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Wave-front curvature in geometrical optics

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This paper develops a general method for calculation of the intensity of light propagating in a medium whose refractive index $n(\mathbf{r})$ varies slowly with position, based on a differential equation for the curvature of wave fronts. The equation can be integrated along rays, one ray at a time, and gives the changes of intensity caused by convergence or divergence of the rays. An explicit solution is obtained for light in a cylindrically symmetric medium having a linear density gradient. Applied to wave mechanics, the method gives a local semiclassical solution of the three-dimensional Schrödinger equation in a form especially suitable for treatment of collisions. We examine the possibility of extending the method to nonlinear optics.
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I. INTRODUCTION

The method of geometrical optics (ray tracing) is very useful in applications where one wishes to calculate wave propagation without the computational expense of a full numerical solution of the wave equation.

Typical applications are the calculation of laser interaction with a fluid or plasma [1]. In these applications the laser refraction must be calculated with a new geometry after each hydrodynamic time step, perhaps thousands of times, and for this reason the laser refraction must be calculated rapidly.

Geometrical optics is a simple and convenient method for tracing ray trajectories but when it is necessary to calculate the light intensity there are difficulties. Of course, geometrical optics becomes inaccurate near focal points or caustic surfaces where the intensity becomes large. This problem can be dealt with by imposing a diffraction limit on the intensity based on the (known) wavelength.

However, there is a second difficulty because the intensity depends on the density of rays. The intensity is usually calculated by numerical sampling; many rays are calculated and an approximate intensity is formed by counting rays passing through each computational zone. It would be more convenient and more accurate to obtain the intensity on each ray as it is being calculated.

The intensity varies inversely as the cross-sectional area of a small tube bounded by rays. When light converges toward a focus, this tube area becomes smaller and the intensity rises. Both the changes of area and the changes of intensity due to convergence of the rays are determined by the *curvature* of the wave front.

In Secs. II and III these ideas are expressed in mathematical form. The equations are written for light propagation in an isotropic medium having a known refractive index $n(\vec{r})$ that varies slowly with position. It appears that the equations can readily be implemented in numerical computations.

In Sec. IV we give the analytic solution for light propagation in a medium having a constant density gradient and cylindrical symmetry. This solution provides the basic algorithm required for the numerical calculation of light propagation in an arbitrary cylindrically symmetric medium.

With small changes the equations can be adapted to solve the one-electron Schrödinger equation for motion in a potential $U(\vec{r})$ (Sec. V). The result is a semiclassical (three-dimensional WKB) general solution of the Schrödinger equation, which is valid near any nonsingular point.

As an illustration we give the analytic solution for scattering by a spherically symmetric potential. In this case a semiclassical scattering wave function is readily obtained and leads to a known semiclassical cross section.

It would be useful if these methods could be applied to the propagation of light in a medium having a nonlinear refractive index. If the index of refraction depends upon the light intensity, one cannot trace rays without knowing the intensity. It appears the method of this paper could be extended to that case by a technique of wave-front tracing (see Sec. VI).

We conclude this introduction with a few citations of relevant literature. The basic equations of geometrical optics are given in many places [2,3]. The relation between wave-front curvature and intensity is discussed in the context of light propagation in vacuum in Refs. [3–5]. Recent efforts to construct a general formula for propagation with a variable index $n(\vec{r})$ are discussed by Kravtsov and Orlov [6].

Results that overlap the work of this paper are likely to be found in the extensive literature of semiclassical dynamics. The overlap may not be immediately apparent due to differences of motivation or notation. For example, Kaufman [7] gives a differential equation that appears equivalent to Eq. (22). In our paper the goal is to develop the theory into a practical computational method for calculating the intensity of light refracted by an inhomogeneous fluid.

II. GEOMETRICAL OPTICS AND WAVE FRONTS

In this section we summarize the equations of geometrical optics for an isotropic medium. It is desired to solve the Helmholtz equation,

$$\{\nabla^2+[n(\vec{r})\omega/c]^2\}\vec{E}(\vec{r})=\vec{0}, \tag{1}$$

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where $n = n(\vec{r})$ is the refractive index, assumed to be a known function of the (vector) position $\vec{r}$. In geometrical optics the changes of $n(\vec{r})$ over one wavelength $\lambda = 2\pi c/(n\omega)$ are assumed to be small. The electric field $\vec{E}(\vec{r})$ has a slowly varying amplitude $\vec{E}_0$ and a rapidly varying phase Φ:

$$\vec{E}(\vec{r}) = \vec{E}_0(\vec{r}) \exp[i\Phi(\vec{r})]. \tag{2}$$

The light intensity is

$$I = (c/8\pi) n(\vec{r}) |\vec{E}_0(\vec{r})|^2. \tag{3}$$

As written, Eq. (3) includes the change of the photon group velocity caused by the index.

