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CAUSTICS ASSOCIATED WITH THE ASYMPTOTIC SOLUTION OF THE DIFFUSION EQUATION*

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Abstract. The Lagrange manifold technique for finding asymptotic solutions of wave equations at turning points is adapted to diffusion-type equations.

1. Introduction. Parabolic differential equations of the form

$$\alpha_0(\mathbf{r}, t)\nabla^2 u + \boldsymbol{\alpha}_1(\mathbf{r}, t) \cdot \nabla u + \alpha_2(\mathbf{r}, t)u = \alpha_3(\mathbf{r}, t)\frac{\partial u}{\partial t}, \tag{1}$$

where $(\mathbf{r}, t)$ are spatial and time coordinates, respectively, occur in physical processes as diverse as neutron transport [1], to heat diffusion [2] and fluid flow [3]. If the α_i actually are functions of $\mathbf{r}$ and t, seldom can such equations be solved exactly. Consequently, approximate solutions are often developed, each valid under situation-special conditions. One technique for obtaining such solutions is the geometrical optics formalism of Keller [4]. Although usually associated with wave propagation, this technique can also be applied to parabolic partial differential equations when a scaling of coordinates allows introduction of the large parameter λ in the time derivative term, i.e.,

$$\alpha_3(\mathbf{r}, t)\frac{\partial u}{\partial t} \to \lambda\alpha_3(\mathbf{r}, t)\frac{\partial u}{\partial t}.$$

Following Cohen and Lewis [2], a solution of the form

$$u = A(\mathbf{r}, t)\exp\{-\lambda S(\mathbf{r}, t)\}, \qquad A(\mathbf{r}, t) \sim \sum_{k=0} A_k(\mathbf{r}, t)\lambda^{-k} \tag{2}$$

is then assumed. (In Eq. (2), $S(\mathbf{r}, t)$ is commonly referred to as the "phase" and the A_k as the "amplitudes.") Then carrying the differentiation in Eq. (1) across the summation in Eq. (2) leads to an eikonal equation for the phase and a transport equation for the amplitudes. However, just as in wave propagation problems, on certain (caustic) curves this procedure can lead to unbounded amplitudes.

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For example, consider the already-scaled diffusion equation ($\mathbf{r} = (x, y)$ for simplicity) of Cohen and Lewis with $\alpha_0(\mathbf{r}, t) = 1$ and $\alpha_3(\mathbf{r}, t) = k - x$, i.e.,

$$\nabla^2 u = \lambda(k - x)\frac{\partial u}{\partial t}.$$

Then, assuming a solution of the form as in Eq. (2) and noting

$$\mathbf{p} = \nabla S, \qquad \omega = -\frac{\partial S}{\partial t},$$

leads to the Hamiltonian

$$H = p_x^2 + p_y^2 - \omega(k - x)$$

and, from Hamilton's equations, the flow

$$x = -\omega\gamma^2 + 2\gamma p_0 \cos\theta + x_0, \qquad y = 2\gamma p_0 \sin\theta + y_0,$$

where γ is a ray-path parameter and θ is an initial direction. If we assume at time zero an initial position at the origin with $p_0 = 2^{1/2}$, $k = 2$, $\omega_0 = 1$, then on the curve obtained by setting the Jacobian determinant $(\partial(x, y)/\partial(\gamma, \theta))$ to zero, i.e., here, $\gamma\cos\theta - 2^{1/2} = 0$, the technique predicts unbounded amplitudes.

One approach to circumventing such problems in wave propagation is the Lagrange manifold formalism [5]. Here we make explicit that with only slight modification, the procedure extends to parabolic partial differential equations, which we illustrate by completing the example above.

2. Formalism. We consider equations of the form

$$\alpha_0(\mathbf{r}, t)\nabla^2 u + \boldsymbol{\alpha}_1(\mathbf{r}, t) \cdot \nabla u + \alpha_2(\mathbf{r}, t)u = \lambda\alpha_3(\mathbf{r}, t)\frac{\partial u}{\partial t}, \tag{3}$$

i.e., parabolic differential equations scaled as discussed above. Analogous to the solution assumed for hyperbolic differential equations, near caustic points we assume a solution of the form

$$u(\mathbf{r}, t) \sim \int d\mathbf{p} \exp\{-\lambda\phi(\mathbf{r}, \mathbf{p}, t)\}A(\mathbf{r}, \mathbf{p}, t, \lambda) \tag{4}$$

where

$$\phi(\mathbf{r}, \mathbf{p}, t) = \mathbf{r} \cdot \mathbf{p} - S(\mathbf{p}, t)$$

