Astigmatic Gaussian beams: exact solutions of the Helmholtz equation in free space

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Abstract

Exact solutions of the 3D Helmholtz equation in free space are presented in the form of a superposition of plane waves. The solutions asymptotically reduce to general astigmatic Gaussian beams and include no backward waves.

1. Introduction

Theoretical descriptions of localized wave propagation demanded in the theory of lasers, have been initially presented for the time-harmonic (monochromatic) regime by means of the parabolic-equation approach (see, e.g. [1–7]). The latter allows for various types of paraxial Gaussian beams which are approximate solutions of the Helmholtz equation

\[ u_{xx} + u_{yy} + u_{zz} + k^2u = 0, \quad k = \text{const} > 0, \tag{1} \]

that is widely accepted as a simple model for the Maxwell equations. Paraxial solutions were presented for axisymmetric and general astigmatic fundamental modes, and for a rich variety of respective higher-order modes. It was immediately understood that paraxial solutions do not exactly satisfy the Helmholtz equation. This was impressively demonstrated recently in [8] where paraxial solutions on the beam axis and in the focal plane were thoroughly studied in the case of axial symmetry.

A challenging problem of derivation of exact solutions of the equation (1), asymptotically showing the same localized behaviour as the paraxial Gaussian beams, has been addressed by several researchers exclusively for the case of axial symmetry. To the best of our knowledge, the studies preceding [9] and [10] describe solutions that either do not satisfy equation (1) in the whole free space or involve a backward propagating wave. The most important example of a research of the first group is the theory of 'complex source' developed after pioneering papers [11, 12] and [13] in both monochromatic and non-monochromatic cases. Singularities due to which these solutions do not satisfy the basic equation (1) in the whole space are described in detail in [14, 15]. As an example of an exact solution satisfying (1) everywhere but involving a backward wave, we mention a nice simple solution found in [16]. In contrast to [16], a discussion of this solution given in [15] is not based on 'sinks and sources in complex space'. A more detailed discussion of the relevant literature can be found in [9, 10] where the required axisymmetric solutions of the Helmholtz equation (1) in the whole space were presented as rather complicated expressions containing double integrals. The construction given in [10] rests on a tricky formula due to Bateman and seems to essentially employ the axial symmetry. The techniques of [9] is based on the classic expansion in plane waves and is generalizable to general astigmatic modes.

It is worthy of notice that simple exact localized non-time-harmonic solutions of the wave equation

\[ U_{xx} + U_{yy} + U_{zz} - \frac{1}{c^2}U_t = 0, \quad c = \text{const}, \tag{2} \]

in the whole space-time, such as Gaussian beams and Gaussian packets, were presented quite a long time ago (see, e.g. pioneering papers [17, 18] and an extensive review [19]). Relatively recently these results were extended to the general astigmatic case in [20].
In the current paper, we present a solution of the Helmholtz equation (1) in the whole free space, having a general astigmatic Gaussian-beam asymptotics and not involving a backward wave. We find it in the form of a classical superposition of plane waves, nontrivially generalizing the techniques developed in [9] for the axisymmetric case. An alternative approach to construction of axisymmetric exact solutions of the equation (1) in the whole space, having a Gaussian-beam behavior, was given recently in [10].

The paper is organized as follows. We start by summarizing the results of the approximate parabolic-equation approach. Then we consider an exact solution presented by a superposition of plane waves with an arbitrary smooth weight function. We find the weight via matching these solutions in a far-field area where \( k z \rightarrow \infty \). Finally we demonstrate that the related exact solution has the desired astigmatic Gaussian-beam asymptotic behaviour at large negative and moderate values of \( k z \).

In what follows we deal with 2D vectors denoted by small bold letters (e.g. \( \mathbf{p}, \mathbf{r} \)) and with 3D vectors denoted by capital letters (e.g. \( \mathbf{R}, \mathbf{N} \)). The scalar product of 2D vectors \( \mathbf{f} \) and \( \mathbf{g} \) will be written as \( \mathbf{f}^\dagger \mathbf{g} \), where \( \dagger \) and \( ^T \) stand for complex conjugation and transposition, respectively. The 3D scalar product of \( \mathbf{F} \) and \( \mathbf{G} \) will be denoted by \( \langle \mathbf{F}, \mathbf{G} \rangle = \mathbf{F}^T \mathbf{G} \). Throughout the paper 3 is standing for the imaginary part.

