Mathematical Models and Methods in Applied Sciences
Vol. 11, No. 2 (2001) 199–228
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COMPUTATION OF HIGH FREQUENCY FIELDS NEAR CAUSTICS

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Communicated by P. A. Markowich
Received 18 September 1998
Revised 18 June 1999

It is well known that although the usual harmonic ansatz of geometrical optics fails near a caustic, uniform expansions can be found which remain valid in the neighborhood of the caustic, and reduce asymptotically to the usual geometric field far enough from it. Such expansions can be constructed by several methods which make essentially use of the symplectic structure of the phase space. In this paper we efficiently apply the Kravtsov–Ludwig method of relevant functions, in conjunction with Hamiltonian ray tracing to define the topology of the caustics and compute high-frequency scalar wave fields near smooth and cusp caustics. We use an adaptive Runge–Kutta method to successfully retrieve the complete ray field in the case of piecewise smooth refraction indices. We efficiently match the geometric and modified amplitudes of the multi-valued field to obtain numerically the correct asymptotic behavior of the solution. Comparisons of the numerical results with analytical calculations in model problems show excellent accuracy in calculating the modified amplitudes using the Kravtsov–Ludwig formulas.

1. Introduction

In the analysis of wave propagation in inhomogeneous media, the method of geometrical optics is often employed (see, e.g., Ref. 35). It is used not only to get a qualitative picture of how the waves propagate, but also to evaluate the fields quantitatively. However, geometrical optics fails either on caustics and focal points where it predicts infinite wave amplitudes (see Sec. 2), or in shadow regions (i.e. regions devoid of rays) where it yields zero fields. On the other hand, formation of caustics is a typical situation in underwater acoustics and seismology due to the multi-path propagation from localized sources. Indeed, even in the simplest oceanic models and geophysical structures (see, e.g. Chap. 5 of Ref. 45 and Chap. 3 of Ref. 21, respectively) a number of caustics occur, depending on the position of the source and the stratification of the wave velocities.

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From the mathematical point of view, formation of caustics and related multivaluedness of the phase function, is the main obstacle in constructing global high-frequency solutions of the Helmholtz equation. The problem of obtaining the multivalued phase function is traditionally handled by resolving numerically the characteristic field related to the eikonal equation (ray tracing methods), see, e.g. Ref. 21. A considerable amount of work has been done recently on constructing the multivalued phase function by properly partitioning the propagation domain and using eikonal solvers (see, e.g., Refs. 1, 10, 23 and 44). A different approach is based on kinetic formulation in the phase space, in terms of a density function which satisfies Liouville's equation. The technique used to capture the multivalued solutions is based on a closure assumption for a system of equations for the moments of the density.[12,43]

Given the geometry of the multivalued phase function, a number of local and uniform methods to describe wave fields near caustics have been proposed. The first type of methods is essentially based on *boundary layer* techniques as they were developed by Babich *et al.* (see, e.g., Refs. 9, 11 and 25). The second type exploits the fact that even if the family of rays has caustics, there are no such singularities for the family of the bicharacteristics in the phase space (see Definition 2.2). This basic fact allows the construction of formal asymptotic solutions (FAS) which are valid near and on the caustics. For this purpose two main asymptotic techniques have been developed. The first one, which we will present in details in Sec. 3, is the *Kravtsov–Ludwig method* (or the *method of relevant functions*).[37,40] This method starts with a modified FAS involving Airy-type integrals, the phase of which take account of the type of caustics (Sec. 3 and Appendix). The second one is the *method of canonical operator* developed by Maslov (closely related to this are the techniques of Orlov's interference integrals[3] and oscillatory spectral integrals.[4,5] Maslov's method exploits the fundamental fact that the Hamiltonian flow associated with the bichararcteristics generates a Lagrangian manifold in the phase space (see, e.g., Ref. 24), on which we can "lift" the phase function in a unique way (see, e.g., Refs. 41, 42 and 46).

Although uniform caustic asymptotics have been widely used by the acoustical and seismological community (see, e.g., Refs. 16, 18, 19 and 29 and the references therein), the problem of the limits of applicability of uniform asymptotic expressions has not been completely resolved yet, as it has been recently observed by Asatryan and Kravtsov[6] who attempted to give a qualitative answer. It seems that the quantitative answer to such a question requires first of all the numerical comparison between uniform asymptotics and ordinary geometrical optics calculations of the wave fields.

In this paper we show how to efficiently apply the Kravtsov–Ludwig method for the numerical calculation of the amplitudes of high-frequency waves near fold and cusp caustics. Comparisons of the numerical results with analytical calculations in model problems show excellent accuracy in calculating numerically the modified amplitudes entering the Kravtsov–Ludwig formulas. We use these modified amplitudes

to compute numerically the field around caustics and show that the uniform asymptotic solution matches efficiently with the ordinary geometrical optics solution far away from the caustic.

In Sec. 2 we present the necessary results from geometrical optics. The Kravtsov–Ludwig method of relevant function for fold and cusp caustics is described in Sec. 3. In Sec. 4 we present the numerical algorithm for tracing the rays and locating the caustics. In Sec. 5 we use the above algorithm in model problems and show that the asymptotic solution obtained by the method of relevant functions numerically, coincides with that obtained analytically, and it matches with the ordinary geometrical optics solution.

2. High Frequency Solutions of the Helmholtz Equation

We consider the propagation of two-dimensional time-harmonic scalar waves in a medium with variable refraction index $n(\mathbf{r}) = c_0/c(\mathbf{r})$, c_0 being the reference wave velocity and $c(\mathbf{r})$ the velocity at the point $\mathbf{r} = (x, z) \in D$, where D is some unbounded domain of $\mathbb{R}^2_{\mathbf{r}}$. We assume that $n \in C^\infty(\mathbb{R}^2_{\mathbf{r}})$ and $n > 0$. The two-dimensional wave field $u(\mathbf{r}, k)$ is governed by the *Helmholtz* equation

$$\Delta u + k^2 n^2(\mathbf{r}) u(\mathbf{r}, k) = F(\mathbf{r}), \quad \mathbf{r} \in D, \tag{2.1}$$

where $k = \omega/c_0$ is the wave number (ω being the frequency of the waves) and F represents a compactly supported source generating the waves. We are interested in the asymptotic behavior of $u(\mathbf{r}, k)$ as $k \to \infty$ (i.e. for very large frequencies ω), assuming that $\mathbf{r}$ remains in a compact subset of D and outside the support of the source function F.

Note that the asymptotic decomposition of scattering solutions when simultaneously $|\mathbf{r}|$ and k go to infinity is a rather complicated problem, as, in general, the caustics of the Lagrangian manifold go off to infinity. This problem has been rigorously studied by Vainberg,[47] when D is a full neighborhood of infinity and $n = 1$ for $|\mathbf{r}| > r_0$, r_0 being a fixed positive constant, and by Kucherenko[38] for the case of a point source (i.e. $f(\mathbf{r}) = \delta(\mathbf{r})$), under certain conditions of decay for $n(\mathbf{r})$ at infinity.

As for fixed $k > 0$ there is, in general, an infinite set of solutions of (2.1), and we need a radiation condition to guarantee uniqueness (cf. Ref. 20 for scattering by compact inhomogeneities, and Ref. 48 for scattering by stratified media). This condition is essentially equivalent to the physical fact that there is no energy flow from infinity, which in geometrical optics is translated to the requirement that the rays must go to infinity.

Definition 2.1. We say that

$$u_N(\mathbf{r}, k) = e^{ik\Phi(\mathbf{r})} \sum_{\ell=0}^{N} (ik)^{-\ell} A_\ell(\mathbf{r}), \tag{2.2}$$

where the phase Φ and the amplitudes A_ℓ are real-valued functions in $C^\infty(\mathbb{R}^2_{\mathbf{r}})$, is a formal asymptotic solution (FAS) of (2.1) if it satisfies

$$(\Delta + k^2 n^2(\mathbf{r}))u_N(\mathbf{r}, k) = O(k^{-N_1}), \quad k \to \infty, \tag{2.3}$$

where $N_1 \to \infty$ as $N \to \infty$, in a bounded domain $|x| \le a$, $|z| \le b$, a, b being positive constants.

According to the well-known WKB procedure we seek an FAS of (2.1) of the form (2.2) in $D \backslash \text{supp } F$. Substituting (2.2) into (2.3) and separating the powers $(ik)^{-\ell}, \ell = 0, 1, \ldots$, we obtain the *eikonal* equation

$$(\nabla\Phi(\mathbf{r}))^2 = n^2(\mathbf{r}), \tag{2.4}$$

for the phase function, and the following hierarchy of transport equations

$$2\nabla\Phi \cdot \nabla A_0 + \Delta\Phi(\mathbf{r})A_0(\mathbf{r}) = 0, \tag{2.5}$$

$$2\nabla\Phi \cdot \nabla A_\ell + \Delta\Phi(\mathbf{r})A_\ell(\mathbf{r}) = -\Delta A_{\ell-1}(\mathbf{r}), \qquad \ell = 1, 2, \ldots, \tag{2.6}$$

for the amplitudes.

A standard way of solving the eikonal equation (2.4) is based on the use of bicharacteristics (see, e.g., Chap. VIII of Ref. 30). Let $H(\mathbf{r}, \mathbf{p})$ be the *Hamiltonian* function

$$H(\mathbf{r}, \mathbf{p}) = \frac{1}{2}\left(|\mathbf{p}|^2 - n^2(\mathbf{r})\right), \quad \mathbf{r} \in D, \ \mathbf{p} \in \mathbb{R}^2_{\mathbf{p}}, \tag{2.7}$$

corresponding to the Helmholtz equation (2.1), where $\mathbf{p} = (p_x, p_z)$ is the momentum conjugate to the position $\mathbf{r} = (x, z)$. The associated Hamiltonian system reads as follows:

$$\frac{d\mathbf{r}}{dt} = \nabla_p H(\mathbf{r}, \mathbf{p}) = \mathbf{p}, \tag{2.8a}$$

$$\frac{d\mathbf{p}}{dt} = -\nabla_r H(\mathbf{r}, \mathbf{p}) = n(\mathbf{r})\nabla n(\mathbf{r}). \tag{2.8b}$$

Let $\mathbf{r} = \mathbf{r}^0(\theta)$, $\theta \in I \subset \mathbb{R}$, be an initial manifold U_0 in $\mathbb{R}^2_r$, and specify on it the initial conditions (for $t = 0$)

$$\mathbf{r}(0) = \mathbf{r}^0(\theta), \qquad \mathbf{p}(0) = \mathbf{p}^0(\theta), \quad \theta \in I, \tag{2.9}$$

$$\Phi(\mathbf{r}) = \Phi^0(\theta), \qquad A_l(\mathbf{r}) = A_l^0(\theta) \qquad \text{for} \qquad \mathbf{r} = \mathbf{r}^0(\theta), \tag{2.10}$$

$\mathbf{p}^0(\theta)$ and $\Phi^0(\theta), A_l^0(\theta)$ being given functions. Note that

$$|\mathbf{p}^0(\theta)|^2 = (n(\mathbf{r}^0(\theta)))^2$$

must be satisfied on the initial manifold (see, e.g., Ref. 38).