and $A(\mathbf{r}, \mathbf{p}, t, \lambda)$ and its derivatives are bounded. Then passing the derivatives in Eq. (3) across the integral in Eq. (4), followed by a re-grouping by powers of λ (noting here $\mathbf{p} = \nabla\phi$, $\omega = -\partial\phi/\partial t = \partial S/\partial t$) obtains

$$\begin{aligned}\int d\mathbf{p} \exp\{-\lambda\phi(\mathbf{r}, \mathbf{p}, t)\}\Big\{&\lambda^2\left[(\alpha_0(\mathbf{r}, t)(\mathbf{p}.\mathbf{p}) - \alpha_3(\mathbf{r}, t)\omega)\right]A \\ &+\lambda\left[2\alpha_0(\mathbf{r}, t)(\mathbf{p} \cdot \nabla A) - (\boldsymbol{\alpha}_1(\mathbf{r}, t) \cdot \mathbf{p})A - \alpha_3(\mathbf{r}, t)\frac{\partial A}{\partial t}\right] \\ &+\lambda^0\left[\alpha_0(\mathbf{r}, t)\nabla^2 A + \boldsymbol{\alpha}_1(\mathbf{r}, t) \cdot \nabla A + \boldsymbol{\alpha}_2(\mathbf{r}, t)A\right]\Big\} \sim O(\lambda^{-\infty}).\end{aligned} \tag{5}$$

The coefficient of the λ^2 term is Maslov's Hamiltonian

$$H = \alpha_0(\mathbf{r}, t)(\mathbf{p} \cdot \mathbf{p}) - \omega\alpha_3(\mathbf{r}, t).$$

The exponential integrals in Eq. (5) are evaluated asymptotically using the Laplace technique [6, 7], i.e., at any field point, $\mathbf{r}$, the principal contribution to the integral comes from those values of $\mathbf{p}$ specified by $\nabla_p\phi = 0$. Here, however, invoking $\nabla_p\phi = 0$ not only identifies the critical points of the phase, but also turns the Hamiltonian into an eikonal equation and determines the Lagrange manifold

$$\mathbf{r} = \nabla_p S(\mathbf{p}, t) \tag{6}$$

which leads to obtaining an explicit phase via Hamilton's equations. First, solving Hamilton's coordinate and momentum equations ($\dot{\mathbf{r}} = \nabla H$, $\dot{\mathbf{p}} = -\nabla_r H$) yields the position coordinates and momenta parametrized by t and ω:

$$\mathbf{r} = \mathbf{r}(\gamma, \theta_1, \theta_2, t, \omega), \qquad \mathbf{p} = \mathbf{p}(\gamma, \theta_1, \theta_2, t, \omega).$$

Next, the momentum map is inverted to obtain

$$\gamma = \gamma(\mathbf{p}, t), \qquad \boldsymbol{\theta} = \boldsymbol{\theta}(\mathbf{p}, t),$$

where Hamilton's time-frequency equations ($\dot{t} = -\partial H/\partial\omega$ and $\dot{\omega} = \partial H/\partial t$) have been used to re-parametrize entirely in t, rather than in t and ω. Finally, a direct substitution in the coordinate space equations (and hence in Eq. (6)) explicitly determines the Lagrange manifold and an integration leads to the phase

$$\phi(\mathbf{r}, \mathbf{p}, t) = \mathbf{r} \cdot \mathbf{p} - S(\mathbf{p}, t).$$

Simpler procedures exist to obtain the phase if the Hamiltonian is cyclic in either a space or time coordinate [6]. We note that the caustic may be determined by setting the Hessian determinant of the phase to zero:

$$\det\left\{\frac{\partial^2\phi}{\partial\mathbf{p}^2}\right\} = 0.$$

Each real set of $\mathbf{p} = (p_x, p_y, p_z)$ satisfying this equation at a given time specifies a caustic point whose configuration space coordinate may be obtained by substituting in the Lagrange manifold, Eq. (6). The locus of these configuration space points is the caustic curve.