Geometrical optics is appropriate when $L \gg \lambda$, where λ is the wavelength and L is a scale length determined by the logarithmic derivative of $\vec{E}_0$. Physically it is evident that L is the smallest of three numbers: the scale length for gradients of $n(\vec{r})$ or the two radii of curvature of the wave front. [This can be verified from Eq. (33) below.]

In deriving the Helmholtz equation from Maxwell's equations, there is a technical issue associated with gradients of the field amplitude and polarization [2,5,6]. In some geometries these gradients generate corrections to Eq. (1) of order L^{-2}, smaller than the terms of order λ^{-2} and $(\lambda L)^{-1}$, which are treated here. Neglecting terms of order L^{-2} we can use Eqs. (1)–(3), but then cannot calculate the polarization dependence of the refraction. This approximation is consistent with the accuracy of geometrical optics.

The gradient of the phase Φ is the wave vector $\vec{k}(\vec{r})$, which can be written as

$$\vec{\nabla}\Phi = \vec{k}(\vec{r}) = (\omega/c) n(\vec{r}) \hat{N}(\vec{r}). \tag{4}$$

Here $\hat{N}(\vec{r})$ is the unit vector normal to the constant-phase surface. The equations that determine the rays are

$$d\vec{r}/ds = \hat{N} = (c/\omega n)\vec{k}, \tag{5}$$

$$d\vec{k}/ds = (\omega/c)\vec{\nabla} n. \tag{6}$$

In Eqs. (5) and (6) the independent variable s is the arc length along a ray. The ray trajectory is the solution $\vec{r}(s)$. Equation (6) is easily proven by analyzing the gradient of $|\vec{k}|^2$ obtained from Eq. (4). Equations (5) and (6) are equivalent to Hamilton's equations for geometrical optics. They can be integrated along one ray in a straightforward manner because they do not require any information about other rays.

By substituting Eq. (2) into Eq. (1), using Eq. (4), and neglecting the second derivative of E_0, which is $O(L^{-2})$, we see that

$$2\vec{k}\cdot\vec{\nabla} E_0 = -(\mathrm{div}\,\vec{k}) E_0. \tag{7}$$

Equation (7) is sometimes called the amplitude transport equation, and its physical content is made clear by writing it as

$$\mathrm{div}[I(\vec{r})\hat{N}(\vec{r})] = \vec{0}. \tag{8}$$

Equation (8) expresses the conservation of energy for a time-independent light wave. Equation (8) applies when there is no absorption, but the theory is easily modified to account for absorption. The difficult point is that Eq. (7) cannot be integrated unless the divergence of $\vec{k}$ is known, but that seems to require information about other rays.

In the geometrical optics approximation for linear optics, we will see that adjacent rays decouple enough so there is a closed equation for the light intensity. This equation makes it possible to propagate the intensity along one ray before calculating the next ray.

III. INTENSITY AND CURVATURE OF WAVE FRONTS

A. Geometrical derivation

Before beginning the mathematics we want to outline the intuitive content of the desired formulas. The intensity varies along a ray for two reasons, first due to physical absorption (or gain) in the propagation medium and second due to convergence or divergence of rays, i.e., due to changes in areas of the small tubes surrounding a ray. Without being precise about the definition of these areas, we expect

$$(1/I)dI/ds = -\alpha - (1/A)dA/ds. \tag{9}$$

Here α is the material absorption coefficient and A is the (infinitesimal) area of a small patch on the wave front bounded by rays. For simplicity, absorption is omitted in most of the following equations. The second negative sign reflects the fact that without absorption the product of intensity I and area A would be constant.

For waves propagating in a homogeneous medium, where the index is constant, two successive wave fronts are separated by a fixed fraction of a wavelength. Because the wavelength is constant, we have

$$(1/A)dA/ds = \kappa_1 + \kappa_2, \tag{10}$$

where κ_1, κ_2 are the two principal curvatures of the wave front. The reciprocal of the curvature is the radius of curvature $R_i = 1/\kappa_i$. The curvature is defined precisely in Eq. (20) below.

For propagation in empty space each radius of curvature changes linearly with distance,

$$R_i = s + R_i^0 \quad (i = 1,2), \tag{11}$$

where R_i^0 is negative for a concave wave front and positive for a convex wave front. (A concave wave front advances toward a focus or caustic, where R_i will approach zero.) Equation (11) is a simple special solution of Eq. (22) given below (see Ref. [5]).