2. Paraxial fundamental astigmatic Gaussian modes

We shortly summarize the common approximate theory of monochromatic Gaussian beams based on the parabolic-equation method.

2.1. Paraxial wavefield at a moderate longitudinal distance

We suppress the time-dependence factor \( e^{-ikz} \) and consider localized wave propagation along the z-axis. The standard parabolic-equation approach (which can be traced back to Leontovich and Fock, see [1]) starts by singling out the plane-wave oscillation along the preferred direction, i.e., via the substitution

\[
u = e^{ikz} w_\nu, \quad w = w(x, y, z; k),
\]

followed by discarding the term \( w_\nu \) in the exact equation \( w_{xx} + w_{yy} + w_{zz} + 2ikw_z = 0 \). We arrive at the so-called parabolic equation

\[
w_{xx} + w_{yy} + 2ikw_z = 0.
\]  \( \text{(4)} \)

The wavefield is assumed to be localized near the z-axis, that is,

\[
w \rightarrow 0 \quad \text{as} \quad k \sqrt{x^2 + y^2} \rightarrow \infty.
\]  \( \text{(5)} \)

Equation (4) has a solution satisfying the paraxiality condition (5),

\[
w = \sqrt{\det \Gamma(z)} \exp \left\{ \frac{ik}{2} r^T \Gamma(z) r \right\},
\]  \( \text{(6)} \)

(see, e.g. [3, 6, 7]) where \( \Gamma(z) \) is a symmetric matrix with a positive definite imaginary part, \( r = (x, y)^T \). We call a real symmetric \( 2 \times 2 \) matrix \( A \) positive definite and write \( A > 0 \) if \( r^T A r > 0 \) for any \( r \in \mathbb{R}^2 \), \( r \neq 0 \), which is equivalent to the assertion that both eigenvalues of \( A \) are strictly positive. For definiteness, the square root in (6) is assumed to have positive imaginary part.

The resulting expression for approximate solution of the Helmholtz equation (1),

\[
u = e^{ikz} w = \sqrt{\det \Gamma(z)} \exp \left\{ i k \left[ z + \frac{1}{2} r^T \Gamma(z) r \right] \right\},
\]  \( \text{(7)} \)

is commonly known as the fundamental general astigmatic Gaussian mode [3, 7, 21]. It describes a beam running along the z-axis and Gaussian-localized at each cross-section with respect to the distance \( |r| = \sqrt{x^2 + y^2} \) from the z-axis.

The matrix \( \Gamma(z) \) satisfies the Riccati equation \( \Gamma_z + \Gamma^2 = 0 \), which implies a useful relation

\[
\Gamma(z) = (\Gamma_0^{-1} + z\mathbb{I})^{-1},
\]  \( \text{(8)} \)

where \( \mathbb{I} \) is the identity \( 2 \times 2 \) matrix and

\[
\Gamma_0 = \Gamma(0),
\]  \( \text{(9)} \)

(see, e.g. [21]). The imaginary part of \( \Gamma_0 \) is positive definite, \( \Im \Gamma_0 > 0 \), whence \( \Im \Gamma_0^{-1} < 0 \), that is, \( -\Im \Gamma_0^{-1} > 0 \).

