Computing High Frequency Waves By the Level Set Method

Hailiang Liu

Department of Mathematics
Iowa State University

Collaborators: Li-Tien Cheng (UCSD), Stanley Osher (UCLA)
Shi Jin (UW-Madison), Richard Tsai (TX-Austin)

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Outline

High Frequency Wave Propagation

⊙ Background:

- Computation of Semiclassical limit of Schrödinger equation
- Computation of high frequency waves applied to: geometrical optics, seismology, medical imaging, ...
- Math Theory: semiclassical analysis, Lagrangian path integral, wave dynamics in nonlinear PDEs ...

⊙ Computing Observables

- Asymptotic methods: WKB method and/or Wigner transform method
- **Level set method** in an augmented space
- Projection + Postprocessing

Dispersive wave equation

- The Schrödinger equation

$$i\epsilon\partial_t u^\epsilon = -\frac{\epsilon^2}{2}\Delta_x u^\epsilon + V(x)u^\epsilon, \quad u_0(x) = A(x)e^{iS_0(x)/\epsilon}.$$

- Semiclassical limit $\epsilon \to 0$: the transition from quantum mechanics to classical mechanics
- Direct computation becomes unrealistic.

The Madelung Equations

- Madelung Transformation (1926) $u^\epsilon = Ae^{iS/\epsilon}$
- Insertion into the Schrödinger equation, and separate into real and imaginary parts

$$\partial_t \rho + \nabla \cdot (\rho v) = 0, \quad v = \nabla S, \rho = A^2,$$
$$\partial_t S + \frac{1}{2}|\nabla_x S|^2 + V + U = 0$$

- Quantum-mechanical potential $U = -\frac{\epsilon^2}{2\sqrt{\rho}}\Delta\sqrt{\rho}$.

$$\partial_t v + v \cdot \nabla_x v = -\nabla V - \nabla U(\rho).$$

Recovering Schrödinger from the Madelung Equations

- v must be a gradient of S;
- we must allow S to be a multi-valued function, otherwise a singularity would appear in

$$\nabla_x u^\epsilon = (\nabla A/A + i\nabla S/\epsilon)u^\epsilon$$

- (enforce quantization) In order for the wave equation to remain single valued, one needs to impose

$$\int_L v \cdot dl = 2\pi j, \quad j \in Z.$$

—phase shift, Keller-Maslov index.

Uncertainty Principle

- The principle of symplectic camel
  Consider phase space ball $B(R) := \{(x,p) : |x|^2 + |p|^2 \leq R^2\}$ and 'symplectic cylinder'

$$Z_j(r) : \{(x,p) : x_j^2 + p_j^2 \leq r^2\}.$$

- Non-squeezing theorem (Gromov 1985): Let f be a symplectomorphism, then

$$f(B(R)) \subset Z_j(r) \Leftrightarrow R \leq r.$$

- Quantum cells $\leftrightarrow$ Keller-Maslov quantization of Lagrangian manifolds. ...

The Wigner equation

- Wigner Transform (1932)

$$w^\epsilon(t,x,k) = \left(\frac{1}{2\pi}\right)^{d/2} \int e^{-ik\cdot y} u^\epsilon(t, x-\epsilon y/2)\bar{u}^\epsilon(x+\epsilon y/2)\, dy.$$

- The Wigner equation as $\epsilon \to 0$ becomes

$$\partial_t w + k \cdot \nabla_x w - \nabla_x V w = 0.$$

- for WKB data $u_0^\epsilon = \sqrt{\rho_0(x)} e^{iS_0(x)/\epsilon}$:

$$w(0,x,k) = \rho_0(x)\delta(k - \nabla_x S_0(x)).$$

Two paths to follow

- Goal: design efficient numerical methods to compute multi-valued geometric observables (phase, phase gradient) and physical observables (density, momentum, energy) for semiclassical limit.
- Two approximations for wave field u^ϵ
  (1) Position density + phase, $u = Ae^{iS/\epsilon}$, WKB method $\rightarrow$ Hamilton–Jacobi + transport equation
  (2)A probability distribution, $f(t, x, \xi)$, Wigner transform $\rightarrow$ Wigner equation + singular data;