The initial manifold is chosen so that to model the source term F in the right-hand side of (2.1). In the case of a point source at $\mathbf{r}_0$, i.e. $F(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_0)$, this has

been exhaustively done by Avila and Keller[2] (see also Ref. 8). In general, the high-frequency modeling of an arbitrary source relies on a Fourier integral representation of the solution of the Helmholtz equation and a stationary-phase approximation of this in the neighborhood of supp F. This procedure has recently been applied, e.g., by Ref. 17 for calculating the local field of a linear array of acoustic transducers (side-scan sonar) and in Ref. 36 for studying the problem of high-frequency cylindrical abberations.

Definition 2.2. The trajectories $\mathbf{r} = \mathbf{r}(t, \theta)$, $\mathbf{p} = \mathbf{p}(t, \theta)$, $t \in \mathbb{R}$, $\theta \in I$, which solve the initial value problem (2.8), (2.9) in the phase space $\mathbb{R}^4_{rp}$ are called bicharacteristics and their projection $\mathbf{r} = \mathbf{r}(\tau, \theta)$, $t \in \mathbb{R}$, $\theta \in I$ onto $\mathbb{R}^2_r$ are called rays.

Assuming that $\mathbf{p}^0(\theta)$ is nowhere tangent to $\mathbf{r}^0(\theta)$, the solution of the (noncharacteristic) Cauchy problem (2.4), (2.10) for the eikonal equation, is given by

$$\Phi(\mathbf{r}(t, \theta)) = \Phi^0(\theta) + \int_0^t \mathbf{p}(\tau, \theta) \frac{d\mathbf{r}(\tau, \theta)}{d\tau} d\tau \,, \tag{2.11}$$

where the integral is calculated along the bicharacteristics. The transformation

$$(t, \theta) \mapsto (x(t, \theta), z(t, \theta)) \,, \tag{2.12}$$

is one-to-one, provided that the Jacobian

$$J = \begin{vmatrix} \dfrac{dx}{dt} & \dfrac{dx}{d\theta} \\ \dfrac{dz}{dt} & \dfrac{dz}{d\theta} \end{vmatrix} \,, \tag{2.13}$$

is nonzero. Although $J \neq 0$ for $t = 0$, it does not necessarily remain nonzero for all t. Whenever $J = 0, (t, \theta)$ may be nonsmooth or multivalued functions of (x, z), and the rays may intersect, overlap, etc., and in general have singularities (although the bicharacteristics never intersect in the phase space). Then, the phase function $\Phi = \Phi(x, z)$ may be a multivalued or a nonsmooth function.

The solution of the transport equation (2.5) for the principal amplitude A_0 on the rays is given by

$$A_0(\mathbf{r}(t, \theta)) = \frac{\alpha_0(\theta)}{\sqrt{J(t, \theta)}} \,, \tag{2.14}$$

where $\alpha_0(\theta) = A_0^0(\theta)$ is the amplitude at the point $\mathbf{r} = \mathbf{r}^0$ on the initial manifold, and $J(t, \theta)$ is the value of the Jacobian, so that $\mathbf{r} = (x(t, \theta), z(t, \theta))$ for the considered time. Note that the amplitude (2.14) is calculated integrating the transport equation (2.5) along the rays.

Definition 2.3. The points $\mathbf{r} = \mathbf{r}(t, \theta)$ at which $J(t, \theta) = 0$ are called focal points, and the manifold generated from these points (i.e. the envelope of the family of the rays) is called caustic.

The amplitude A_0 calculated by (2.14), blows up on the caustics and therefore the WKB procedure fails to predict the correct amplitudes there. Fortunately, the caustics only appear as apparent singularities when we apply the WKB procedure, and as we already mentioned in the Introduction, it is possible to construct uniform solutions which remain finite on the caustics.

3. Kravtsov–Ludwig Method of Relevant Functions

3.1. *Motivation*

The idea of obtaining global high-frequency solutions of the Helmholtz equation (2.1) by the method of relevant functions, is to replace (2.2) by an integral of the form (see, e.g., Refs. 22, 37 and 40)

$$u(\mathbf{r}) = \left(\frac{ik}{2\pi}\right)^{1/2} \int_{\Xi} e^{ikS(\mathbf{r},\xi)} a(\mathbf{r},\xi)\, d\xi\,, \qquad \xi \in \Xi \subset \mathbb{R}_\xi\,. \tag{3.1}$$

Here S and a satisfy the eikonal equation (2.4) and the transport equation (2.5), respectively, identically with respect to ξ. Such an integral can be regarded as a continuous superposition of oscillatory functions of the form (2.2). The physical motivation underlying the method of relevant functions is the fact that in every small region in which the refraction index of the medium can be considered as constant and the wave front as plane, the field can be represented as a superposition of plane waves ae^{iS}, where a and ∇S vary slowly in transition from one region to the next.

In the case of single phase geometrical optics we can take $S(\mathbf{r},\xi) = \phi(\mathbf{r}) - \xi^2$. Then the only stationary point $\xi = 0$ is simple and by stationary phase lemma (see, e.g., p. 219 of Ref. 13), the oscillatory integral (3.1) reduces asymptotically to (2.2). If there are more than one simple stationary point $\xi_j(\mathbf{r})$, i.e. $\partial_\xi S(\mathbf{r},\xi_j(\mathbf{r})) = 0$ and $\partial_\xi^2 S(\mathbf{r},\xi_j(\mathbf{r})) \neq 0$, we have the asymptotic expansion

$$u(\mathbf{r}) \sim \sum_j A_0^j(\mathbf{r}) e^{ikS_j(\mathbf{r})}\,, \tag{3.2}$$

where

$$S_j(\mathbf{r}) = S(\mathbf{r},\xi_j(\mathbf{r})) \tag{3.3a}$$

and

$$A_0^j(\mathbf{r}) = \exp\left(i\left(\frac{\pi}{2} + \operatorname{sgn}(\partial_\xi^2 S(\mathbf{r},\xi_j(\mathbf{r})))\right)\right) \frac{a(\mathbf{r},\xi_j(\mathbf{r}))}{\sqrt{|\partial_\xi^2 S(\mathbf{r},\xi_j(\mathbf{r}))|}}\,, \tag{3.3b}$$

and the summation in (3.2) extends over all the stationary points. The amplitudes A_0^j are solutions of the zero-order transport equation (2.5).

The expansion fails whenever $\partial_\xi^2 S(\mathbf{r},\xi_j(\mathbf{r})) = 0$, i.e. for the stationary points of multiplicity greater than one, and in this case a modified stationary phase lemma must be applied (p. 222 of Ref. 13). The appearance of multiple stationary points is

associated with the formation of caustics. Near caustics the phase is a multivalued function and, in general, it cannot be derived by integration using (2.11). Representation theorems for the phase function S are derived by the methods of singularity theory (see, e.g., Ref. 7), according to the type of caustic appearing. For simple caustics (fold, cusp), these results are briefly presented in the Appendix.

3.2. *Smooth caustic (fold)*

It can be shown that near a smooth caustic (fold) the correct form of the phase is (see Appendix; also Proposition 6.1 of Ref. 26, and Ref. 37)

$$S(\mathbf{r},\xi) = \phi(\mathbf{r}) + \xi\rho_1(\mathbf{r}) - \frac{\xi^3}{3}\,, \tag{3.4}$$

and the amplitude admits the decomposition

$$a(\mathbf{r},\xi) = g_0(\mathbf{r}) + \xi g_1(\mathbf{r}) + h(\mathbf{r},\xi)\partial_\xi S(\mathbf{r},\xi)\,, \tag{3.5}$$

where $h(\mathbf{r},\xi)$ is a smooth function. Substituting (3.4) and (3.5) into (3.1), applying the stationary phase lemma for $k \to \infty$ to get rid of the third term in (3.5), and using the standard integral representation of the Airy function Ai(.) (see, e.g., Ref. 39), we obtain the asymptotic expansion

$$\begin{aligned} u(\mathbf{r}) &= \sqrt{2\pi}k^{1/6}e^{i\pi/4}e^{ik\phi(\mathbf{r})} \\ &\quad\times\Big(g_0(\mathbf{r})\mathrm{Ai}(-k^{2/3}\rho_1(\mathbf{r})) + ik^{-1/3}g_1(\mathbf{r})\mathrm{Ai}'(-k^{2/3}\rho_1(\mathbf{r}))\Big) + O(k^{-1})\,. \end{aligned} \tag{3.6}$$

Using the asymptotic expansion of the Airy function for large negative argument, we obtain from (3.6) for $\rho_1 \neq 0$ and $k \to \infty$, the expansion

$$\begin{aligned} u(\mathbf{r}) &= \frac{1}{\sqrt{2}}\left(g_0(\mathbf{r}) + g_1(\mathbf{r})\sqrt{\rho_1(\mathbf{r})}\right)\rho_1^{-1/4}e^{ik\tilde{S}_+(\mathbf{r})} \\ &\quad + \frac{1}{\sqrt{2}}\left(g_0(\mathbf{r}) - g_1(\mathbf{r})\sqrt{\rho_1(\mathbf{r})}\right)\rho_1^{-1/4}e^{ik\tilde{S}_-(\mathbf{r})}e^{i\pi/2}\,, \end{aligned} \tag{3.7}$$

where

$$\tilde{S}_\pm(\mathbf{r}) = S(\mathbf{r},\xi_\pm(\mathbf{r})) = \phi(\mathbf{r}) \pm \frac{2}{3}\rho_1^{3/2}(\mathbf{r}) \tag{3.8}$$

are the values of the phase function at the points $\xi_\pm(\mathbf{r}) = \pm\sqrt{\rho_1(\mathbf{r})}$, i.e. the roots of the stationary phase equation $\partial_\xi S(\mathbf{r},\xi) = 0$. On the other hand, if two rays, which pass through any point M in the region of the fold (Fig. 1), are far enough from the caustic, the geometrical optics expansion has the form

$$u(\mathbf{r}) = A_+(\mathbf{r})e^{ik\Phi_+(\mathbf{r})} + A_-(\mathbf{r})e^{ik\Phi_-(\mathbf{r})}\,, \tag{3.9}$$

where $\Phi_\pm(\mathbf{r})$ are the geometrical phases. The symbol $(-)$ (respectively $(+)$) indicates the ray which arrives at M directly from the initial manifold (respectively, after "reflection" from the caustic). $A_\pm$ are the values of the zeroth-order amplitudes

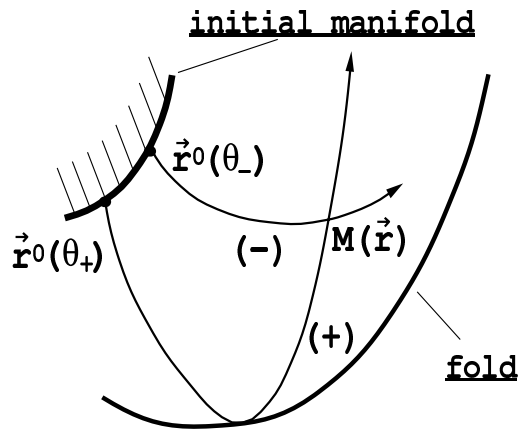

Fig. 1. The geometry of a fold caustic.