2.2. Paraxial far-field

It is well known (see, e.g. [19, 22]) that at a large longitudinal distance, i.e., as \( k z \rightarrow \pm \infty \), the plane wave \( e^{ikz} \) in (3) does not correctly describe the leading oscillation of the beam. There, the expression (7) requires modification and must be matched with spherical waves, outgoing and incoming, respectively,
\[ u \approx \frac{\exp(ikR)}{R} F^+(N), \; kz \to +\infty, \] \hspace{2cm} (10)

and

\[ u \approx \frac{\exp(-ikR)}{R} F^-(N), \; kz \to -\infty. \] \hspace{2cm} (11)

The patterns \( F^\pm(N) \) are smooth functions of angular variables

\[ N = \frac{R}{R}, \] \hspace{2cm} (12)

where \( R = (x, y, z)^T \) and \( R = |R| = \sqrt{x^2 + y^2 + z^2}. \)

It is convenient to employ classical spherical coordinates which we introduce as follows:

\[ x = R \sin \chi \cos \varphi, \; y = R \sin \chi \sin \varphi, \; z = R \cos \chi, \] \hspace{2cm} (13)

\( 0 \leq \chi \leq \pi, 0 \leq \varphi < 2\pi, 0 \leq R < \infty. \) Therefore,

\[ N = (\sin \chi \cos \varphi, \sin \chi \sin \varphi, \cos \chi)^T. \] \hspace{2cm} (14)

We will use notation for patterns \( F^\pm(N) = F^\pm(\chi, \varphi). \) It will be seen that patterns \( F^\pm \) are not negligibly small only in a neighborhood of the z-axis, where

\[ \frac{r}{R} \ll 1, \] \hspace{2cm} (15)

\( r = |r| = \sqrt{x^2 + y^2}, \) that is, either \( \chi \ll 1 \) or \( \pi - \chi \ll 1. \)

Consider the expression (7) for large values of \(|z|\). Under condition (15), we have

\[ R \approx |z| + \frac{r^2}{2|z|}. \] \hspace{2cm} (16)

The identity (8) implies

\[ \Gamma(z) = \left( \Gamma_0^{-1} + izI \right)^{-1} = \frac{1}{z} \left( I + \frac{1}{z} \Gamma_0^{-1} \right)^{-1} \approx \frac{1}{z} - \frac{1}{z^2} \Gamma_0^{-1}. \] \hspace{2cm} (17)

Under the assumption that (15) holds, the amplitude and the phase in (7) become:

\[ \sqrt{\det \Gamma(z)} \approx \frac{1}{z} \approx \pm \frac{1}{R}, \; z \to \pm \infty, \] \hspace{2cm} (18)

and

\[ ikz + ikr \left( \frac{1}{z} - \frac{1}{z^2} \right) \approx \pm ik \frac{r}{R} - \frac{ik}{2} \bar{r} \Gamma_0^{-1} \bar{r}, \; kz \to \pm \infty, \] \hspace{2cm} (19)

where \( \bar{r} \) is the following 2D vector:

\[ \bar{r} = \frac{r}{R} = (\sin \chi \cos \varphi, \sin \chi \sin \varphi)^T = \sin \chi (\cos \varphi, \sin \varphi)^T. \] \hspace{2cm} (20)

To summarize, we found that in the paraxial area described by (15), the wavefield (6) matches with outgoing spherical wave (10) as \( kz \to \infty \) and with incoming spherical wave (11) as \( kz \to -\infty \), respectively, where the patterns are

\[ F^+(N) = \exp \left\{ -\frac{ik}{2} \bar{r} \Gamma_0^{-1} \bar{r} \right\} \] \hspace{2cm} (21)

and

\[ F^-(N) = -\exp \left\{ -\frac{ik}{2} \bar{r} \Gamma_0^{-1} \bar{r} \right\}. \] \hspace{2cm} (22)

By paraxial fundamental astigmatic Gaussian beam we mean a matched asymptotic expression equal to incoming spherical wave (11), (22) for large negative \( z \), to the parabolic-equation expression (7) for moderate \( z \) and to outgoing spherical wave (10), (21) for large positive \( z \). The area where (7) is valid overlap with areas of validity of representations of the wavefield by spherical waves (see, e.g. [22]). Throughout the paraxial area, this matched wavefield propagates solely in the directions close to that of the positive z-axis, with no backward waves.
3. Gaussian localization of the far-field with respect to the angle $\chi$. Large parameter

Consider the paraxial expression for outgoing spherical wave in more detail. Let $b_1$ and $b_2$ be the eigenvalues of the positive definite matrix $-\mathcal{H}_0$ and

$$b = \min \{b_1, b_2\}. \quad (23)$$

Under the paraxiality condition (15), we obviously have for $kz \to \infty$:

$$|F^+ (N)| = \left| \exp \left\{ -\frac{ik}{2} r^2 \right\} \right| \leq \exp \left\{ -\frac{kb}{2} \right\} = \exp \left\{ -\frac{kb}{2} \sin^2 \chi \right\}$$

which shows that the pattern $F^+$ is strongly localized in the vicinity of the positive direction of the $z$-axis if $kb \gg 1$.

