Computational high frequency waves through interfaces/barriers

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Outline

- Problems and motivation

  semiclassical limit through barriers (classical particles)

  geometrical optics (any high frequency waves) through interfaces

- Mathematical formulation and numerical methods

  Liouville equations and Hamiltonian systems with singular Hamiltonians

- Applications and extensions:

  semiclassical model for quantum barriers;

  computation of diffractions

High frequency waves

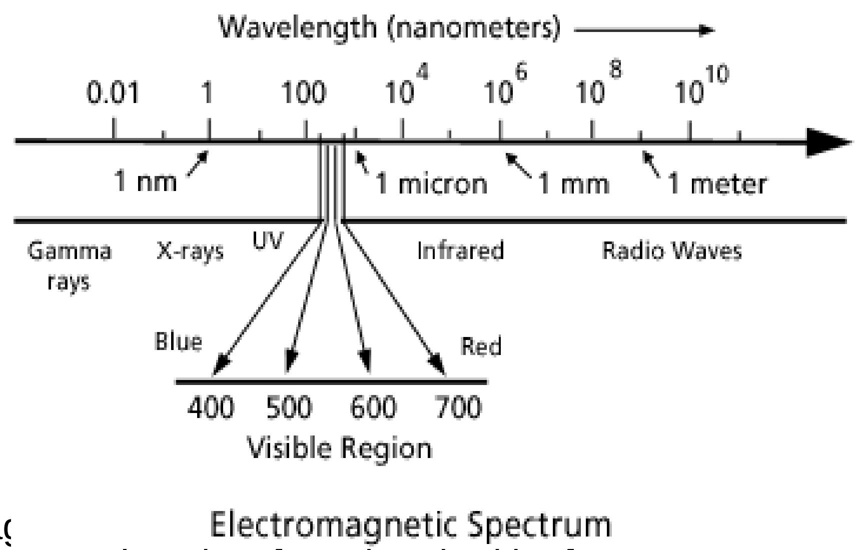


Fig. 1. The electromag ion of light, extends from gamma rays with wave lengths of one hundredth of a nanometer to radio waves with wave lengths of one meter or greater.

- High frequency waves: wave length/domain of computation <<1
- Seismic waves: elastic waves from Sichuan to Beijing (2.5$\times$ 10^3 *km*)

Difficulty of high frequecy wave computation

- Consider the example of visible lights in this lecture room:

wave length: $\sim 10^{-6}$ m

computation domain $\sim$ m

1d computation: $10^6 \sim 10^7$

2d computation: $10^{12} \sim 10^{14}$

3d computation: $10^{18} \sim 10^{21}$

do not forget time! Time steps: $10^6 \sim 10^7$

Example: Linear Schrodinger Equation

$$i\epsilon\,\psi_t + \frac{\epsilon^2}{2}\Delta\psi - V\psi = 0 \qquad \mathbf{x} \in R^d, \quad t > 0$$

$$\psi(\mathbf{x}, 0) = A_0(\mathbf{x})e^{i\frac{S_0(\mathbf{x})}{\epsilon}}$$

In this equation, $\psi(\mathbf{x}, t)$ is the complex-valued *wave function*, ϵ is or is playing the role of *Planck's constant*. It is assumed to be small here. The solution ψ and the related physical observables become *oscillatory* in space and time in the order of $O(\epsilon)$, causing all the mathematical and numerical challenges.

The WKB Method

We assume that solution has the form (*Madelung Transform*)