Applied to other wave equations

- Hyperbolic waves —Basic wave equation

$$\partial_t^2 u = c(x)^2 \Delta u, \quad u(t,x) = Ae^{i\omega S}, \quad \omega >> 1.$$

- Symmetric hyperbolic systems of the form

$$A(x)\frac{\partial \mathbf{u}_\epsilon}{\partial t} + \sum_{j=1}^{n} D^j \frac{\partial \mathbf{u}_\epsilon}{\partial x^j} = 0. \quad (1)$$

where $\mathbf{u}_\epsilon \in C^M$ is a complex valued vector and $\mathbf{x} \in R^d$.

- Examples include: acoustic wave equations, Maxwell equation, equations of linear elasticity.

WKB approach $\Rightarrow$ the WKB system

- For a smooth nonlinear Hamiltonian $H(\mathbf{x}, \mathbf{k}) : R^n \times R^n \to R^1$, the WKB method typically results in a weakly coupled system of an eikonal equation for phase S and a transport equation for position density $\rho = |A|^2$ respectively:

$$\partial_t S + H(\mathbf{x}, \nabla S) = 0, \quad (t, \mathbf{x}) \in R^+ \times R^n, \tag{2}$$

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \nabla_{\mathbf{k}} H(\mathbf{x}, \nabla_{\mathbf{x}} S)) = 0. \tag{3}$$

- Two canonical examples: the semiclassical limit of the Schrödinger equations ($H = \frac{1}{2}|\mathbf{k}|^2 + V(\mathbf{x})$) and geometrical optics limit of the wave equations ($H = c(\mathbf{x})|\mathbf{k}|$).
- Advantage and disadvantage: ϵ-free, superposition principle lost ...

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Known Methods? surveyed by Engquist and Runborg

- **Ray tracing** (rays, characteristics), ODE based;
- **Hamilton-Jacobi Methods**—nonlinear PDE based
  [Fatemi, Engquist, Osher, Benamou , Abgrall, Symes, Qian ...]
- **Kinetic Methods** — linear PDE based
  (i)Wave front methods:
  [Engquist, Tornberg, Runborg, Formel, Sethian, Osher-Cheng-Kang-Shim and Tsai ...]
  (ii)Moment closure methods:
  [Brenier, Corrias, Engquist, Runborg, Gosse, Jin-Li, Gosse-Jin-Li...]
- **Level set method ...**

Outline

Capturing multi-valued solutions

- 1-D Burgers' equation

$$\partial_t u + u\partial_x u = 0, \quad u(x,0) = u_0(x).$$

Characteristic method gives $u = u_0(\alpha), \quad X = \alpha + u_0(\alpha)t$

- In physical space (t, x): $u(t,x) = u_0(x - u(t,x)t)$.
- In the space (t, x, y) (graph evolution)

$$\phi(t,x,y) = 0, \quad \phi(t,x,y) = y - u_0(x - yt),$$

with $\phi(t,x,y)$ satisfying

$$\partial_t \phi + y\partial_x \phi = 0, \quad \phi(0,x,y) = y - u_0(x).$$

Giga, Osher and Tsai (2002), for capturing entropy solution

Multi-valued phase (Cheng, Liu and S. Osher (03))

Jet Space Method

Consider the HJ equation

$$\partial_t S + H(x, \nabla_x S) = 0, \quad H(x,k) = \frac{1}{2}|k|^2 + V(x).$$

For this equation the graph evolution is not enough to unfold the singularity since H is also nonlinear in $\nabla_x S$.

Therefore we choose

- to work in the **Jet space** (x, k, z) with $z = S(x,t)$ and $k = \nabla_x S$;
- to select and evolve an implicit representative of the solution manifold.