Essentially, the parameter $kb$ is the large parameter of the paraxial asymptotic theory describing astigmatic Gaussian beams. The wavefield (10) sufficiently differs from zero only for small $\chi$ (more precise, $\chi < (kb)^{-1/2} + \epsilon$, where $\epsilon$ is an arbitrarily small fixed positive number). Similarly,

$$|F^- (N)| \leq \exp \left\{ -\frac{kb}{2} \sin^2 (\pi - \chi) \right\}$$

as $kz \to -\infty$.

4. Exact theory based on expansion in plane waves

Any solution of the Helmholtz equation (1)\(^4\) can be presented as a superposition of plane waves:

$$u(x, y, z) = \iiint_{|P|=1} A(P)e^{i\mathbf{R} \cdot \mathbf{P}^*}dS(P). \quad (26)$$

Here, $(\mathbf{R}, \mathbf{P})$ is a scalar product of a vector $\mathbf{R} = (x, y, z)^T$ and a unit real 3D vector $\mathbf{P}$, $|\mathbf{P}|^2 = 1$, that parameterizes points of a unit sphere over which integration proceeds, and $dS(P)$ stands for its area element. The weight function $A(P)$ is an arbitrary generalized function.

Let us parameterize the integrand in (26) by spherical coordinates, putting

$$\mathbf{P} = (\sin \chi \sin \varphi', \sin \chi \sin \varphi', \cos \chi')^T$$

and $A(\mathbf{P}) = A(\varphi', \chi')$, and taking into account that $dS(\mathbf{P}) = \sin \chi' d\chi' d\varphi'$. Now (26) takes the form

$$u = \int_0^{2\pi} \int_0^\pi A(\chi', \varphi')e^{i\mathbf{R} \cdot \mathbf{P}^*} \sin \chi' d\varphi' d\chi', \quad (27)$$

with

$$\Psi = \Psi(\chi', \varphi') = \sin \chi \sin \chi' \cos (\varphi - \varphi') + \cos \chi \cos \chi'$$. \quad (28)

The desired weight function will be found by asymptotic matching of the integral (26) and the paraxial solution in the far-field zone.

Consider the asymptotics of the integral (26) as $kR \to \infty$. We assume that the weight $A(\mathbf{P})$ is infinitely differentiable on the unit sphere, which allows for application of the standard stationary-phase techniques (e.g. [24–26]). The integral asymptotically reduces to a sum of contributions of critical points of the phase $(\mathbf{R}, \mathbf{P})$ on the sphere $|\mathbf{P}| = 1$ (critical points $\mathbf{P} = \mathbf{P}^*$ are those where $\Psi_{\chi'} |_{\mathbf{P}^*} = \Psi_{\varphi'} |_{\mathbf{P}^*} = 0$). Such a calculation is described, e.g. in [9]. It proves that the phase has two critical points

$$\mathbf{P} = \mathbf{P}_{\pm} = \pm \mathbf{N},$$

where $\mathbf{N}$ is given by (14). As $kR \to \infty$, the integral in equation (26) asymptotically reduces to

$$u = u^+ + u^-,$$

where

$$u^* \approx \pm \frac{2\pi i}{k} \frac{\exp(\pm ikR)}{R} A(\pm \mathbf{N})$$

are the contributions coming from $\pm \mathbf{N}$ (see, e.g. [9, 19]). For large $kz$, $u^+$ and $u^-$ describe outgoing and incoming spherical waves, respectively. For $z > 0$, they are forward and backward propagating ones. Since we aim at finding a solution with no backward wave, the function $A(\mathbf{N})$ must vanish where the projection of $\mathbf{N}$ on the direction of the $z$-axis is negative.

