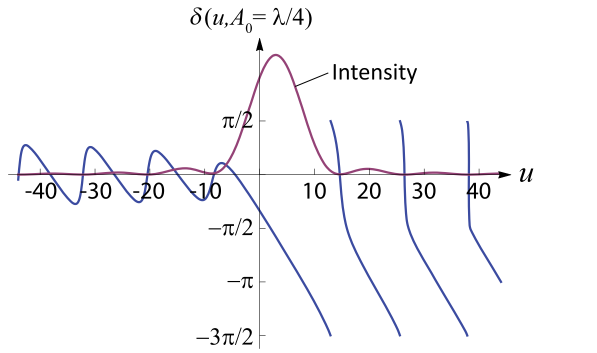

Fig. 6. Gouy phase and the intensity distribution of the field along the axis for the case $A_0 = \lambda/4$.

Table 1. Wavefront Spacings (in Free-Space Wavelengths λ) near the Diffraction Focus for Different Amounts of Spherical Aberration, for the Case $a/f = 1/2$

N	$A_0 = 0$	$A_0 = \lambda/4$	$A_0 = -\lambda/4$
−4	1.06683	1.06087	1.08080
−3	1.06871	1.06530	1.07540
−2	1.06948	1.06767	1.07304
−1	1.06982	1.06918	1.07162
1	1.06995	1.07034	1.07050
2	1.06991	1.07144	1.06935
3	1.06971	1.07279	1.06789
4	1.06923	1.07495	1.06567

increasing N. This means that the spacings to the right of the diffraction focus ($N \geq 1$) are systematically larger than those to the left of the diffraction focus ($N \leq -1$). The difference between the smallest and the largest spacing ($N = -4$ and $N = 4$) is more than 1%. This is considerably larger than the typically aspired metrological accuracy levels.

- When the aberration parameter is slightly increased (not shown) the systematic increase in wavefront spacing with increasing N gets larger.
- For negative values of the aberration parameter ($A_0 = -\lambda/4$), the wavefront spacings decrease with increasing N. This is in agreement with the symmetry expressed by Eq. (6), and Figs. 5 and 6.

In summary, we have derived expressions for the Gouy phase of a focused field in the presence of primary spherical aberration. Its behavior around the diffraction focus is found to be highly asymmetric. This coincides with a wavefront spacing that is systematically larger on one side of the intensity maximum than on the other side. The distance between successive wavefronts is found to increase with increasing spherical aberration and is typically larger than predicted by previous analyses that relied on the Debye approximation. Since even for a small amount of spherical aberration like $\lambda/4$ the difference in fringe spacing can exceed 1%, these results may put restrictions on the accuracy that can be achieved in optical metrology and calibration.

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