A_0 (see Eq. (2.5)) computed along the $(\pm)$ rays. Therefore, the geometrical amplitudes $A_\pm(\mathbf{r})$ solve the transport equations (2.5), and, according to (2.14), they are given by

$$A_\pm(\mathbf{r}) = \frac{\alpha_0(\theta_\pm)}{\sqrt{J_\pm(\mathbf{r})}}\,, \tag{3.10}$$

where $\theta_\pm = \theta_\pm(\mathbf{r})$ are the values of the parameter at the initial manifold corresponding to the rays $(\pm)$ passing from M, $\alpha_0(\theta_\pm)$ are the corresponding initial amplitudes, and $J_\pm(\mathbf{r})$ are the values of the Jacobian at the point $\mathbf{r}$ calculated along the $(\pm)$ rays. The value of the square root $\sqrt{J_\pm}$ is calculated by the formula $\sqrt{J_\pm} = \sqrt{|J_\pm|}e^{i(\pi/2)\gamma_\pm}$ where $\gamma_+ = 1$ and $\gamma_- = 0$. Note that $\gamma_\pm$ counts the number of tangencies of the rays with the caustic along their course from the points $\mathbf{r}_0(\theta_\pm)$ on the initial manifold to the point M. The geometrical phases $\Phi_\pm(\mathbf{r})$ in (3.9) are computed by integration along the rays using (2.11).

According to the matching principle, the expansions (3.7) and (3.9) must coincide away from the caustic. From the matching conditions for the amplitudes

$$\frac{1}{\sqrt{2}}\left(g_0(\mathbf{r}) + g_1(\mathbf{r})\sqrt{\rho_1(\mathbf{r})}\right)\rho_1^{-1/4} = A_+(\mathbf{r})\,, \tag{3.11a}$$

$$\frac{1}{\sqrt{2}}\left(g_0(\mathbf{r}) - g_1(\mathbf{r})\sqrt{\rho_1(\mathbf{r})}\right)\rho_1^{-1/4}e^{i\pi/2} = A_-(\mathbf{r})\,, \tag{3.11b}$$

we obtain the modified amplitudes

$$g_0(\mathbf{r}) = \frac{\rho_1^{1/4}}{\sqrt{2}}(A_+(\mathbf{r}) - iA_-(\mathbf{r}))\,, \tag{3.12a}$$

$$g_1(\mathbf{r}) = \frac{\rho_1^{-1/4}}{\sqrt{2}}(A_+(\mathbf{r}) + iA_-(\mathbf{r}))\,. \tag{3.12b}$$

The functions ϕ and ρ_1 are found from the matching condition of the phases $\tilde{S}_\pm(\mathbf{r}) = S_\pm(\mathbf{r})$, and they are given by

$$\phi(\mathbf{r}) = \frac{1}{2}(\Phi_+(\mathbf{r}) + \Phi_-(\mathbf{r})) \quad \text{and} \quad \rho_1(\mathbf{r}) = \left(\frac{3}{4}(\Phi_+(\mathbf{r}) - \Phi_-(\mathbf{r}))\right)^{2/3}. \tag{3.13}$$

3.3. *The cusp caustic*

In the case of a cusp caustic the phase function must have the form (GS, Proposition 7.1 for $k = 4$ of Ref. 26, and Ref. 37)

$$S(\mathbf{r}, \xi) = \phi(\mathbf{r}) + \rho_1(\mathbf{r})\xi - \rho_2(\mathbf{r})\frac{\xi^2}{2} + \frac{\xi^4}{4}, \tag{3.14}$$

and the amplitude admits the representation

$$a(\mathbf{r}, \xi) = g_0(\mathbf{r}) + \xi g_1(\mathbf{r}) + \xi^2 g_2(\mathbf{r}) + f(\mathbf{r}, \xi)\partial_\xi S(\mathbf{r}, \xi), \tag{3.15}$$

where $f(\mathbf{r}, \xi)$ is a smooth function. Note that again by the stationary phase formula we will get rid of the third term in (3.15). The stationary points $\xi_j(\mathbf{r})$ are the roots of the cubic equation

$$\partial_\xi S(\mathbf{r}, \xi) = \rho_1(\mathbf{r}) - \rho_2(\mathbf{r})\xi + \xi^3 = 0, \tag{3.16}$$

and they are given by the formulas

$$\xi_1(\rho_1, \rho_2) = A + B, \tag{3.17a}$$

$$\xi_2(\rho_1, \rho_2) = -\frac{1}{2}(A + B) + i\frac{\sqrt{3}}{2}(A - B), \tag{3.17b}$$

$$\xi_3(\rho_1, \rho_2) = -\frac{1}{2}(A + B) - i\frac{\sqrt{3}}{2}(A - B), \tag{3.17c}$$

with

$$A = \left(\frac{\rho_1}{2} + \sqrt{D}\right)^{1/3}, \qquad B = \left(\frac{\rho_1}{2} - \sqrt{D}\right)^{1/3} \tag{3.17d}$$

and

$$D = \frac{\rho_1^2}{4} - \frac{\rho_2^3}{27}. \tag{3.17e}$$

From (3.17e) it follows that there are three real stationary points in Region I, a double one on the sides of the cusp, and a triple one, equal to zero, at the "beak" of the cusp, and only one real stationary point in Region II (Fig. 2). Regions I and II are separated by the cusp which is the locus of multiple (double or triple) roots of (3.16), i.e. the points where

$$\rho_1^2 = \frac{4\rho_2^3}{27}. \tag{3.18}$$

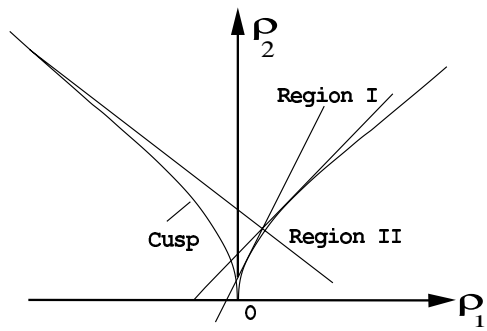

Fig. 2. The geometry of a cusp caustic.

Note that each real stationary point corresponds to a ray, and therefore there are three rays passing through any point inside the cusp (Region I) and only one ray through each point outside the cusp (Region II). At the sides of the cusp the double stationary point corresponds to a pair of coalescing rays tangent to the caustic, while the third one corresponds to the ray crossing the caustic transversely. Finally, at the "beak" of the caustic (3.18), the triple stationary point, equal to zero, corresponds to the three rays coalescing at this point.

Again according to the matching principle, we apply the stationary phase lemma for the integral (3.1) with phase (3.14) (see, e.g., p. 221 of Ref. 13, Chap. VII of Ref. 49), and we match the obtained amplitudes and phases with the geometrical ones. From the matching of the amplitudes we obtain the system

$$\begin{aligned} g_0(\mathbf{r}) + \xi_j g_1(\mathbf{r}) + \xi_j^2 g_2(\mathbf{r}) &= A_j(\mathbf{r})(\partial_\xi^2 S(\mathbf{r}, \xi_j(\mathbf{r})))^{1/2} \\ &= A_j(\mathbf{r})(3\xi_j^2(\mathbf{r}) - \rho_2(\mathbf{r}))^{1/2}\,, \quad j = 1, 2, 3\,, \end{aligned} \tag{3.19}$$

where $A_j(\mathbf{r})$ are the geometrical amplitudes calculated using (2.14) by the formula

$$A_j(\mathbf{r}) = \frac{\alpha_0(\theta_j)}{\sqrt{J_j(\mathbf{r})}}\,. \tag{3.20}$$

Here θ_j are the values of the parameter at the initial manifold corresponding to the jth ray, while $\alpha_0(\theta_j)$ is the corresponding initial amplitude and $J_j(\mathbf{r})$ is the value of the Jacobian calculated for the jth ray.

From the matching of the phases $\tilde{S}_j(\phi, \rho_1, \rho_2) = S(\mathbf{r}, \xi_j(\rho_1, \rho_2))$ with the geometrical phases $\Phi_j(\mathbf{r})$ which are computed by (2.11) along the jth ray ($j = 1, 2, 3$), we obtain

$$\begin{aligned} \tilde{S}(\phi, \rho_1, \rho_2) &= \phi(\mathbf{r}) + \rho_1 \xi_j(\rho_1, \rho_2) - \rho_2 \frac{\xi_j^2(\rho_1, \rho_2)}{2} + \frac{\xi_j^4(\rho_1, \rho_2)}{4} \\ &= \Phi_j(\mathbf{r})\,, \qquad j = 1, 2, 3\,. \end{aligned} \tag{3.21}$$

Solving the nonlinear system (3.21) for $\rho_1(\mathbf{r})$, $\rho_2(\mathbf{r})$ and $\phi(\mathbf{r})$, and thereafter calculating $\xi_j(\mathbf{r}) = \xi_j(\rho_1(\mathbf{r}), \rho_2(\mathbf{r}))$ from the relations (3.17a)–(3.17c), we compute

the modified amplitudes g_0, g_1, g_2 from the linear system (3.19). It can be shown using (3.20) and the system (3.19), that the modified amplitudes g_0, g_1 and g_2 remain finite on the caustic.[40]

Introducing the *Pearcey's integral* (generalized Airy function)

$$Y_0(-a,b) = \int_{\mathbb{R}} \exp\left(i\left(\frac{t^4}{4} - a\frac{t^2}{2} + bt\right)\right) dt\,, \tag{3.22}$$

and using (3.1), (3.14) and (3.15) we obtain the asymptotic expansion

$$\begin{aligned} u(\mathbf{r}) = {} & (2\pi)^{-1/2} e^{i\pi/4} e^{ik\phi(\mathbf{r})} (g_0(\mathbf{r}) k^{1/4} Y_0(-a,b) - ik^{-1/2} g_1(\mathbf{r}) \partial_b Y_0(-a,b) \\ & + 2ik^{-1/2} g_2(\mathbf{r}) \partial_a Y_0(-a,b)) + O(k^{-1})\,, \qquad k \to \infty\,, \end{aligned} \tag{3.23}$$

where we have put

$$a = k^{1/2}\rho_2 \qquad \text{and} \qquad b = k^{3/4}\rho_1\,. \tag{3.24}$$

Note that

$$b = \mu a^{3/2}\,, \qquad \mu = \frac{\rho_1}{\rho_2^{3/2}}\,. \tag{3.25}$$

Here μ plays the role of the uniformity parameter for the uniform asymptotic expansion of Y_0 constructed by Kaminski,[33] and it provides a measure of the distance of the point (ρ_1, ρ_2) from the caustic, where μ takes the value $\mu_c = 2/\sqrt{27}$.