\(^4\)To be precise, a solution in a class of tempered distributions, see, e.g. [23].
5. Matching at $kz \to \infty$ and small $\chi$. The weight

Following the approach developed earlier for the axisymmetric case in [9], we will match the functions given by equations (10), (21) and (29), (30) at large values of $kz$. We start with a suggestive consideration.

Denote Cartesian coordinates of the vector $P$ by $\zeta, \eta$, and $\zeta$,

$$P = (\zeta, \eta, \zeta)^T, \quad \zeta^2 + \eta^2 + \zeta^2 = 1,$$

and introduce a 2D vector $p$ by

$$p = (\zeta, \eta)^T = (\sin \chi' \cos \chi', \sin \chi' \sin \chi')^T,$$

so that we can write $P = (p, \zeta)^T$. Note that $|p| = \sin \chi'$.

For $kz \to +\infty$ and small values of $|p|$, we match $u^+$ with the outgoing spherical wave described by (10) and (21) by putting

$$A(P) = -\frac{ik}{2\pi} \exp \left\{ -\frac{ik}{2} p^T \Gamma_0^{-1} p \right\}, \quad |p| \ll 1. \quad (33)$$

However, the undesirable, albeit small, contribution $u^-$ of the stationary point $-N$ must be eliminated. This can be done if we multiply the expression (33) by a factor equal to 1 for small $|p|$ and vanishing for $\zeta = \cos \chi' < 0$.

An immediate candidate for such a function is the Heaviside step function

$$H(\zeta) = \begin{cases} 1 & \text{for } \zeta > 0 \\ 0 & \text{for } \zeta \leq 0. \end{cases} \quad (34)$$

The weight in (26) defined as a product of (33) and (34) has a jump at $\chi' = \frac{\pi}{2}$ which gives undesirable, though small, contribution to wavefield, and an extra smooth factor vanishing at $\chi' = \frac{\pi}{2}$ should be introduced. Let $\sigma(s)$ be the standard neutralizer function widely used in asymptotic evaluation of integrals (see, e.g. [24–26])

$$\sigma(s) = \begin{cases} \exp \left( -\frac{s^2}{\alpha^2 - s^2} \right) & \text{for } 0 \leq |s| < \alpha \\ 0 & \text{for } |s| \geq \alpha, \end{cases} \quad (35)$$

where $\alpha$ is arbitrarily fixed within the interval $0 < \alpha < 1$.

We define the weight function on the unit sphere by

$$A(P) = -\frac{ik}{2\pi} \exp \left\{ -\frac{ik}{2} p^T \Gamma_0^{-1} p \right\} H(\cos \chi') \sigma(\sin \chi'). \quad (36)$$

This function is smooth and asymptotically coincides with (33) for small $\chi'$ where $\sigma(\sin \chi') \approx 1$. Asymptotic behaviour of the integral (26), (36) does not depend on the value of $\alpha$.

To complete the analysis of the far-field asymptotics of the integral (26), we now assume that $kz \to -\infty$ and $\pi - \chi$ is small. In the asymptotics (29), the term $u^-$ equals zero because the critical point $P = N$ lies in the area where the Heaviside factor (34) vanishes. Consider the contribution $u^+$ of the critical point $P = -N$. In its vicinity, $\sigma(\sin \chi') \approx 1$, $H(\cos \chi') = 1$, whence $u^+ (-N)$ approximately coincides with (11) where $F^-$ is given by (22).

We established that the choice of the weight function in accordance with (36) ensures asymptotic reduction of the integral (26) to the paraxial solution at large values of $k|z|$.

6. Integral (26) at moderate values of $kz$

Now we consider asymptotic behavior of the integral (26) with the weight function (36) without the assumption that $kz$ is large. The integrand is a product of a rapidly varying exponential function and a slowly varying amplitude. The standard techniques of finding leading-term asymptotics of such integrals (see, e.g. [24–26]) is based on expanding the phase of the rapidly varying factor up to quadratic terms inclusively at its critical points and taking the zero-order approximation for the amplitude. Thereafter, the limits of integration are extended to infinity.