Equations (9)–(11) immediately lead to an equation for the intensity of light propagating without absorption in a homogeneous medium[4,5],

$$I \propto (R_1 R_2)^{-1}. \tag{12}$$

At a caustic or focal point one or both radii R_i approach zero and Eq. (12) diverges, which indicates a breakdown of geometrical optics. However, the formula is again valid, with the same coefficient, on the far side of the singularity.

Equations (11) and (12) tell how intensity changes as one moves along a ray, but do not describe the intensity variation over the wave front. For example, we can imagine light coming through a lens from a source and can imagine drawing any pattern on the lens, producing a nearly arbitrary variation of intensity on the first wave front after the lens. (If the edges of the drawing are too sharp, diffraction will invalidate the geometrical optics approximation.) Thus the variation of intensity over any wave front is essentially arbitrary except for the general requirement of geometrical optics that the derivatives must be not too large.

In this paper we want to extend Eqs. (9)–(12) to include the effect of refraction by a variable index $n(\vec{r})$. The key results are Eqs. (22) and (25) below, which show how the curvature of the wave fronts is changed by refraction and then how the intensity changes are determined by the curvature.

Two useful formulas immediately follow from Eqs. (1)–(6):

$$dn/ds = \hat{N}\cdot\vec{\nabla}n, \tag{13}$$

$$d\hat{N}/ds = (1/n)\underline{\Pi}\cdot\vec{\nabla}n. \tag{14}$$

Here $\hat{N}$ is the unit vector parallel to $\vec{k}$, which points along the ray, and we use the symbol

$$\underline{\Pi} = \underline{1} - \hat{N}\hat{N}. \tag{15}$$

$\underline{\Pi} = \underline{\Pi}(\vec{r})$ is a symmetric tensor (dyadic). A dot product with $\underline{\Pi}$ projects vectors into the plane tangent to the wave front at the point $\vec{r}$ under consideration. $\underline{\Pi}$ and $\hat{N}$ obey two obvious equations,

$$\underline{\Pi}\cdot\underline{\Pi} = \underline{\Pi}, \tag{16}$$

$$\hat{N}\cdot\underline{\Pi} = \underline{\Pi}\cdot\hat{N} = \vec{0}. \tag{17}$$

The curvature of the wave front at the point $\vec{r}$ is described by the curvature tensor $\underline{K}(\vec{r})$ whose defining properties are (1) $\underline{K}$ is a symmetric tensor; (2) $\underline{K}$ operates on (and produces) vectors in the plane

$$\hat{N}\cdot\underline{K} = \underline{K}\cdot\hat{N} = \vec{0}, \tag{18}$$

$$\underline{\Pi}\cdot\underline{K} = \underline{K}\cdot\underline{\Pi} = \underline{K}; \tag{19}$$

(3) For any small displacement $d\vec{r}$ on the wave front, the change of the surface normal is

$$d\hat{N} = \underline{K}\cdot d\vec{r}. \tag{20a}$$

In general, there are two directions on the wave front called principal directions, for which the change $d\hat{N}$ is parallel to $d\vec{r}$. The eigenvalues κ_1, κ_2 of $\underline{K}$ are the two curvatures of the wave front. The reader can make small sketches to convince himself that the change $d\hat{N}$ is parallel to $d\vec{r}$ with a positive coefficient for a surface locally convex in the direction $d\vec{r}$, corresponding to positive curvature and a diverging family of rays. The sign of the curvature depends on the

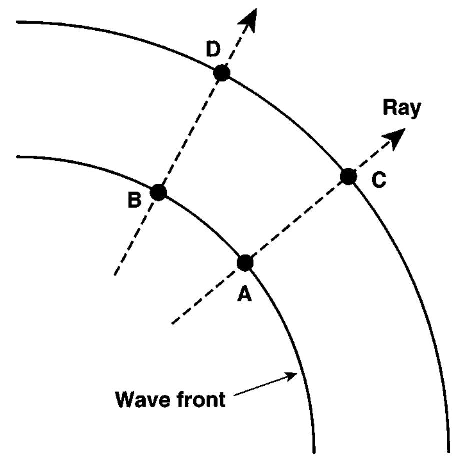

FIG. 1. The diagram illustrates the derivation of Eq. (22). Points A, B, C, and D are all understood to be close together. A and C are one ray while B and D are on a nearby ray. A and B are on the same wave front, and C and D are on a nearby wave front. The changes in surface normal from A to B are given by the curvature formula, Eq. (20a). The changes from A to C and from B to D are given by Eq. (14). Then the changes AC, AB, and BD are all known, and together give a projection of Eq. (22) for the change CD.

orientation of the wave front, which is determined by the direction of the unit vector $\hat{N}(\vec{r})$.