The stable numerical computation of the modified amplitudes g_0, g_1 by (3.11) and of g_0, g_1 and g_2 through the solution of the linear system (3.19) is, in general, a nontrivial task, since the geometrical amplitudes $A_\pm$ and $A_j, j = 1,2,3$ blowup on the caustics, and their singularities must eventually cancel in the course of numerical computation to obtain the correct field. Besides that, possible numerical errors in locating the caustic can further introduce instabilities in the computations. The last task is successfully dealt with using the procedure described in the next section.

4. Numerical Ray Tracing and Caustic Location

A crucial step for applying the Kravtsov–Ludwig method is to locate the caustic. Recall that by Definition 2.3 the caustic is the locus of points where $J = 0$. It follows from (2.13) that the Hamiltonian system (2.8) is not sufficient to evaluate the Jacobian J. Differentiating this system with respect to the parameter θ we obtain

$$\frac{d}{dt}\left(\frac{d\mathbf{r}}{d\theta}\right) = \nabla_p \nabla_x H(\mathbf{r},\mathbf{p}) \frac{d\mathbf{r}}{d\theta} + \nabla_p \nabla_p H(\mathbf{r},\mathbf{p}) \frac{d\mathbf{p}}{d\theta}\,, \tag{4.1a}$$

$$\frac{d}{dt}\left(\frac{d\mathbf{p}}{d\theta}\right) = -\nabla_x \nabla_x H(\mathbf{r},\mathbf{p}) \frac{d\mathbf{r}}{d\theta} - \nabla_x \nabla_p H(\mathbf{r},\mathbf{p}) \frac{d\mathbf{p}}{d\theta}\,. \tag{4.1b}$$

Therefore, we must consider (2.8) together with (4.1a), (4.1b), i.e. the following system of ordinary differential equations

$$\begin{cases} \dfrac{dx}{dt} = p_x & \dfrac{dp_x}{dt} = \dfrac{1}{2}\dfrac{\partial \varepsilon}{\partial x}\,, \\ \dfrac{dz}{dt} = p_z & \dfrac{dp_z}{dt} = \dfrac{1}{2}\dfrac{\partial \varepsilon}{\partial z}\,, \\ \dfrac{dX}{dt} = P & \dfrac{dP}{dt} = \dfrac{1}{2}\left(\dfrac{\partial^2 \varepsilon}{\partial x^2}X + \dfrac{\partial^2 \varepsilon}{\partial x \partial z}Z\right)\,, \\ \dfrac{dZ}{dt} = Q & \dfrac{dQ}{dt} = \dfrac{1}{2}\left(\dfrac{\partial^2 \varepsilon}{\partial z \partial x}X + \dfrac{\partial^2 \varepsilon}{\partial z^2}Z\right)\,, \end{cases} \tag{4.2}$$

where $\varepsilon = n^2$ and

$$X = \frac{dx}{d\theta}\,, \qquad Z = \frac{dz}{d\theta}\,, \qquad P = \frac{dp_x}{d\theta}\,, \qquad Q = \frac{dp_z}{d\theta}\,,$$

which is subjected to the initial conditions

$$\begin{aligned} x(0) &= x_0(\theta)\,, & p_x(0) &= p_{0x}(\theta)\,, \\ z(0) &= z_0(\theta)\,, & p_z(0) &= p_{0z}(\theta)\,, \\ X(0) &= 0\,, & P(0) &= \frac{dp_{0x}(\theta)}{d\theta}\,, \\ Z(0) &= 0\,, & Q(0) &= \frac{dp_{0z}(\theta)}{d\theta}\,. \end{aligned} \tag{4.3}$$

$p_{0x}(\theta)$ and $p_{0z}(\theta)$ being the components of the vector $\mathbf{p}^0(\theta)$, and $x_0(\theta), z_0(\theta)$ being the components of $\mathbf{r}^0(\theta)$ (see Eq. (2.9)).

In the special case of a point source, the geometrical optics solution near a point source has been constructed by Avila and Keller,[2] combining the WKB method with the boundary layer technique to deal with the peculiarities of the two-dimensional case. For a point source located at the point (x_0, z_0), the appropriate initial conditions are

$$\begin{aligned} x(0) &= x_0\,, & p_x(0) &= n_0 \cos\theta\,, \\ z(0) &= z_0\,, & p_z(0) &= n_0 \sin\theta\,, \\ X(0) &= 0\,, & P(0) &= -n_0 \sin\theta\,, \\ Z(0) &= 0\,, & Q(0) &= n_0 \cos\theta\,, \end{aligned} \tag{4.4}$$

where θ is the shooting angle of the ray (i.e. the polar angle at the source point (x_0, z_0)), and $n_0 = n(x_0, z_0)$ is the value of the refraction index at the source. The numerical solution of the above system gives us the points of the rays $(x(t,\theta), z(t,\theta))$ as well as the values of the derivatives $X(t,\theta), Z(t,\theta)$. The caustic is identified as the locus of the points $(x(t,\theta), z(t,\theta))$ where $J(t,\theta) = p_x Z - X p_z = 0$.

The system (4.2), (4.4) cannot be solved analytically for a general refraction index n^2, although this is possible in some important special situations (see the examples in Sec. 5). Therefore, we have to rely on direct numerical methods to solve it.

For a given θ, that is along a fixed ray, the system (4.2), (4.3) becomes a standard initial-value problem (IVP), the solution of which can in general be approximated using Runge–Kutta (RK) methods for marching with respect to t. These methods have excellent stability properties which, as follows from several numerical experiments,[34] are extremely important for defining with accuracy the topology of the caustics, especially when the refraction index n^2 has discontinuous derivatives. It has been observed that when the refraction index has continuous derivatives, the *Standard RK*-method (SRK) gives satisfactory results. However, in the case where n^2 has discontinuous derivatives, it is necessary to apply an adaptive RK-method (ARK), since (SRK) fails to produce an adequate solution.

For locating numerically the caustic we proceed as follows. We choose a sufficiently large time interval $[0, T]$ and a wide sector of initial angles $[\theta_I, \theta_F]$, which depend, in general, on the ray picture obtained by the ray tracing. For fixed positive integers M, N and $\Delta t = T/N$ and $\Delta\theta = (\theta_F - \theta_I)/M$, we define the partition

$$\Omega_{N,M} = \{(t_n, \theta_m)\,,\ t_n = n\Delta t\,,\ \theta_m = \theta_I + m\Delta\theta\,,\ n = 0, \ldots, N\,,\ m = 0, \ldots, M\}\ ,$$

of $\Omega = [0, T] \times [\theta_I, \theta_F]$. Then, solving the IVP in the interval $0 \le t \le T$, for any fixed θ_m in our partition, we find the points $x_{mn} = x(t_n, \theta_m)$, $z_{mn} = z(t_n, \theta_m)$ of the rays, and the corresponding quantities X_{mn}, Z_{mn}, P_{mn}, Q_{mn} to compute the value of the Jacobian $J_{mn} = J(t_n, \theta_m)$ at the point $x_{mn},\ z_{mn}$. To locate the caustic we collect the points where $|J_{mn}| \le \delta$, the tolerance δ being a small number, which in general depends on the smoothness of the refraction index. In the case of a fold caustic, this condition is satisfied by taking a sufficiently fine grid in time, that is taking large enough N. However, in the case of a cusp this simple approach requires an extremely large value of N, which makes the whole computation slow and inefficient. Thus we are led to a different approach which is based on the fact that J changes sign whenever the ray intersects the caustic. More specifically, let t_b and $t_a = t_b + \Delta t$ be two points in our partition, such that $J(t_b) > 0$ and $J(t_a) < 0$, i.e. the ray intersects the caustic, for some t_0 in the interval (t_b, t_a), and J has a zero for $t = t_0$. At this point we can follow two different ways. Either we introduce a partition for the interval (t_b, t_a) and solve again the IVP to get a more accurate approximation of the root of J, or we apply a root-finding algorithm, like the bisection method, to locate the zero of J up to a desired accuracy in (t_b, t_a). It turns out from several numerical experiments we have done that the second way works much better in capturing the caustics in relatively complicated stratified media.

In order to test the efficiency of our ray tracing and caustic identification code, we have compared our results with analytical ones for various continuous profiles $n^2(z)$ which however have discontinuous derivative at $z = 0$ (weak interface). For example, in Figs. 3 and 4 we show the results of the numerical ray tracing for

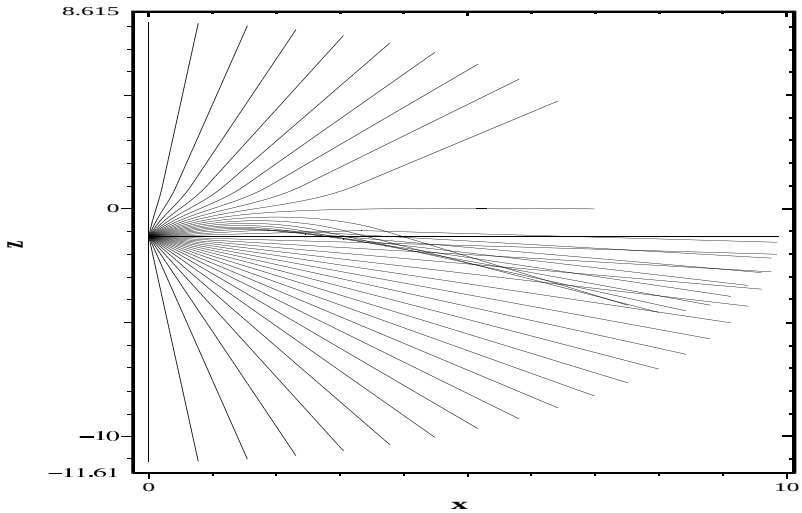

Fig. 3. Rays from a point source.