The transport equation proceeds by Taylor expanding the Hamiltonian near the Lagrange manifold,

$$\begin{aligned}\alpha_0(\mathbf{r}, t)(\mathbf{p} \cdot \mathbf{p}) - \alpha_3(\mathbf{r}, t)\omega &= \alpha_0(\nabla_p S, t)(\mathbf{p} \cdot \mathbf{p}) - \alpha_3(\nabla_p S, t)\omega + (\mathbf{r} - \nabla_p S) \cdot \mathbf{D} \\ &= (\mathbf{r} - \nabla_p S) \cdot \mathbf{D},\end{aligned}$$

where

$$\mathbf{D} = \int_0^1 \nabla_r H\big(\xi(\mathbf{r} - \nabla_p S) + \nabla_p S, \mathbf{p}, t, \omega\big)\, d\xi.$$

Substituting into Eq. (5) obtains

$$\int d\mathbf{p} \exp\{-\lambda\phi(\mathbf{r},\mathbf{p},t)\}\Big\{\lambda\Big(\nabla_p A\cdot\mathbf{D} + A\nabla_p\cdot\mathbf{D} - 2(\mathbf{p}\cdot\nabla_r A)\alpha_0(\mathbf{r},t) - \boldsymbol{\alpha}_1(\mathbf{r},t)\cdot\mathbf{p}A - \alpha_3(\mathbf{r},t)\frac{\partial A}{\partial t}\Big) + \alpha_0(\mathbf{r},t)\nabla_r^2 A + \boldsymbol{\alpha}_1(\mathbf{r},t)\cdot\nabla_r A + \alpha_2(\mathbf{r},t)A\Big\} = O(\lambda^{-\infty}),$$

which, upon introducing the flow

$$\dot{\mathbf{r}} = -2\alpha_0(\mathbf{r},t)\mathbf{p}, \qquad \dot{\mathbf{p}} = \mathbf{D}$$

and (analogous to Cohen and Lewis) the differential operator

$$\frac{d}{d\gamma} = \alpha_3(\mathbf{r},t)\frac{\partial}{\partial t} + 2\alpha_0(\mathbf{r},t)\mathbf{p}\cdot\nabla_r + \mathbf{D}\cdot\nabla_p$$

leads to the transport equation (cf. [5])

$$\frac{dA_k}{d\gamma} + (\boldsymbol{\alpha}_1\cdot\mathbf{p} - \nabla_p\cdot\mathbf{D})A_k = \alpha_0(\mathbf{r},t)\nabla_r^2 A_{k-1} + \boldsymbol{\alpha}_1(\mathbf{r},t)\cdot\nabla_r A_{k-1} + \alpha_2(\mathbf{r},t)A_{k-1}.$$

To find $u(\mathbf{r},t)$ it is necessary to evaluate the resulting integrals, i.e.,

$$\int \exp\{-\lambda\phi(\mathbf{r},\mathbf{p},t)\}A_k(\mathbf{r},\mathbf{p})\,d\mathbf{p}$$

asymptotically. As this has been detailed elsewhere [6, 7, 8], we do not repeat it here.

3. Example. To illustrate the technique we return to the example above,

$$\nabla^2 u = (k - x)\frac{\partial u}{\partial t},$$

where for a point source beginning radiation at $t = 0$ at the origin, $p_0 = 2^{1/2}$, $k = 2$, and $\omega_0 = 1$. On the caustic curve ($\gamma\cos\theta - 2^{1/2} = 0$), we assume a solution of the form given in Eq. (4), which leads to the same Hamiltonian (and Hamiltonian flow, hence the same caustic) as above. At any γ, θ on the caustic, we can find (x, y, p_x, p_y) from Hamilton's equations. Explicitly, let $(\gamma, \theta) = (1.58, 26.6°)$, then at $t = .79$, a caustic point occurs at $(x, y, p_x, p_y) = (1.5, 2.0, -.32, .63)$. Proceeding along the algorithm we obtain the Lagrange manifold

$$x = -.5p_x + p_x^2 + p_y^2, \qquad y = 2 + 2p_x p_y - 2p_y(2 - p_y^2)^{1/2}$$

and hence the phase

$$\phi(x, y, p_x, p_y, t) = xp_x + yp_y + \frac{1}{3}p_x^3 + p_x p_y^2 - 2p_x + \frac{2}{3}(2 - p_y^2)^{3/2} - t.$$

(We note that at $(p_x, p_y) = (-.32, .63)$ the Hessian determinant of the phase is zero, confirming the level-equivalence of the Hamiltonian and Lagrange manifold maps, i.e., regular points are carried to regular points and caustic points are carried to caustic points.) For this simple case,

$$\mathbf{D} = \omega\hat{\mathbf{i}} + 0\hat{\mathbf{j}},$$

leading to the transport equation

$$\frac{dA_k}{dt} + \nabla^2 A_{k-1} = 0.$$

Finally, if $A_0 = 1$ at the emitter, the first two terms in the asymptotic series for $u(\mathbf{r}, t)$ at $(\mathbf{r}, t) = (1.5, 2.0, .79)$ are

$$u(\mathbf{r}, t) \sim \varepsilon^{-1.038\lambda}\{.0659\lambda^{-7/6} - .0447\lambda^{-4/3}\}.$$

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