Equations (18)–(20a) are summarized by the statement that $\underline{K}$ is the projection of grad $\hat{N}$ into the plane tangent to the wave front, i.e.,

$$\underline{K} = \underline{\Pi}\cdot\vec{\nabla}\hat{N}\cdot\underline{\Pi}. \tag{20b}$$

Because $\hat{N}^2$ is a constant (equal to unity) the right-hand projection has no effect and can be omitted.

To calculate the derivative $d\underline{K}/ds$ we compare two successive wave fronts that differ by a small phase change $\delta\Phi$. A first constraint on the derivative of $\underline{K}$ comes from the requirement that Eq. (18) hold everywhere. This condition, obtained with the help of Eq. (14), is

$$\hat{N}\cdot d\underline{K}/ds = d\underline{K}/ds\cdot\hat{N} = -(1/n)\underline{K}\cdot\vec{\nabla}n. \tag{21}$$

The equations needed to determine $d\underline{K}/ds$ are obtained by examining four nearby points labeled A, B, C, and D in Fig. 1. Points A and B are in the same wave front, and C and D are in a nearby wave front. Points A and C are on the same ray, and B and D are on an adjacent ray. Equations (5) and (14) determine the changes $d\vec{r}$ and $d\hat{N}$ from A to C and from B to D, while Eq. (20) gives the change $d\hat{N}_{AB}$ between points A and B in terms of $d\vec{r}_{AB}$. Combining these relations we obtain the change $d\hat{N}_{CD}$ from C to D, and the corresponding change $d\vec{r}_{CD}$. Then $d\hat{N}_{CD}$ is the dot product of $(\underline{K}+ds\ d\underline{K}/ds)$ with $d\vec{r}_{CD}$. The calculation can be repeated with a second linearly independent vector $d\vec{r}_{AB'}$. The formulas described, in conjunction with Eq. (21), yield Eq. (22) below for $d\underline{K}/ds$.

In this calculation the two surfaces are wave fronts, and so the calculation produces $d\underline{K}/d\Phi$, which is converted into $d\underline{K}/ds$ with the help of Eq. (4). The result is

$$d\underline{K}/ds = -\underline{K}\cdot\underline{K} - (1/n)(\hat{N}\cdot\vec{\nabla}n)\underline{K} + (1/n)\underline{\Pi}\cdot\vec{\nabla}\vec{\nabla}n\cdot\underline{\Pi} - (2/n^2)\underline{\Pi}\cdot\vec{\nabla}n\vec{\nabla}n\cdot\underline{\Pi} - (1/n)[(\underline{K}\cdot\vec{\nabla}n)\hat{N} + \hat{N}(\vec{\nabla}n\cdot\underline{K})]. \tag{22}$$

In checking Eq. (22) the reader will want to remember that because $\underline{K}$ is symmetric, dot products of vectors with $\underline{K}$ can be written in either order. Equation (22) implies that the derivative of $\underline{K}$ is also symmetric. It is easily verified that Eq. (22) is consistent with Eq. (21).

Equation (22) can be derived in various ways. Using a coordinate system on the wave fronts, several pages of classical differential geometry lead to Eq. (22). Another formal derivation of Eq. (22) is indicated in Sec. III B.

If the index is constant, so its gradient is zero, Eq. (22) simplifies to

$$d\underline{K}/ds = -\underline{K}\cdot\underline{K} \quad (n=\text{const}). \tag{23}$$

The solution of this equation is just Eq. (11).

It follows from Eq. (20b) that the divergence of the unit vector $\hat{N}$ is given by

$$\text{div } \hat{N} = \text{Tr}[\underline{K}] = \kappa_1 + \kappa_2. \tag{24a}$$

Equation (4) and Eq. (24a) can be combined to give a formula for div $\vec{k}$:

$$\text{div } \vec{k} = (\omega n/c)(\kappa_1+\kappa_2) + (\omega/c)dn/ds. \tag{24b}$$

Equation (24b) leads through Eq. (7) to

$$dI/ds = -(\kappa_1+\kappa_2)I. \tag{25}$$

This agrees with Eqs. (9) and (10) and therefore the refraction does not change the geometrical relation between curvature and intensity.

To summarize, if we know $\hat{N}$, $\underline{K}$, and I at a point on one ray, then we can evaluate the right-hand sides of Eqs. (14), (22), and (25) and thereby integrate the intensity along that ray *without* knowing about other rays. However, when we later examine a nearby ray, its direction is already constrained by the assumed initial value of $\underline{K}$. Thus there is a requirement that rays launched from the source be consistent with the assumed curvature of the first wave front. This requirement is not difficult when the light source is a beam or is light emerging from a simple lens.