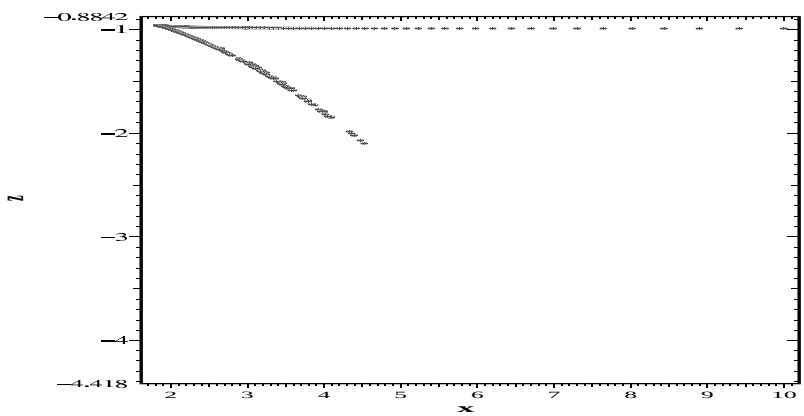

Fig. 4. Caustic located by ARK algorithm.

the rays and the caustic generated by a point source at $z = z_0$ in a medium with refraction index

$$n^2(z) = \begin{cases} 1\,, & z \le 0\,, \\ (1 + az)^{-2}\,, & |z| \ge 0 \end{cases}$$

for $z_0 = -1.25$ and $a = 0.5$. In this case, SRK fails to capture any points of the caustic, while ARK can efficiently locate the cusp shown in Fig. 4, which is clearly suggested by the ray pattern in Fig. 3. It should be emphasized that the rays and the caustics traced are in excellent accuracy numerically with those plotted using their analytical parametric equations.

5. Examples

In this section we analyze two models in order to show that the Geometrical Optics (GO) and the Kravtsov–Ludwig (KL) solutions match each other far away from the caustic for high enough frequency. In these examples most of the necessary calculations for computing the modified amplitudes entering the KL formula can be performed analytically. In this way we are able to compare the results obtained by direct numerical computation of the modified amplitudes with those obtained by analytical computation of these amplitudes and to ensure the accuracy of our computations for the high frequency field.

Example 5.1. (Linear layer[37]). We consider the field generated by a point source at $(x, z) = (0, z_0)$ in a stratified medium, occupying the half-space $z \leq d$, with refraction index which increases linearly off its boundary, i.e.

$$n^2(z) = 1 - \frac{z}{d}\,, \qquad z \leq d\,, \qquad d > 0\,. \tag{5.1}$$

In this case the system (4.2) with initial conditions (4.4) can be easily solved to derive the parametric equations of the rays

$$x(t, \theta) = n_0 t \cos\theta\,, \tag{5.2a}$$

$$z(t, \theta) = -\frac{1}{4d} t^2 + n_0 t \sin\theta + z_0\,, \tag{5.2b}$$

where $n_0 = \sqrt{1 - z_0/d}$. Eliminating the parameter t from (5.2a), (5.2b) we find the Cartesian equation of the rays

$$z(x, \theta) = -\frac{1}{4(d - z_0)\cos^2\theta} x^2 + x \tan\theta + z_0 \tag{5.2c}$$

parametrized with the initial angle θ of the ray. In the sequel we put $H = d - z_0$. As the field is symmetric with respect to the z-axis, we consider only the rays in the half-plane $x > 0$, i.e. those with initial angle $-\pi/2 < \theta < \pi/2$.

The turning points of the rays are defined from the condition $p_z = dz/dt = 0$, which implies $t_{ud} = 2dn_0 \sin\theta$ (the subscript ud means that the rays turn downwards), and they are given by

$$x_{ud} = 2H \sin\theta \cos\theta \tag{5.3a}$$

$$z_{ud} = z_0 + H \sin^2\theta\,, \qquad 0 < \theta < \pi/2\,. \tag{5.3b}$$

Obviously $z_{ud} \leq d$ for any $\theta \in (0, \pi/2)$, and therefore only the ray with angle $\theta = \pi/2$ reaches the boundary $z = d$.

The Jacobian (2.13) takes the form

$$J(\tau, \theta) = n_0 \left(1 - t\frac{\sin\theta}{2dn_0}\right) t\,, \tag{5.4}$$

and it vanishes for $t = 0$ which corresponds to the point source, and for $t = 2dn_0/\sin\theta$ which corresponds to the caustic. The parametric equations of the caustic are

$$x_c(\theta) = \frac{2H}{\tan\theta}\,, \tag{5.5a}$$

$$z_c(\theta) = 2H\left(1 - \frac{1}{2\sin^2\theta}\right) + z_0\,, \tag{5.5b}$$

and therefore the caustic is the parabola (fold)

$$z_c(x) = d - \frac{x^2}{4H}\,. \tag{5.5c}$$

From (5.2c) we see that the rays from the source $(0, z_0)$ with angles $\theta_\pm$ satisfying

$$\tan\theta_\pm = \frac{2H}{x}\left\{1 \pm \left[1 - \frac{x^2}{4H^2} - \frac{z - z_0}{H}\right]^{1/2}\right\}, \tag{5.6}$$

pass through the point (x, z) at

$$t_\pm = 2\sqrt{2}\left\{1 - \frac{z - z_0}{H} \pm \left[1 - \frac{x^2}{4H^2} - \frac{z - z_0}{H}\right]^{1/2}\right\}^{1/2}\sqrt{\frac{H}{d}}\,. \tag{5.7}$$

The corresponding values of the Jacobian J are

$$J_\pm = \tau_\pm\left(1 - \frac{z - z_0}{2H} - \frac{\tau_\pm^2}{8H^2}\right), \tag{5.8}$$

where $\tau_\pm = n_0 t_\pm$. Putting

$$f_\pm = 1 - \frac{z - z_0}{2H} \pm \frac{R}{2H}\,, \qquad R^2 = x^2 + (z - z_0)^2\,, \tag{5.9}$$

we have

$$\tau_\pm = 2H\left(\sqrt{f_+} \pm \sqrt{f_-}\right) \tag{5.10}$$

and

$$J_\pm = \mp 2H\left(f_+\sqrt{f_-} \pm f_-\sqrt{f_+}\right)\,. \tag{5.11}$$

Note that in the illuminated zone we have $\tau_\pm > 0$ and $\tau_+ > \tau_-$. Also, since $f_+ > 0$ and $f_+ f_- = 0$ on the caustic, it follows that $f_- = 0$ there. The choice of the $\pm$ indices is made according to the convention introduced in Sec. 3 for the rays approaching or leaving the fold. Therefore, J_- must be positive since the corresponding ray has not intersected the caustic yet.

The phase function is given by

$$\begin{aligned}\Phi(x,z)-\Phi(0,z_0) &= \int_0^\tau n^2(z(t,\theta))\,dt \\ &= \int_0^\tau \left(1-\frac{1}{H}\left(-\frac{t^2}{4H}+t\sin\theta+z_0\right)\right)dt \\ &= \tau\left\{\left(1-\frac{z-z_0}{2H}\right)-\frac{\tau^2}{24H^2}-\frac{z_0}{H}\right\}. \end{aligned} \tag{5.12}$$

Using the initial condition $\Phi(0,z_0)=0$, we obtain the two phases

$$\Phi_+(x,z)=\frac{2H}{3}(f_+^{3/2}+f_-^{3/2})-2z_0\left(\sqrt{f_+}+\sqrt{f_-}\right), \tag{5.13a}$$

$$\Phi_-(x,z)=\frac{2H}{3}(f_+^{3/2}-f_-^{3/2})-2z_0\left(\sqrt{f_+}-\sqrt{f_-}\right). \tag{5.13b}$$

Using Eqs. (3.8) we compute the quantities

$$\phi(x,z)=\frac{2H}{3}f_+^{3/2}-2z_0\sqrt{f_+}, \tag{5.14a}$$

$$\rho_1(x,z)=\left(Hf_-^{3/2}-3z_0\sqrt{f_-}\right)^{2/3} \tag{5.14b}$$

and substitute into KL formula (3.6). We observe that, in fact, $\rho_1=0$ on the caustic since $f_-=0$ implies $\Phi_-=\Phi_+=\phi$ there.

In the sequel for simplicity we assume that $z_0=0$ (then $H=d$ and $n_0=1$). From (3.12) we find the geometrical amplitudes

$$A_+=\frac{-i\alpha_0}{\sqrt{\tau}_+(f_+f_-)^{1/4}}, \tag{5.15a}$$

$$A_-=\frac{\alpha_0}{\sqrt{\tau}_-(f_+f_-)^{1/4}}, \tag{5.15b}$$

and using (3.11) we calculate the modified amplitudes

$$g_0=\frac{-iH^{1/6}\alpha_0}{\sqrt{2}f_+^{1/4}}\left(\frac{1}{\sqrt{\tau}_+}+\frac{1}{\sqrt{\tau}_-}\right), \tag{5.16a}$$

$$g_1=\frac{iH^{1/6}\alpha_0}{\sqrt{2}f_+^{1/4}}\frac{1}{f_-^{1/2}}\left(\frac{1}{\sqrt{\tau}_+}-\frac{1}{\sqrt{\tau}_-}\right). \tag{5.16b}$$

It can be easily seen from (5.16a) that g_0 remains finite on the caustic, and the same holds for g_1 since

$$\frac{1}{\sqrt{\tau}_+}-\frac{1}{\sqrt{\tau}_-}=\frac{-4H\sqrt{f}_-}{\sqrt{\tau_+\tau_-}(\tau_++\tau_-)}$$

and

$$g_1 = \frac{iH^{-1/6}\alpha_0}{\sqrt{2}f_+^{1/4}} \frac{-4H}{\sqrt{\tau_+\tau_-}(\sqrt{\tau_+}+\sqrt{\tau_-})}\,. \tag{5.17}$$

In order to define the initial amplitude at the source, which should be independent of the polar angle θ because of the local symmetry of the field, we approximate (5.16a) and (5.16b) for small R, and we find that near the source

$$A_- \sim \frac{\alpha_0}{\sqrt{R}} \qquad \text{and} \qquad \Phi_- \sim R\,, \tag{5.18}$$

while A_+ remains bounded. Then, the expansion (3.9) leads to the near source approximation

$$u \sim A_- e^{ikS_-} \sim \alpha_0 \frac{e^{ikR}}{\sqrt{R}}\,. \tag{5.19}$$

On the other hand, according to the high-frequency approximation of the point-source field constructed in Ref. 2 (see also Ref. 9), the solution near the source has the asymptotic expansion

$$u \sim \frac{e^{-i\pi/4}}{2i\sqrt{2\pi}} \frac{e^{ikR}}{\sqrt{R}}\,. \tag{5.20}$$

Comparing (5.19) and (5.20) we find

$$\alpha_0 = \frac{e^{-i\pi/4}}{2i\sqrt{2\pi}}\,. \tag{5.21}$$

Finally, using the KL formula (3.6) we obtain the high-frequency field

$$u(x,z) = -\frac{1}{4\sqrt{2}} \frac{1}{f_+^{1/4}\sqrt{R}} \lambda^{1/6} e^{i2/3\lambda f_+^{3/2}} \left(\frac{1}{\sqrt{H}} (\sqrt{\tau_+}+\sqrt{\tau_-}) \mathrm{Ai}\left(-\lambda^{2/3} f_-\right) \right.$$

$$\left. + i\lambda^{-1/3} \frac{4\sqrt{H}}{\sqrt{\tau_+}+\sqrt{\tau_-}} \mathrm{Ai}'\left(-\lambda^{2/3} f_-\right) \right), \tag{5.22}$$

where $\lambda = kH = kd$ is the dimensionless wave number. Recall that $\mathrm{Ai}(\cdot)$ is the *Airy* function.