In order to apply this machinery to the integral (27), we parameterize the unit vector $P$ by Cartesian coordinates, see (31). Taking into account that

$$dS(P) = \frac{dp}{\sqrt{1 + \zeta^2 + \eta^2}}, \quad dp = d\zeta \, d\eta,$$
the integral (26) with the weight (36) reads
\[ -\frac{ik}{2\pi} \int_{\mathbb{R}^3} \exp \left\{ -\frac{ik}{2} \mathbf{p}^\dagger \mathbf{G}_0^{-1} \mathbf{p} \right\} \sigma(|\mathbf{p}|) \exp \{ ik[\mathbf{p}^\dagger \mathbf{r} + \sqrt{1 - \mathbf{p}^2} z]\} \frac{d\mathbf{p}}{\sqrt{1 + \mathbf{p}^2}}, \]
where the factor \( H(\zeta) \) in (36) results in taking the positive value of the square root.

A simple estimate analogous to (24),
\[ \left| \exp \left\{ -\frac{ik}{2} \mathbf{p}^\dagger \mathbf{G}^{-1} \mathbf{p} \right\} \right| \leq \exp \left\{ -\frac{kb}{2} \mathbf{p}^2 \right\}, \]
shows that only small values of \( \zeta \) and \( \eta \) give a non-negligible contribution to the integral. With an exponentially small error, the integration domain can be reduced to \( \mathbb{R} \) where \( \varepsilon > 0 \) is small, e.g. \( \varepsilon = (kb)^{-1/2} \). In this domain we simplify in the amplitude factor
\[ \sigma(|\mathbf{p}|) \sqrt{1 + \mathbf{p}^2} \approx 1, \]
and write in the phase \( \sqrt{1 - \mathbf{p}^2} \approx 1 - \mathbf{p}^2/2 \). Further, we extend the limits of integration to the whole \((\zeta, \eta)\)-plane, which gives
\[ u \approx -\frac{ik}{2\pi} \int_{|\mathbf{p}|<\varepsilon} \exp \left\{ -\frac{ik}{2} \mathbf{p}^\dagger \mathbf{G}_0^{-1} \mathbf{p} \right\} \exp \{ ik[\mathbf{p}^\dagger \mathbf{r} + (1 - \mathbf{p}^2/2)z]\} d\mathbf{p} \approx -\frac{ik}{2\pi} \exp(ikz) \int_{\mathbb{R}^2} \exp \left\{ -\frac{ik}{2} \mathbf{p}^\dagger (\mathbf{G}_0^{-1} + zI) \mathbf{p} \right\} \exp \{ ik\mathbf{p}^\dagger \mathbf{r}\} d\mathbf{p}. \]

Using (8) we obtain
\[ u \approx -\frac{ik}{2\pi} \exp(ikz) \int_{\mathbb{R}^2} \exp \left\{ -\frac{ik}{2} \mathbf{p}^\dagger (\mathbf{G}_0^{-1} + zI) \mathbf{p} \right\} \exp \{ ik\mathbf{p}^\dagger \mathbf{r}\} d\mathbf{p}. \]

The integral (37) which appears to be the Fourier transform of an exponential of a quadratic form, is known in explicit form (see, e.g. [27]). It equals
\[ \sqrt{\det \mathbf{G}(z)} \exp \left\{ ikz + \frac{ik}{2} \mathbf{r}^\dagger \mathbf{G}(z) \mathbf{r} \right\}, \]
where the square root has positive imaginary part. The resulting expression coincides with the right-hand side of formula (7). Thus, we established that a superposition of plane waves with the weight (36) asymptotically coincides with the paraxial Gaussian beam described in section 2.

7. Conclusions

We presented an exact solution of the Helmholtz equation in the whole 3D space, which asymptotically reduces to a general astigmatic fundamental Gaussian beam and does not include a backward wave. The construction can be generalized to higher-order modes and to vector equations such as those describing electromagnetic wave propagation in crystals.

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