B. Formal derivation

We now give another derivation of Eq. (22) in which the mathematics is more straightforward while the geometry is less evident.

We examine the tensor

$$\vec{\nabla}\vec{\nabla}\Phi = (\omega/c)\vec{\nabla}[n(\vec{r})\hat{N}(\vec{r})]. \tag{26}$$

From Eq. (26) it is clear this tensor is symmetric.

Equation (20b) implies

$$\vec{\nabla}\hat{N} = \underline{K} + \hat{N}\ d\hat{N}/ds \tag{27}$$

and therefore

$$\vec{\nabla}(n\hat{N}) = n\underline{K} + d(n\hat{N}\hat{N})/ds. \tag{28}$$

Thus from an equation that propagates $\vec{\nabla}(n\hat{N})$ along the rays, we are able to propagate the curvature tensor itself.

For any function $f(\vec{r})$ (scalar, vector, or tensor) we have

$$df/ds = \hat{N}\cdot\vec{\nabla}f \tag{29}$$

and therefore

$$\vec{\nabla}\ df/ds = \vec{\nabla}\hat{N}\cdot\vec{\nabla}f + d(\vec{\nabla}f\ )/ds. \tag{30}$$

We apply these equations to $\vec{f} = n\hat{N}$. Equation (29) gives

$$d(n\hat{N})/ds = \vec{\nabla}n \tag{31}$$

in agreement with Eq. (6). Using Eq. (31) and the simple formula

$$\vec{\nabla}\vec{\nabla}n^2 = 2\vec{\nabla}n\vec{\nabla}n + 2n\vec{\nabla}\vec{\nabla}n, \tag{32}$$

Eq. (30) can be rearranged to give

$$nd[\vec{\nabla}(n\hat{N})]/ds = -\vec{\nabla}(n\hat{N})\cdot\vec{\nabla}(n\hat{N}) + \tfrac{1}{2}\vec{\nabla}\vec{\nabla}n^2. \tag{33}$$

This tensor differential equation includes Eq. (22) among its components. For example, when we project Eq. (33) into the plane tangent to the surface using the tensor $\underline{\Pi}$ it is easily shown that we obtain the corresponding projection of Eq. (22). This is the additional derivation of Eq. (22) mentioned above. When the index is constant Eq. (33) is very simple. In Sec. IV we solve Eq. (33) for an index with a nonzero gradient.

Returning to the equation for the intensity, and including the absorption coefficient α, from Eq. (25) we expect

$$dI/ds = -(\kappa_1+\kappa_2)I - \alpha I. \tag{34}$$

Using Eq. (28), this can be transformed to read

$$d\ \ln(I/n)/ds = -\alpha - (1/n)\text{Tr}[\vec{\nabla}(n\hat{N})] \tag{35}$$

and this form is also convenient.

IV. SOLUTION FOR CYLINDRICAL SYMMETRY

In this section we solve Eqs. (22) and (25) for a cylindrically symmetric wave in a cylindrically symmetric medium having a constant density gradient, corresponding to a linear dependence of dielectric function on position.

Any smooth density profile can be approximated on a grid of triangular zones containing locally linear densities, so the results of this section form the basis for a numerical calculation of light propagation in a cylindrically symmetric medium having any index $n = n(r,z)$.

Cylindrical symmetry means two things here: First, the index depends only on the variables r,z, and this is a constraint on the propagation medium. In addition the phase Φ depends only on r,z so the wave fronts are surfaces of revolution about the z axis, and this is a constraint on the wave being traced. The second assumption is consistent with the first.

The solution gives a closed-form expression for the light intensity.

The dielectric function $\varepsilon = n^2$ is usually a linear function of the material density and so we assume that its gradient is independent of r and z over the region considered. This means

$$\vec{a} = \tfrac{1}{2}\vec{\nabla} n^2 = \vec{a}(\theta). \tag{36}$$

We assume that $\vec{a}$ is independent of r and z, but underline the fact that any vector that lies in the r-z plane depends on θ because the radial unit vector $\hat{r} = \hat{r}(\theta)$ depends on θ. (We use cylindrical polar coordinates r,θ,z.)

The equations simplify when the ray is written $\vec{r} = \vec{r}(u)$ in terms of an independent variable $u(s)$ defined by

$$ds/du = n[\vec{r}(u)]. \tag{37}$$

In the equations that follow, derivatives with respect to u are directional derivatives along a ray.