In Figs. 5–7, we compare the amplitude $|u|$ of the field predicted by the ordinary GO (solid line) with that predicted by KL formula (5.22) (dashed line) for various wave numbers k, in the case $z_0 = 0$, $d = 1$ (then $H = 1$). The amplitude $|u|$ of the field is calculated along the ray at $\theta_* = \pi/4$ from the source, at the points where this ray intersects the rays with angle in the interval $(-\Delta\theta + \theta_*, \theta_* + \Delta\theta)$ where $\Delta\theta = 0.45\pi$, and are plotted as functions of the dimensionless parameter $q = x/d$. As the initial angle θ moves far from θ_*, the intersection point moves away from the caustic, and GO matches with KL solution. In both cases all the computations have been performed numerically.

For the numerical approximation of the quantities $J_\pm, \Phi_\pm$, entering the formulas (3.11) and (3.13) we numerically compute the modified amplitudes g_0, g_1 as

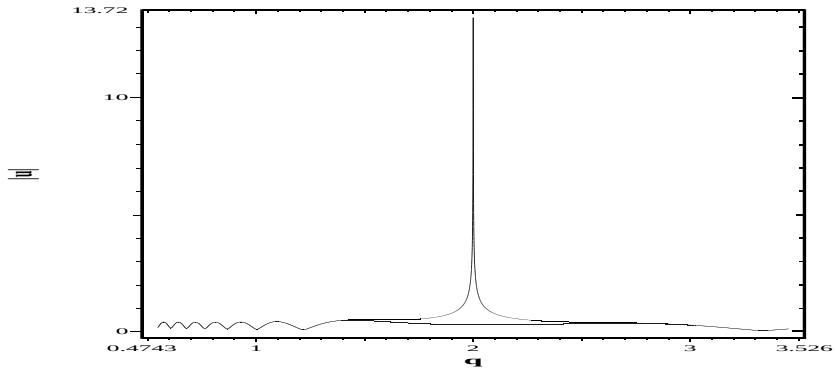

Fig. 5. $|u|$ vs q for $k = 100$.

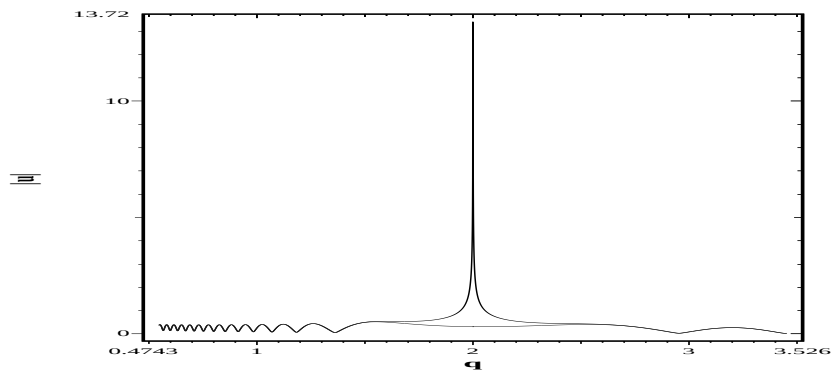

Fig. 6. $|u|$ vs q for $k = 200$.

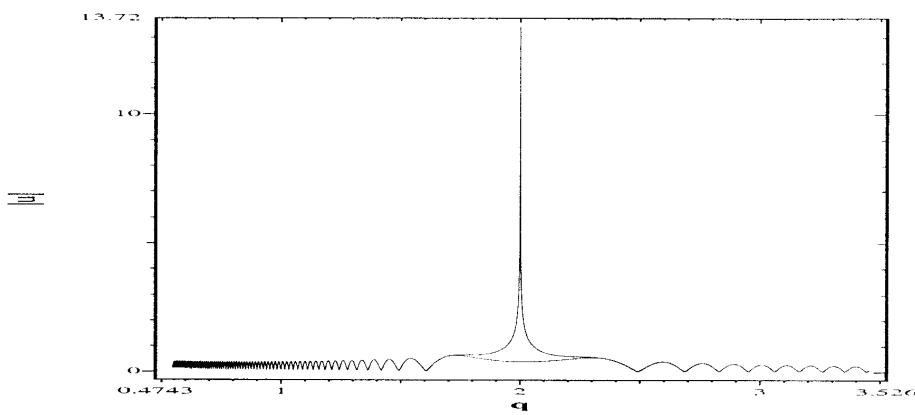

Fig. 7. $|u|$ vs q for $k = 1000$.

follows: We start by shooting two rays, with initial angles θ_* and $\theta_* + \Delta\theta$ for some small $\Delta\theta$. Then, there is a $t_\sigma \in [0, T]$ such that the two rays intersect each other, and one of them has already touched the caustic while the other has not. If $\Delta\theta$ is small enough, we expect that the intersection point is very close to the caustic. To find t_σ we first solve the IVP for sufficiently large T to guarantee that the two rays have an intersection point. Next, we find the minimal distance between the two rays sampled on the underlying partition $\{t_n = n\Delta T,\ n = 0, \ldots, N\}$, where $\Delta T = T/N$. If N is sufficiently large, then there are points $t_s^+,\ t_s^-, 0 < s < N$, on the two rays $(\pm)$, respectively that are "close" to t_σ. After locating $t_s^+,\ t_s^-$ we define a small neighborhood around these points, and we solve again the IVP there with smaller Δt to improve the accuracy for the intersection point. In this way we also get much more precise values for the other quantities. Finally, for the computation of the phases $S_\pm$ we approximate the integral formula (2.11) using the Gauss–Legendre quadrature rule (in this example, four quadrature points give very good approximation of the integral). The required values of n^2 along the rays at the quadrature points are obtained using cubic spline interpolation at the points on the rays corresponding to t_n.

It turned out that the numerical values for the Jacobian $J_\pm$ and the phase $\Phi_\pm$, and thereafter of the field amplitudes, are in excellent accuracy with those obtained using the analytical formulas (5.8) and (5.13a), (5.13b).

Note finally that in the case where we restrict the propagation domain to $z \le h$, $h < d$, there is a pencil of rays shot with angle $\theta \in (\arcsin\sqrt{\frac{h-z_0}{H}}, \pi/2)$, which are reflected at the boundary $z = h$ as their turning points satisfy $t_{ud} > h$. This pencil is separated from the pencil of rays which are refracted downwards by a *boundary ray* which is tangent to the boundary $z = h$ and also to the caustic which in this case is an open arc of the parabola (5.5c). The boundary ray and this arc define the shadow boundary (cf. Ref. 32). The representation of the phase function in this case is radically different from (3.4), and it can be derived by the methods of singularity theory (Ref. 31, cf. Ref. 28).

Example 5.2. (Evolution of a parabolic wave front in a homogeneous medium) The high-frequency approximation of the focusing in cylindrical abberation (see, e.g., Ref. 35) leads to solve the eikonal equation (see also p. 172 of Ref. 46)

$$|\nabla\Phi(x, z)| = 1 \tag{5.23}$$

with initial data

$$\Phi|_\Gamma = 0\,, \qquad \partial_\nu\Phi|_\Gamma = 1\,. \tag{5.24}$$

Here Γ is the parabola

$$\Gamma = \left\{(x, z)|z = \zeta, \quad x = \frac{\zeta^2}{2\sigma}, \zeta \in \mathbb{R}\right\}\,, \tag{5.25}$$

σ being a fixed positive parameter, and ν denotes the interior unit normal vector on Γ.

The Hamiltonian (2.7) is given in this case by $H(\mathbf{r},\mathbf{p}) = \frac{1}{2}(|\mathbf{p}|^2 - 1)$. Solving the system (2.8) we find that the rays are given by

$$x(\tau) = \frac{\sigma}{\sqrt{\sigma^2+\zeta^2}}\tau + \frac{\zeta^2}{2\sigma}\,, \tag{5.26a}$$

$$z(\tau) = -\frac{\zeta}{\sqrt{\sigma^2+\zeta^2}}\tau + \zeta\,. \tag{5.26b}$$

The Jacobian (2.13) is given by

$$J(\tau,\zeta) = \frac{1}{\sigma}\sqrt{\sigma^2+\zeta^2} - \frac{\sigma}{\sigma^2+\zeta^2}\tau\,, \tag{5.27}$$

and accordingly the caustic is the curve

$$x = \sigma + \frac{3\sigma^{1/3}}{2}z^{2/3}\,. \tag{5.28}$$

Eliminating the parameter τ from Eqs. (5.26a) and (5.26b) we obtain the cubic equation

$$\zeta^3 + 2\sigma(\sigma - x)\zeta - 2\sigma^2 z = 0\,. \tag{5.29}$$

Performing the trivial change of coordinates

$$\xi = \frac{\zeta}{\sqrt{2\sigma}}\,, \qquad \rho_1 = -z\sqrt{\frac{\sigma}{2}}\,, \qquad \rho_2 = x - \sigma \tag{5.30}$$

we rewrite the equation of the caustic (5.28) in the form (3.17), while the cubic equation (5.29) is written in the form (3.16). Note that the coordinates ρ_1, ρ_2 introduced in (5.30) do not represent globally the correct (Kravtsov–Ludwig) coordinates which have to be found from the solution of the nonlinear system (3.21).