Multi-valued phase and velocity

- Characteristic equation: In the jet space (x, k, z) the HJ equation is governed by ODEs

$$
\begin{aligned}
\frac{dx}{dt} &= \nabla_k H(x,k), \quad x(0,\alpha) = \alpha, \\
\frac{dk}{dt} &= -\nabla_x H(x,k), \quad k(0,\alpha) = \nabla_x S_0(\alpha), \\
\frac{dz}{dt} &= k \cdot \nabla H_k(x,k) - H(x,k), \quad z(0,\alpha) = S_0(\alpha).
\end{aligned}
$$

- level set function $\simeq$ global invariants of the above ODEs.
- level set equation
  We introduce a level set function $\phi = \phi(t, x, k, z)$ so that the graph $z = S$ can be realized as a zero level set

$$\phi(t,x,k,z) = 0, \quad z = S(t,x,k),$$

$$\partial_t \phi + (\nabla_k H, \quad -\nabla_x H, \quad k \cdot \nabla_k H - H)^\top \cdot \nabla_{\{x,k,z\}} \phi = 0.$$

Multi-valued velocity—Phase space method

- **Hamitonian dynamics**: If we just want to capture the velocity $k = \nabla_x S$ or to track the wave front, z direction is unnecessary.

$$\frac{dx}{dt} = \nabla_k H(x,k), \quad x(0,\alpha) = \alpha,$$
$$\frac{dk}{dt} = -\nabla_x H(x,k), \quad k(0,\alpha) = \nabla_x S_0(\alpha).$$

- **Liouville equation**

$$\partial_t \phi + \nabla_k H(x,k) \cdot \partial_x \phi - \nabla_x H(x,k) \cdot \nabla_k \phi = 0, \quad \phi \in \mathbb{R}^n.$$

Note here ϕ is a geometric object — level set function, instead of the distribution function.

- Independent work by S. Jin & S. Osher (03').

1st-order nonlinear PDEs (Liu, Cheng and Osher (04))

Consider $F(x, u, u_x) = 0$. In the jet space (x, z, p) with $z = u$ and $p = u_x$, the equation becomes a manifold

$$F(x, z, p) = 0.$$

Let its integral manifold be denoted by a zero set of a vector valued function $\phi = \phi(x, p, z)$, then the function ϕ is transported by the characteristic flow

$$L\phi = 0$$

with the characteristic field defined by

$$L := \nabla_p F \cdot \nabla_x + p \cdot \nabla_p F \partial_z - (\nabla_x F + p\partial_z F) \cdot \nabla_p.$$

Remarks

- Reduction to lower dimension space whenever possible [say, jet space to phase space];
- Number of level set functions$= m - k$, $m =$reduced space dimension, $k =$dimension of domain to be simulated [whole domain $k = d$, or wave front $k = d - 1$];
- Choice of initial data is not unique, but the zero level set should uniquely embed the given initial data.

Outline

Evaluation of density (Jin, Liu, Osher and Tsai, JCP04)

- For semiclassical limit of the Schrödinger equation $H = |k|^2/2 + V(x)$.
- we evaluate the multi-valued density in the physical space by projecting its value in phase space $(\mathbf{x}, \mathbf{k})$ onto the manifold $\phi = 0$, i.e., for any x we compute

$$\bar{\rho}(\mathbf{x}, t) = \int \tilde{\rho}(t, \mathbf{x}, \mathbf{k})|J(t, \mathbf{x}, \mathbf{k})|\delta(\phi)d\mathbf{k},$$

  where $J := \det(\nabla_{\mathbf{k}}\phi) = \det(Q)$.
- A new quantity $f(t, \mathbf{x}, \mathbf{k}) := \tilde{\rho}(t, \mathbf{x}, \mathbf{k})|J(t, \mathbf{x}, \mathbf{k})|$ also solves the Liouville equation

$$\partial_t f + k \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V(x) \cdot \nabla_{\mathbf{k}} f = 0, \quad f_0 = \rho_0.$$

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General Hamiltonian(Jin, Liu, Osher and Tsai, JCP05)

- In the physical space the density equation is

$$\partial_t \rho + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} \rho = -\rho G$$

where $G := \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{k}} H(\mathbf{x}, \mathbf{k}), \quad \mathbf{k} = \nabla_{\mathbf{x}} S(t, \mathbf{x}) = \mathbf{v}(t, \mathbf{x})$.