The Hamilton equations, Eqs. (5) and (6), become

$$d\vec{r}/du = \vec{v}, \tag{38}$$

$$d\vec{v}/du = \vec{a}, \tag{39}$$

with

$$\vec{v} = n\hat{N}. \tag{40}$$

Here $\vec{v}$ is a dimensionless quantity proportional to the wave vector $\vec{k} = (\omega/c)\vec{v}$; and $\hat{N}$ is the unit vector along $\vec{k}$.

For the case considered here, $\vec{a}$ does not vary with u and Eqs. (38) and (39) are easily solved for the ray trajectory:

$$\vec{v} = \vec{v}_0 + u\vec{a}, \tag{41}$$

$$\vec{r} = \vec{r}_0 + u\vec{v}_0 + \tfrac{1}{2}\vec{a}u^2. \tag{42}$$

This is a simple special solution of the equations of geometrical optics. Now we find the intensity implied by this solution.

The intensity I is found by solving Eq. (33), which can be written as

$$d\underset{\sim}{G}/du = -\underset{\sim}{G}\cdot\underset{\sim}{G} + \tfrac{1}{2}\vec{\nabla}\vec{\nabla} n^2, \tag{43}$$

where

$$\underset{\sim}{G} = \vec{\nabla}(n\hat{N}). \tag{44}$$

The solution of Eq. (43) will then be used to solve Eq. (35) (with $\alpha = 0$), which can be written as

$$(d/du)\ln(I/n) = -\mathrm{Tr}\ \underset{\sim}{G}. \tag{45}$$

The first step is to remove the θ dependence. By assumption the phase Φ is independent of θ, but the radial unit vector $\vec{r}$ depends on θ. Then we easily see

$$\hat{\theta}\cdot\vec{\nabla}\vec{\nabla}\Phi = (1/r)(\partial\Phi/\partial r)\hat{\theta}. \tag{46}$$

In Eq. (46), $\hat{\theta}$ is the unit vector in the θ direction. Comparing the left side to Eq. (28) and the right side to Eq. (4), we can see Eq. (46) gives one eigenvalue of the curvature tensor $\underset{\sim}{K}$,

$$\underset{\sim}{K}\cdot\hat{\theta} = \kappa_\theta\hat{\theta} \tag{47}$$

with

$$\kappa_\theta = (\hat{N}\cdot\hat{r})/r. \tag{48}$$

In Eq. (48) the two vectors $(\hat{N},\hat{r})$ in the numerator are unit vectors, so the units are still correct. Equation (48) can also be written as

$$n\kappa_\theta = d(\ln r)/du. \tag{49}$$

In Eq. (49) the scalar radius r appears on the right-hand side. Equation (49) will help solve Eq. (45). We can also form the tensor derivative,

$$d(n\kappa_\theta\hat{\theta}\hat{\theta})/du = -(n\kappa_\theta\hat{\theta}\hat{\theta})\cdot(n\kappa_\theta\hat{\theta}\hat{\theta}) + (\vec{a}\cdot\hat{r}/r)\hat{\theta}\hat{\theta}. \tag{50}$$

Here the combination $\hat{\theta}\hat{\theta}$ is a tensor made from the unit vector $\hat{\theta}$ and the numerator of the last term contains $(\vec{a}\cdot\hat{r})$, where $\hat{r}$ is again the radial unit vector, while the denominator is the scalar radius r. Equation (50) will help solve Eq. (43).

Equations (47)–(50) have a geometrical interpretation that is worth comment. The curvature of a surface is determined by the sphere which has second-order contact with the surface in a principal direction.

When the wave front is a surface of revolution, one sphere makes contact with the wave front around a circle of fixed r,z. The radius of this sphere is determined by the distance to the z axis along the local normal to the surface. In simple language, all rays launched from points around this circle would arrive in phase on the axis (although they may be further refracted as they move). So for the curvature in the θ direction, the center of curvature is always on the z axis. The intensity changes associated with this curvature κ_θ are easily determined because the total energy inside a given cone of rays is conserved.

To complete the solution of Eq. (43) we remove the known part of $\underset{\sim}{G}$, defining

$$\underset{\sim}{Q} = \underset{\sim}{G} - n\kappa_\theta\hat{\theta}\hat{\theta}. \tag{51}$$

From Eq. (47) we easily see that

$$\underset{\sim}{Q}\cdot\hat{\theta} = 0 \tag{52}$$

and then the differential equation for $\underset{\sim}{Q}$ is

$$d\underset{\sim}{Q}/du = -\underset{\sim}{Q}\cdot\underset{\sim}{Q}. \tag{53}$$

This equation is easily solved,

$$\underline{Q}=\underline{Q}_0/(\underline{1}+u\underline{Q}_0), \tag{54}$$

where $\underline{Q}_0$ is the initial value corresponding to $u=0$.