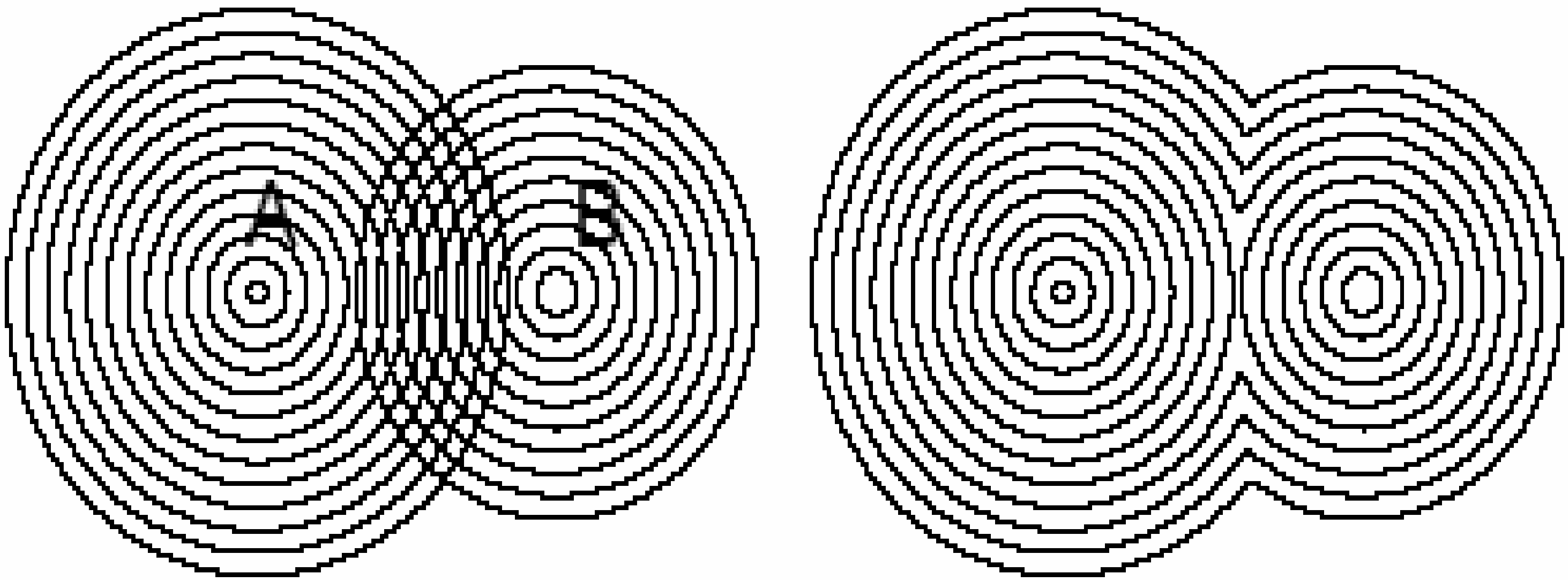
$$\psi(\mathrm{x}, t) = A(\mathrm{x}, t) e^{i\frac{S(\mathrm{x},t)}{\epsilon}}$$

and apply this ansatz into the Schrodinger equation with initial data.
To leading order, one can get

$$S_t + \frac{1}{2}|\nabla S|^2 + V = 0 \qquad \text{eiconal equation}$$

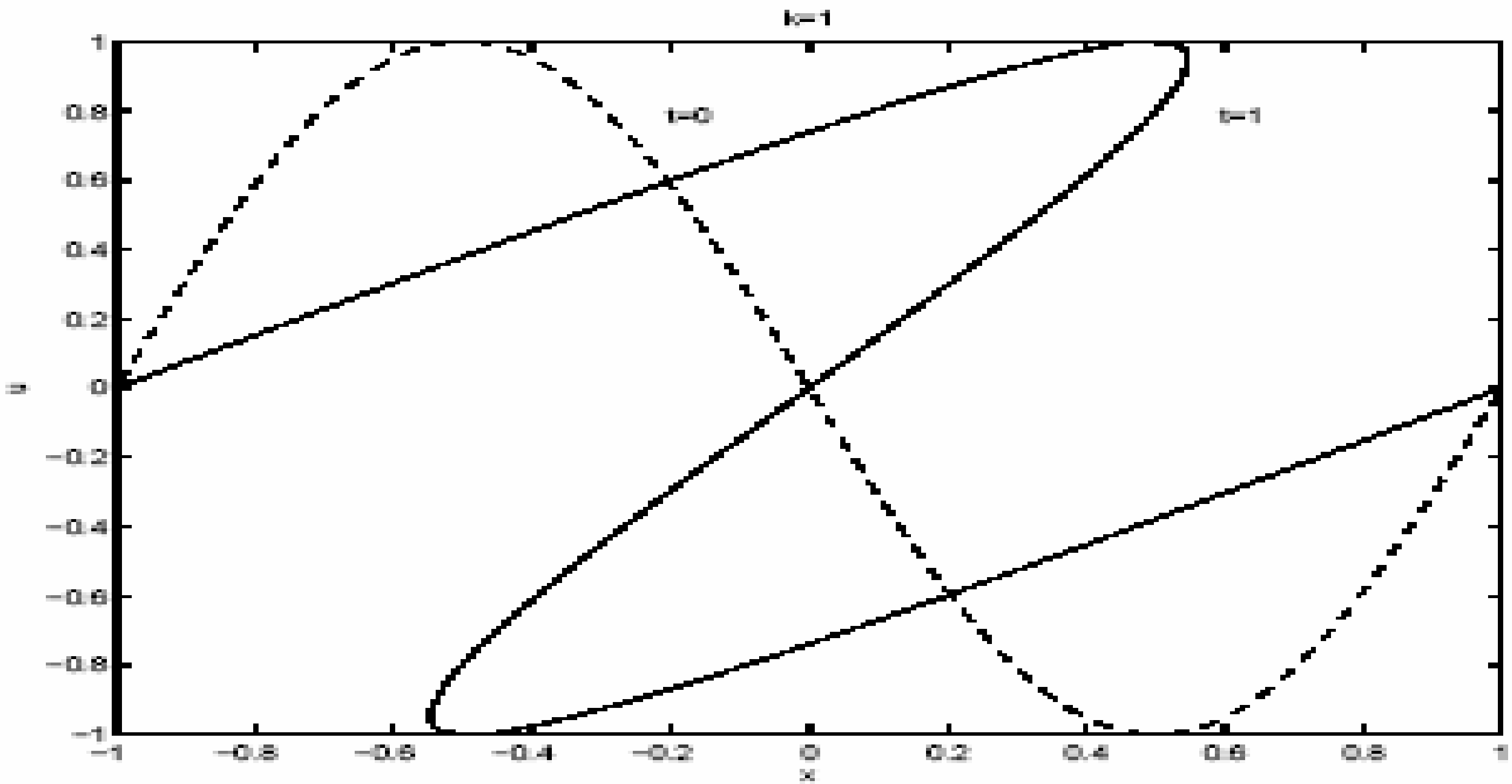
$$(|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) = 0 \quad \text{transport equation}$$