Recall that the roots of the cubic equation (3.17), and therefore of (5.29), are real in Region I (see Fig. 2), while in Region II there is only one real root, the other two being complex. On the cusp (where the discriminant D, given by (3.17e), vanishes) two of the three real roots coalesce to a double one, and at the beak O all the real roots coalesce to the triple root $\zeta = 0$. In Region I the rays go through each point $\mathbf{r} = (x,z)$ at the times $\tau_j = \tau_j(x,z), j = 1,2,3$, originating at the points of the initial parabola Γ corresponding to the values $\zeta_j = \zeta_j(x,z) = \xi_j(\rho_1,\rho_2)\sqrt{2\sigma}$. The times τ_j are calculated from either (5.26a) or (5.26b) for $\zeta = \zeta_j$.

In order to calculate the modified amplitudes g_0, g_1, g_2 we apply the procedure described in Sec. 3.3 as follows.

Step 1. We compute the geometrical phases by integration along the rays, using

$$\Phi_j(x,z) = \int_0^{\tau_j(x,z)} n^2(x(t,\zeta_j), z(t,\zeta_j))\,dt \tag{5.31a}$$

$$= \tau_j(x,z) = (\zeta_j - z)\frac{\sqrt{\sigma^2+\zeta_j^2}}{\zeta_j}\,. \tag{5.31b}$$

We also compute the geometrical amplitudes

$$A_j(\mathbf{r}) = \frac{\alpha_0(\zeta_j)}{\sqrt{J_j(\mathbf{r})}}\,,$$

where $J_j(\mathbf{r}) = J(\tau_j, \zeta_j)$ are obtained from (5.27).

In the sequel, for simplicity, we assume that $\alpha_0 = 1$ everywhere on Γ.

Step 2. We substitute (5.31a)–(5.31c) into (3.19) to obtain $\tilde{S}(\phi, \rho_1, \rho_2)$. These phases must be equal to the geometrical phases $S_j(\mathbf{r})$, given by (5.32b), so we have to solve the nonlinear system

$$\begin{aligned}\tilde{S}(\phi, \rho_1, \rho_2) &= \phi(\mathbf{r}) + \rho_1 \xi_j(\rho_1, \rho_2) - \rho_2 \frac{\xi_j^2(\rho_1, \rho_2)}{2} + \frac{\xi_j^4(\rho_1, \rho_2)}{4} \\ &= \Phi_j(\mathbf{r})\,, \qquad j = 1, 2, 3\,, \end{aligned} \tag{5.32}$$

to derive $\phi(\mathbf{r})$, $\rho_1(\mathbf{r})$ and $\rho_2(\mathbf{r})$. Note that, even for this simple case, the system (5.32) cannot be solved analytically, and so we cannot calculate explicitly the modified amplitudes.

The numerical solution of this nonlinear system is performed as follows. We rewrite the system in the form

$$\phi = -\rho_1 \xi_1 + \rho_2 \frac{\xi_1^2}{2} - \frac{\xi_1^4}{4} + \Phi_1\,, \tag{5.33a}$$

$$\rho_1(\xi_1 - \xi_2) - \frac{\rho_2}{2}(\xi_1^2 - \xi_2^2) + \frac{1}{4}(\xi_1^4 - \xi_2^4) = \Phi_1 - \Phi_2\,, \tag{5.33b}$$

$$\rho_1(\xi_2 - \xi_3) - \frac{\rho_2}{2}(\xi_2^2 - \xi_3^2) + \frac{1}{4}(\xi_2^4 - \xi_3^4) = \Phi_2 - \Phi_3\,. \tag{5.33c}$$

Using the formulas

$$\xi_1 + \xi_2 + \xi_3 = 0\,, \qquad \xi_1\xi_2\xi_3 = -\rho_1\,, \quad \xi_1\xi_2 + \xi_2\xi_3 + \xi_1\xi_3 = \rho_2\,, \tag{5.34}$$

connecting the roots of the cubic equation (3.16) with the coefficients ρ_1, ρ_2, we write Eqs. (5.33b), (5.33c) as a system with respect to ξ_2, ξ_3 only, the roots of which correspond to the rays which coalesce as we approach the caustic. This system reads as follows:

$$F(\xi_2, \xi_3) = -\xi_3^4/4 - 2\xi_2^3\xi_3 - 3\xi_2\xi_3^3/2 - 3\xi_2^2\xi_3^2 = \Phi_1 - \Phi_2\,, \tag{5.35a}$$

$$G(\xi_2, \xi_3) = -\xi_2^4/4 + \xi_3^4/4 + \xi_2^3\xi_3/2 - \xi_3^3\xi_2/2 = \Phi_2 - \Phi_3\,. \tag{5.35b}$$

The system (5.35a), (5.35b) is solved by Newton's method assuming as convergence criterion the absolute distance between successive approximations of the roots to be less than a given tolerance ε which in this particular example is $\varepsilon = 10^{-12}$.

Note that as we approach the beak of the cusp, the Jacobian of the system (5.36a), (5.36b) goes to zero as ξ_2, ξ_3 go to zero with the same order with respect to the distance from the beak. However, since $(\Phi_2 - \Phi_3)$ also goes to zero and

$(\Phi_2 - \Phi_3)/G(\xi_2, \xi_3)$ remains bounded away from zero, the computation is stable up to distances of the order 10^{-10} from the beak (the value of the uniformity parameter μ at this distance is $\mu = 0.312\,499\,961\,215\,455\,2$, while on the caustic it has the value $\mu = 2/\sqrt{27} = 0.384\,900\,18\ldots$).

Step 3. Finally we substitute $\phi(\mathbf{r}), \rho_1(\mathbf{r}), \rho_2(\mathbf{r})$ found by Step 3 into (5.31a)–(5.31c), to get $\xi_j(\mathbf{r})$, and we compute the modified amplitudes by solving explicitly the linear system (3.18), i.e.

$$g_0(\mathbf{r}) + \xi_j(\mathbf{r})g_1(\mathbf{r}) + \xi_j^2(\mathbf{r})g_2(\mathbf{r}) = a_j(\mathbf{r})\left((\partial_\xi^2 S(\mathbf{r}, \xi_j(\mathbf{r})))\right)^{1/2}$$
$$= A_j(\mathbf{r})(3\xi_j^2(\mathbf{r}) - \rho_2(\mathbf{r}))^{1/2}, \quad j = 1, 2, 3. \quad (5.36)$$

Then the field is evaluated using formula (3.22).

In Figs. 8, 9 and 10, we compare the amplitudes of the field predicted by GO with that predicted by KL formula for relatively high frequencies ($k = 100$) along the three rays passing through the point $(x_0, z_0) = (1.7937, -0.382)$ inside the cusp (5.28) with $\sigma = 1$. We compute the amplitudes as functions of $|z|$. The solid line represents the GO solution which blows up along each ray as we approach the caustic. The dashed line represents the KL solution when the Pearcey integral is computed using the uniform asymptotic expansion by Kaminski,[33] while the dotted line represents the KL solution when we compute the Pearcey integral by direct numerical integration. In the latter case the numerical integration fails for large enough $k|z|$. However, uniform asymptotics and numerical integration give almost identical results for a satisfactory range of $|z|$ for each k, giving thus enough evidence that the asymptotic expansion is accurate for large values of $k|z|$. Obviously GO tends to match the KL solution far away from the caustic. The distance from the caustic for satisfactory matching depends, in general, on the particular wave number k.

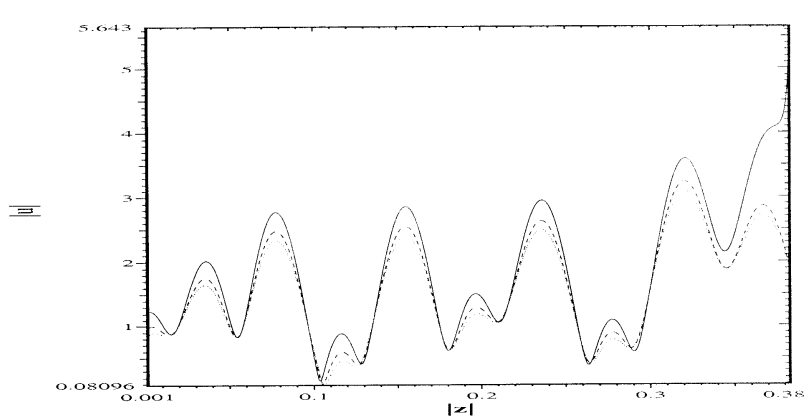

Fig. 8. $|u|$ vs $|z|$ along ray 1.

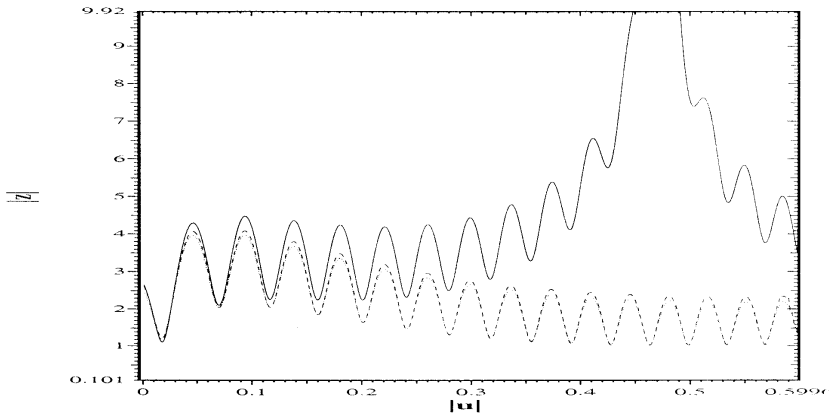

Fig. 9. $|u|$ vs $|z|$ along ray 2.

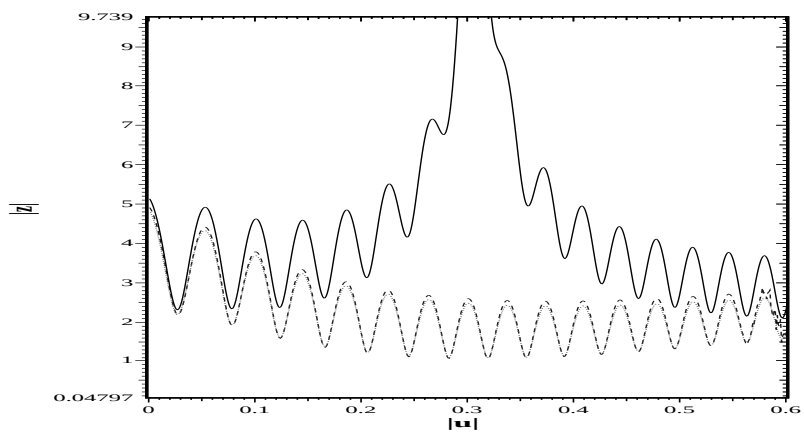

Fig. 10. $|u|$ vs $|z|$ along ray 3.