We define a function

$$D=\det(\underline{1}+u\underline{Q}_0). \tag{55}$$

The form of $\underline{Q}_0$ can be found from Eq. (28) and gives

$$D=(1+un_0\kappa_r^0)(1+u\vec{a}\cdot\hat{N}_0/n_0)-u^2(\hat{t}_0\cdot\vec{a}/n_0)^2. \tag{56}$$

In Eq. (56), $\hat{t}=\hat{N}\times\hat{\theta}$ is a unit vector tangent to the wave front, the subscript or superscript 0 denotes the initial value at $u=0$, and κ_r^0 is the initial curvature in the $\hat{t}$ direction.

We now observe

$$\mathrm{Tr}\ \underline{Q}=d(\ln D)/du, \tag{57}$$

which follows from the formula

$$\mathrm{Tr}\ \underline{Q}=(d/du)\mathrm{Tr}\ \ln(\underline{1}+u\underline{Q}_0). \tag{58}$$

With this the solution to Eq. (45) is immediately found:

$$(d/du)(IrD/n)=0 \tag{59}$$

or

$$I=(n/rD)(r_0/n_0)I_0 \tag{60}$$

as $D_0=1$.

Equation (60) gives the intensity along the ray in terms of initial values. The initial point is an arbitrary point along the ray. It is necessary to know κ_r^0, which must be consistent with the initial directions of the nearby rays.

We close this section with an expression for κ_r:

$$n\kappa_r=-(\vec{a}\cdot\hat{N})/n+(d/du)\ln D. \tag{61}$$

This is the curvature in the direction defined by the unit vector $\hat{t}$. It is easily seen that Eq. (61) reproduces the assumed initial value.

To help the reader understand Eq. (60) we point out that there is another derivation. One could have taken three nearby rays, differenced their positions (at equal values of the phase), and formed the area of the small triangle defined by them. Then using the relation between intensity and area, this would again give Eq. (60).

V. APPLICATION TO WAVE MECHANICS

The one-electron Schrödinger equation is a special case of the wave equation, obtained by the substitution

$$[n(\vec{r})\omega/c]^2=k^2=(2m/\hbar^2)[E-U(\vec{r})]. \tag{62}$$

Here E is the particle energy and $U(\vec{r})$ is the potential energy. With this substitution, Eqs. (22) and (25) translate into the following equations:

$$k\ d\underline{B}/ds=-\underline{B}\cdot\underline{B}+\tfrac{1}{2}\vec{\nabla}\vec{\nabla}k^2, \tag{63}$$

$$k\ dP/ds=-P\ \mathrm{Tr}\ \underline{B}, \tag{64}$$

where P is the electron probability density and $\underline{B}$ is the tensor gradient of the wave vector $\vec{k}$:

$$P=|\Psi|^2, \tag{65}$$

$$\underline{B}=\vec{\nabla}\vec{k}. \tag{66}$$

Solution of Eq. (63) gives a practical way to construct the prefactor for the semiclassical wave function. The prefactor is usually constructed by evaluating the Van Vleck determinant, which can be written in various ways [8], but can be evaluated only if one knows the action as a function of a complete set of independent constants of the motion. Thus one needs a complete solution to the problem in order to use the Van Vleck formula. In contrast to this, the method based on Eq. (63) gives the prefactor at $\vec{r}$ based on information about one trajectory passing through $\vec{r}$ without requiring any additional information.

Equations (22) and (25) can be applied as follows: an atom or molecule is described by a potential $U(\vec{r})$, which need not be spherically symmetric. An electron scattering from this target is described by a scattering wave function having the asymptotic form

$$\psi\to\exp(ikz)+(1/r)f(\theta)\exp(ikr). \tag{67}$$

This wave function can be approximately represented by a finite number of classical trajectories [9]. The trajectories begin on a source plane at $z\to-\infty$. Solution of Eqs. (63) and (64) will give the wave function, trajectory by trajectory, without requiring an overall normalization.

While the angular momentum $\hbar L$ is constant along each trajectory, the scattering function of Eq. (67) is not an eigenfunction of angular momentum and different trajectories have different values of L determined by their initial impact parameters.

To illustrate the method, we solve Eqs. (63) and (64) for the scattering produced by a spherically symmetric potential $U(r)$. Various classical and semiclassical solutions are available in the literature [10].