- Lift to phase space (x, k): Let $\tilde{\rho}(t, \mathbf{x}, \mathbf{k})$ be a representative of $\rho(t, \mathbf{x})$ in the phase space such that $\tilde{\rho}(t, \mathbf{x}, \mathbf{v}(t, \mathbf{x})) = \rho(t, \mathbf{x})$. Then

$$L\tilde{\rho}(t, \mathbf{x}, \mathbf{k}) = -\tilde{\rho} G$$

and

$$L(J) = JG$$

where the Liouville operator:

$$L := \partial_t + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{k}}.$$

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A new quantity f

$$f(t, \mathbf{x}, \mathbf{k}) := \tilde{\rho}(t, \mathbf{x}, \mathbf{k})|J(t, \mathbf{x}, \mathbf{k})|$$

indeed solves the Liouville equation

$$\partial_t f + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{k}} f = 0, \quad f_0 = \rho_0 |J_0|.$$

⊙ *Here f is similar to, but different from*

$$\rho(t, x) \det \left(\frac{\partial X}{\partial \alpha} \right),$$

which remains unchanged along the ray in physical space, $\det \left(\frac{\partial X}{\partial \alpha} \right)$ *called 'geometrical divergence'*

Post-processing

The combination of the vector level set function ϕ and the function f enables us to compute the desired physical observables, for example, density and the velocity via integrations against a delta function

$$\bar{\rho}(x,t) = \int f(t,x,k)\delta(\phi)dk,$$

$$\bar{u}(x,t) = \int kf(t,x,k)\delta(\phi)dk/\bar{\rho}.$$

$\delta(\phi) := \prod_{j=1}^{n} \delta(\phi_j)$ with ϕ_j being the j-th component of ϕ.

$O(nlogn)$ minimal effort, local level set method.

Application I: Scalar wave equation

- Wave equation:

$$\partial_t^2 u - c^2(\mathbf{x})\Delta u = 0, \quad (t, \mathbf{x}) \in \mathcal{R}^+ \times \mathcal{R}^n,$$

  where $c(\mathbf{x})$ is the local wave speed of medium.
- Eikonal equation: $\partial_t S + c(\mathbf{x})|\nabla_{\mathbf{x}} S| = 0$.
- Amplitude equation:

$$\partial_t A_0 + c(\mathbf{x})\frac{\nabla_{\mathbf{x}} S \cdot \nabla_{\mathbf{x}} A_0}{|\nabla_{\mathbf{x}} S|} + \frac{c^2 \Delta S - \partial_t^2 S}{2c|\nabla_{\mathbf{x}} S|} A_0 = 0.$$

- $\partial_t A_0^2 + c^2 \nabla_{\mathbf{x}} \cdot \left(A_0^2 \frac{\nabla_{\mathbf{x}} S}{c(\mathbf{x})|\nabla_{\mathbf{x}} S|} \right) = 0.$

  This suggests that for $H(\mathbf{x}, \mathbf{k}) = c(\mathbf{x})|\mathbf{k}|$, $\rho = A_0^2/c^2$ solves

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Application II: Acoustic waves

- $$\rho(\mathbf{x})\partial_t \mathbf{v} + \nabla_{\mathbf{x}} p = 0, \quad \kappa(\mathbf{x})\partial_t p + \nabla_{\mathbf{x}} \cdot \mathbf{v} = 0.$$