Appendix A. Lagrangian Manifold and Phase Functions

Consider the partial differential equation

$$P(x, k^{-1}D_x)u(x,k) = 0\,, \qquad x \in X \tag{A.1}$$

where k is a large parameter and P is the differential operator

$$P(x, D_x) = \sum_{|\alpha|=0}^{m} c_\alpha(x) D_x^\alpha\,, \tag{A.2}$$

with $\alpha = (\alpha_1, \ldots, \alpha_m)$, α_j being non-negative integers, $|\alpha| = \alpha_1 + \cdots + \alpha_m$, $D_x = (\frac{1}{i}\partial_{x_1}, \ldots, \frac{1}{i}\partial_{x_m})$, and $D_x^\alpha = (\frac{1}{i}\partial_{x_1})^{\alpha_1} \cdots (\frac{1}{i}\partial_{x_m})^{\alpha_m}$, $i = \sqrt{-1}$. In general, X can be an m-dimensional smooth manifold, but for simplicity we can think of X

as $\mathbb{R}^m$. The function

$$P(x,p) = \sum_{|\alpha|=0}^{m} c_\alpha(x) p^\alpha \,, \tag{A.3}$$

where $p = (p_1, \ldots, p_m)$ is called the symbol of the differential operator (A.2).

Substituting the FAS

$$u(x,k) = e^{ik\Phi(x)} \sum_{\ell=0}^{\infty} (ik)^{-\ell} A_\ell(x) \,, \tag{A.4}$$

into (A.1) and separating powers of k, and putting $p = \nabla\Phi(x)$, we obtain the Hamilton–Jacobi equation

$$H(x,p) = 0 \,, \tag{A.5}$$

where $H(x,p)$ is the principal symbol of the operator P. In the case, for example, of the Helmholtz operator $P = -\Delta + k^2 n^2(x)$, the Hamilton–Jacobi equation (A.5) is the usual eikonal equation $|\nabla\Phi|^2 = n^2$.

The bicharacteristics of (A.2) are given by the Hamiltonian system

$$\frac{dx}{dt} = \nabla_p H \,, \qquad \frac{dp}{dt} = -\nabla_x H \,, \tag{A.6}$$

with initial data

$$x(0,u) = x^0(u) \,, \qquad p(0,u) = p^0(u) \,, \qquad u \in U \,, \tag{A.7}$$

U being an open subset of $\mathbb{R}^{m-1}$. Suppose that the initial data are such that $H(x^0(u), p^0(u)) = 0$ (compatibility condition for the Cauchy problem (A.6), (A.7)), and define $\Phi^0(u)$, $u \in U$, by $p^0(u)\, dx^0(u) = d\Phi^0(u)$.

Let L_H be the Hamiltonian vector field

$$L_H = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial H}{\partial x_i}\frac{\partial}{\partial p_i} \,. \tag{A.8}$$

Obviously $L_H H = 0$, and therefore L_H is tangent to $H^{-1}(0)$ in the cotangent space T^*X. The integral curves of L_H in H^{-1} are called *bicharacteristic strips* of the hypersurface $H^{-1}(0)$, and because $H^{-1}(0)$ is the characteristic variety of the operator P we call these integral curves the bicharacteristic strip for P. The images in X of these curves under the projection $\pi : (x,p) \to x$ from T^*X into X are called *bicharacteristic curves* for P (rays).

A smooth submanifold Λ of T^*X is locally of the form $\{(x, \nabla\Phi(x)) \in T^*X;\ x \in D\}$, that is the graph of $\nabla\Phi$ for some smooth real-valued function Φ on an open subset D of X, if and only if it satisfies the following geometric conditions

$$\dim \Lambda = m \tag{A.9a}$$

$$\Lambda \text{ is transversal to the fibers } x = \text{const. in } T^*X \tag{A.9b}$$

$$\sigma(\zeta,\eta) = 0 \quad \text{if} \quad (\zeta,\eta) \in T_{(x,p)}\Lambda \,, \tag{A.9c}$$

where σ is the canonical two-form on T^*X, given by

$$\sigma(\zeta,\eta) = \sum_{l=1}^{m} (\zeta_{2l}\eta_{1l} - \zeta_{1l}\eta_{2l}) \ , \tag{A.10a}$$

in local coordinates

$$\zeta = (\zeta_1, \zeta_2)\,, \qquad \eta = (\eta_1, \eta_2)\,. \tag{A.10b}$$

The relations (A.9a) and (A.9b) mean that Λ is locally the graph $\{(x, p(x)) \in T^*X; x \in D\}$ of some one-form p, and then (A.9c) express the fact that $dp = 0$ which locally implies that $p = d\Phi$ for some function Φ. A submanifold Λ satisfying (A.9c) is called *isotropic*. If, in addition, its dimension is equal to m (maximal), then it is called a *Lagrangian submanifold* in T^*X.

Therefore, finding local solutions Φ *of the Hamilton–Jacobi equation* (A.5) *is equivalent to finding pieces of Lagrangian manifolds* Λ *which are transversal to the fibers on which* $H = 0$.

It can be shown that if $\Lambda \subset H^{-1}(0)$ in T^*X, then L_H is tangent to Λ and therefore Λ is the union of parts of bicharacteristic strips. Conversely, if Λ_0 is an $(m-1)$-dimensional smooth isotropic submanifold of T^*X, $\Lambda_0 \subset H^{-1}(0)$ and L_H is transversal to Λ_0, then the local flow-out Λ of Λ_0 along a bicharacteristic strip is a Lagrangian manifold in $H^{-1}(0)$, and locally the only one containing Λ_0. Therefore, assuming that L_H is nowhere tangent to the initial submanifold $\Lambda_0 = \{(x^0(u), p^0(u)), u \in U\}$ (which means that the Cauchy problem is locally well-posed), we construct the phase function $\Phi = \Phi(x)$ integrating the equation

$$\frac{d\breve{\Phi}}{dt} = p \cdot \nabla_p H\,, \tag{A.11}$$

along the rays $x = x(t,u)$, with initial condition $\breve{\Phi}(0,u) = \Phi^0(u)$, and then, if possible, changing from the coordinates (t,u) to x, and setting $\Phi(x) = \breve{\Phi}(t, x^{-1}(t,x))$.

This procedure fails in the following cases:

Case 1: If $H(x_0,p_0) = \nabla H(x_0,p_0) = 0$ at a certain point (x_0,p_0) in Λ_0 which makes even a local solution impossible.

Case 2: If following a bicharacteristic strip the tangent space $T\Lambda$ of the Lagrangian manifold "turns vertically", and it is not transversal to the fibers (i.e. the condition (A.9b) is not satisfied), even if $\nabla H \neq 0$ all the time. This case corresponds to the formation of *caustics* and there the projections of the bicharacteristic strips on X get singularly concentrated.

Case 3: If Λ itself has singularities, e.g. self-intersections.

In all these cases it is not possible to construct global asymptotic expansions by means of the formal ansatz (A.4) because it is not possible to construct the phase function by the above described procedure. However, a phase function parametrizing the Lagrangian manifold Λ still can be found by appealing to the methods of singularity theory. More precisely, the following proposition holds.

Proposition A.1. (Ref. 26) *Let $\pi : \Lambda \to X$ the projection of Λ onto X, and assume that $d\pi$ has rank $m - \nu$ at the point (x_0, p_0). Then, there exists a phase function $S = S(x, \zeta_0)$ on $X \times \mathbb{R}^\nu$, such that the critical set $C_\zeta = \{(x, \zeta) : d_\zeta S = 0\}$ is an m-dimensional submanifold of $X \times \mathbb{R}^\nu$ and the map $C_\zeta \to T^*X, (x, \zeta) \mapsto (x, d_x S)$ maps a neighborhood of $(x_0, 0)$ diffeomorphically onto a neighborhood of (x_0, p_0) in Λ.*

Note that the dimension of the phase variable ζ, i.e. the rank $m - \nu$ of the projection $\pi : \Lambda \to X$, is equal to the nullity of the Hessian $D^2 S$.

Then, we can represent the solution as a compound asymptotic generated by the Lagrangian distribution associated with the Lagrangian pair (Λ, S) (Chap. VII of Ref. 26), i.e. as an oscillatory integral of the form

$$u(x, k) = \left(\frac{ik}{2\pi}\right)^{\nu/2} \int_Z e^{ikS(x,\zeta)} A(x, \zeta, k)\, d\zeta\,, \qquad Z \subset \mathbb{R}^\nu_\zeta\,, \tag{A.12}$$

where

$$A(x, \zeta, \lambda) \sim \sum_{l=0}^{\infty} A_l(x, \zeta) k^{\mu - l}\,, \tag{A.13}$$

μ being a positive real constant.

The construction of global asymptotic solutions starting from the oscillatory integral (A.12) requires the transformation of the phase function $S(x, \zeta)$ to a canonical form by changing the fiber variable $\zeta \in Z$, so that to be able to apply stationary-phase type lemmas for the transformed integral. In the general case such a transformation is provided by the techniques of singularity theory, but the presentation of any general results in this direction goes beyond the purpose of this Appendix.

In the special case of simple caustics (of the type A_λ, Sec. 17 of Ref. 7), including fold ($\lambda = 2$) and cusp caustics ($\lambda = 3$), it is enough to take $\nu = 1$, and then the following representation theorem holds.

Theorem A.1. (*Ref.* 26) *Let X be a neighborhood of the origin of $\mathbb{R}^m$ and $S = S(x, \zeta)$ a phase function on $X \times \mathbb{R}$. Suppose that at the origin*

$$\frac{\partial^l S}{\partial \zeta^l} = 0 \quad for \quad l = 1, \ldots, q-1 \quad and \quad \frac{\partial^q S}{\partial \zeta^q} \neq 0\,. \tag{A.14}$$

Then there exists a function $\xi = \xi(x, \zeta)$ and functions of $x : f_0(x), \ldots, f_{q-2}(x)$ such that $\xi(0, 0) = 0$ and $f_0(0), \ldots, f_{q-2}(0) = 0$,

$$\frac{\partial \xi}{\partial \zeta} \neq 0 \quad at \quad 0 \tag{A.15}$$

and

$$S(x, \zeta) = f_0 + f_1 \xi + \cdots + f_{q-2} \xi^{q-2} + \frac{\xi^q}{q} + \varepsilon(x, \zeta)$$

with $\varepsilon(x, \zeta)$ vanishing to infinite order at $x = 0$.

Acknowledgment

The authors are grateful to the anonymous referee for his valuable suggestions. This work has been partially supported by the TMR Programme "Hyperbolic Systems of Conservation Laws" (CT96-0033).

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