Along each electron trajectory the angular momentum $\hbar L$ is constant. The trajectories begin at $z\to-\infty$. We use the notations

$$q(r)=\sqrt{(k^2-L^2/r^2)}, \tag{68}$$

$$A(r)=\int_r^{r_0}k^2dr/(r^2q^3). \tag{69}$$

Here $q(r)$ is the radial wave vector, $k(r)$ is the three-dimensional wave vector from Eq. (62), and $A(r)$ is an integral related to the angular position,

$$A(r)=-d\theta(r)/dL, \tag{70}$$

$$\theta(r)=\pi-\int_r^{r_0}dr/(r^2q). \tag{71}$$

In Eqs. (69) and (71), for the incoming portion of the orbit the integrals run from the current radius r to a fixed large radius ($=r_0$, say). This means that the derivative of θ with respect to r is positive. For very large r on the incoming portion of the orbit the angle θ is approximately π, consistent with Eq. (67).

While the calculation is generally straightforward, there is one interesting technicality: Eq. (63) is a vector (dyadic) equation, and to evaluate $d\underline{B}/ds$ in spherical polar coordinates it is necessary to differentiate unit vectors as well as components of $\underline{B}$. In guessing the solution, we were helped by the result given in Eq. (48), which also applies here. Letting these clues suffice, we simply indicate the result and the reader can confirm that it is a solution by differentiation. The components of $\underline{B}$ are

$$B_{rr}=-dq/dr+L^2/(r^4q^2A), \tag{72a}$$

$$B_{r\theta}=L/r^2-L/(r^3qA), \tag{72b}$$

$$B_{\theta\theta}=1/(r^2A)-q/r, \tag{72c}$$

$$B_{\phi\phi}=-q/r-L\cos\theta/(r^2\sin\theta). \tag{72d}$$

These are verified by showing that they solve Eq. (63). For example,

$$-q\,dB_{rr}/dr-(2k/r)(\hat{N}\cdot\hat{\theta})B_{r\theta}=-(B_{rr}^2+B_{r\theta}^2)-(m/\hbar^2)d^2U/dr^2. \tag{73}$$

The minus sign on the first term $(-q\,dB/dr)$ appears for the incoming part of the trajectory, because the radial velocity points toward the origin.

From Eqs. (72) for $\underline{B}$ the probability density is found to be

$$P=|\psi|^2=\text{const}/[r^2q(r)A(r)\sin\theta]. \tag{74}$$

We have not found this formula in the literature of semiclassical scattering theory (e.g., it does not appear in Ref. [10]). Equation (74) gives the prefactor for a semiclassical scattering function of the asymptotic form given in Eq. (67), which of course differs from the prefactor for partial-wave eigenfunctions.

In the asymptotic region $|\psi|^2$ is simply related to the scattering cross section. Equation (74) leads to a known semiclassical differential cross section (obtained by a different method in Ref. [10]). The agreement confirms the method given in Eqs. (63) and (64).

In summary, the semiclassical probability density changes along the particle orbits in a way controlled by the local curvature(s) of the wave fronts, and these changes are determined by a simple tensor differential equation for the wave-front curvature. The theory gives the expected result for a simple test case.

VI. APPLICATION TO NONLINEAR OPTICS

We briefly consider the possibility of calculating light propagation in a nonlinear medium.

For this purpose one must be clear about the limitations of geometrical optics and ray tracing. These methods apparently cannot easily calculate harmonic production or even fine-scale (diffraction-limited) nonlinear beam breakup. However, geometrical optics might be able to correctly model large-scale self-focusing or channel formation produced by the nonlinear index.

For this purpose the challenge is that one requires the intensity to evaluate the nonlinear part of the index of refraction. Equation (25) gives the required intensity. However, Eq. (22) asks for the gradient of the index, and to evaluate this it would be necessary to insert information about the gradient of the intensity. This is not available in a calculation that proceeds one ray at a time.

The obvious solution to this difficulty is to treat an entire wave front at once. For cylindrically symmetric systems, this is essentially the same computational and storage problem as the original ray-tracing calculation, but for the general three-dimensional case would require more computer memory. However, if one has the curvature and intensity data on one wave front, then Eqs. (22) and (25) tell one how to construct the corresponding information on the next wave front.

VII. CONCLUSION

This paper has presented the formulation of a general method for directly calculating the intensity of light in geometrical optics. The method is based on a geometrical study of wave-front curvature and the way in which the curvature evolves as light moves along a ray. The most important feature of the method is that the adjacent rays decouple enough so the intensity can be calculated *one ray at a time*, even though the intensity changes physically reflect the bunching or dispersal of rays associated with convergent or divergent beams.

Two examples show how the general equations can be solved. The equations are suitable for numerical applications, which are under way. We expect that this method will provide a simple and convenient way to obtain approximate information about the intensity of light refracted through a dense inhomogeneous fluid, potentially including effects of the index nonlinearity.

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