  Here $\rho =$ density and $\kappa =$ compressibility. With oscillatory initial data $\mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}) \exp(iS_0(\mathbf{x})/\epsilon)$ where $\mathbf{u} = (\mathbf{v}, p)$ and S_0 is the initial phase function. Seeking WKB asymptotic solution

  $$\mathbf{u}(t, \mathbf{x}) = A(t, \mathbf{x}, \epsilon) \exp(iS(t, \mathbf{x})/\epsilon).$$

- There are four wave modes: $H(\mathbf{x}, \mathbf{k}) = \{0, 0, v(x)|\mathbf{k}|, -v(x)|\mathbf{k}|\}$= transverse waves (no propagation) + acoustic waves (longitudinal, propagate with sound speed $v = 1/\sqrt{k(x)\rho(x)}$).

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- Let $\hat{k} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the vector

$$\mathbf{b}^+(\mathbf{x}, \hat{k}) := \left(\frac{\hat{k}}{\sqrt{2\rho}}, \frac{1}{\sqrt{2\kappa}}\right),$$

and define an amplitude function $\mathcal{A}$ in the direction of $\mathbf{b}^+$ as

$$u_0(\mathbf{x}) = \mathcal{A}(0, x)(\mathbf{x})\mathbf{b}^+(\mathbf{x}, \nabla_\mathbf{x} S_0).$$

- The nonnegative function $\eta = |\mathcal{A}|^2(t, x)$ satisfies

$$\partial_t\eta + \nabla_\mathbf{x}\cdot(\eta\nabla_k H(\mathbf{x}, \nabla_\mathbf{x} S)) = 0$$

coupled with the eikonal equation

$$\partial_t S + H(\mathbf{x}, \nabla_\mathbf{x} S) = 0, \quad H(x, \mathbf{k}) = v(x)|\mathbf{k}|.$$

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Outline

Wigner approach

- The limiting Wigner function $w(t, x, k)$ solves the Liouville equation

$$\partial_t w + \nabla_p H \cdot \nabla_x w - \nabla_x H \cdot \nabla_k w = 0.$$

$$w(0, x, k) = \rho_0(x)\delta(k - \nabla S_0(x))$$

- How to link this to the WKB approach?

Building 'level set devices' into the Wigner equation

- Level set formulation

$$
\begin{aligned}
&\partial_t\phi + \nabla_k H(x,p)\cdot\nabla_x\phi - \nabla_x H(x,p)\cdot\nabla_k\phi = 0,\\
&\phi(0,x,k) = \phi_0(x),
\end{aligned}
$$

, where $\phi_0 = k - \nabla_x S_0$ for smooth S_0.

- the bounded quantity f

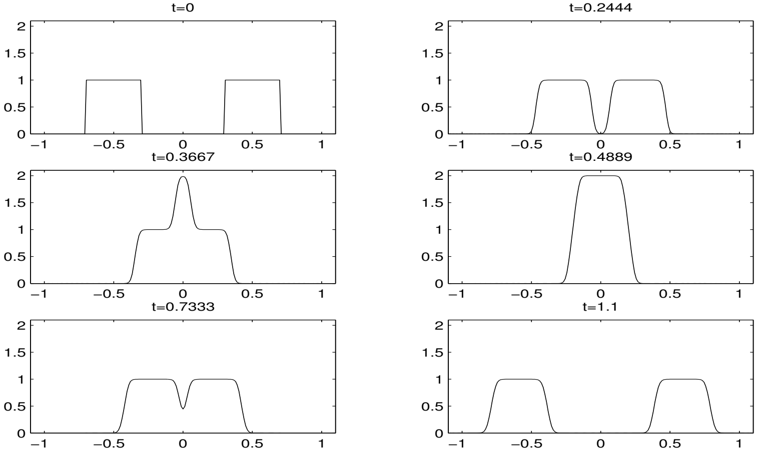
$$
\begin{aligned}
&\partial_t f + \nabla_k H(x,k)\cdot\nabla_x f - \nabla_x H(x,k)\cdot\nabla_k f = 0,\\
&f(0,x,k) = \rho_0(x).
\end{aligned}
$$

- Let $\phi = (\phi^1, \cdots, \phi^n)^\top$. The solution is given by

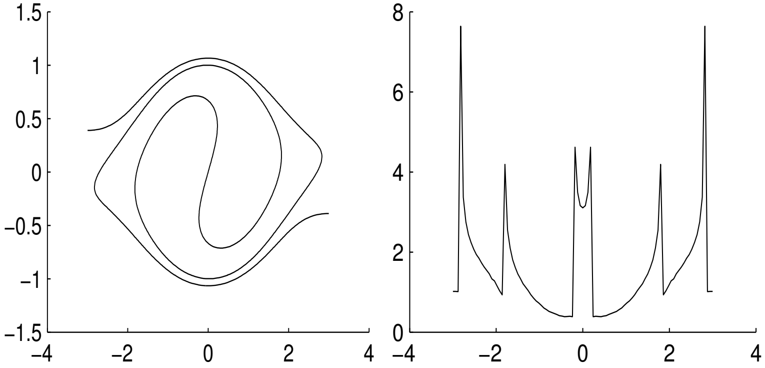
$$
w(t,x,k) = f(t,x,k)\delta(\phi(t,\mathbf{x},\mathbf{k})).
$$

Outline

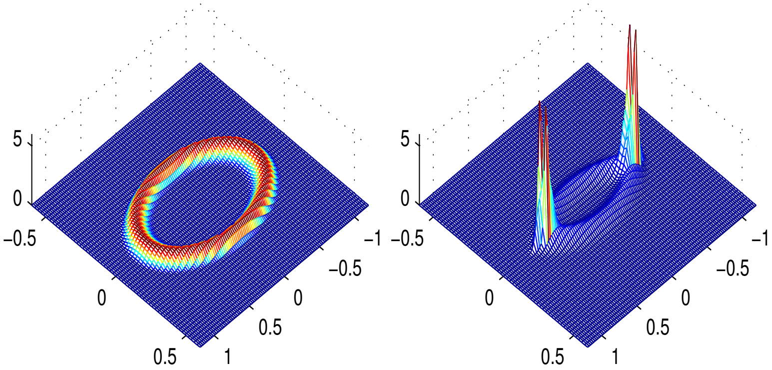
1D Self-crossing wave fronts



Wave Guide



Contracting ellipse in 2D



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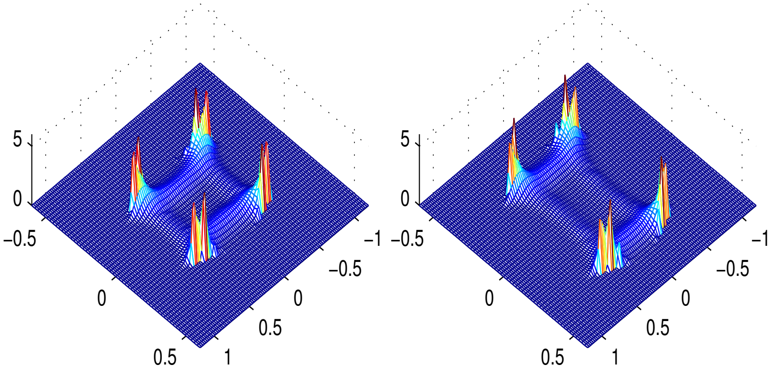

Concluding remarks

⊗ Summary

- The phase space based method introduced may be regarded as a compromise between *ray tracing* and the *kinetic method*, and the jet space method is for computing the multi-valued phase.
- The evaluation of density and high moments is performed by a post-processing step.
- The techniques discussed here are naturally geometrical and well suited for handling multi-valued solutions, arising in a large class of problems.

⊗ Future work: nonlinear dispersive waves equations; handling wave scattering; recovering the radiation loss ...