Linear superposition vs viscosity solution



(a) Correct solution (b) Eikonal equation

Shock vs. multivalued solution



Eulerian computations of multivalued solutons

- Brenier-Corrias
- Engquist-Runborg
- Gosse
- Jin-Li
- Fomel-Sethian
- Jin-Osher-Liu-Cheng-Tsai

Kinetic equations, moment methods, level set

Semiclassical limit in the phase space

Wigner Transform

$$W^{\epsilon}(\mathrm{x},\mathrm{k}) = \left(\frac{1}{2\pi}\right)^{d} \int_{R^d} e^{i\mathrm{k}\cdot\mathrm{y}} \psi(\mathrm{x}-\frac{\mathrm{y}}{2})\overline{\psi}(\mathrm{x}+\frac{\mathrm{y}}{2})d\mathrm{y}$$

A convenient tool to study the semiclassical limit:

Lions-Paul, Gerard-Markowich-Mauser-Poupaud, Papanicolaou-Ryzhik-Keller

Moments of the Wigner function

The connection between W^ε and ψ is established through the moments

$$\int_{R^d} W^\epsilon(\mathrm{x},\mathrm{k})\,d\mathrm{k} = |\psi(\mathrm{x})|^2$$
$$\int_{R^d} \mathrm{k}W^\epsilon(\mathrm{x},\mathrm{k})\,d\mathrm{k} = \frac{1}{2i}(\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi)$$
$$\int_{R^d} |\mathrm{k}|^2 W^\epsilon(\mathrm{x},\mathrm{k})d\mathrm{k} = |\nabla\phi(\mathrm{x})|^2$$

The semiclassical limit (for smooth V)

As $\epsilon \to 0$, the limit Wigner equation is the **Liouville equation** in phase space

$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the initial condition

$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

The wigner tranform works for any linear symmetric hyperbolic systems: elastic waves, electromagneticwaves, etc. (Ryzhik-Papanicolaou-Keller)

High frequency wave equations

$$u_{tt} – c(x)^2 \Delta u = 0$$

$$u(0, x) = A_0(x) \exp (S_0(x)/\varepsilon)$$

By using the Wigner transform, the enegry density satisfies

$$f_t + c(x) \{\xi / |\xi|\} \cdot \nabla_x f - |\xi| \nabla c \cdot \nabla_\xi f = 0$$

Discontinuous Hamiltonians in Liouville equation

$$f_t + \nabla_\xi H \cdot \nabla_{\mathbf{x}} f - \nabla_x H \cdot \nabla_\xi f = 0$$

- $H=1/2|\xi|^2+V(x)$: V(x) is **discontinuous-** potential barrier,
- $H=c(x)|\xi|$: c(x) is discontinuous- different index of refraction

- quantum tunneling effect, semiconductor devise modeling, plasmas, geometric optics, interfaces between different materials, etc.

Analytic issues

$$f_t + \nabla_\xi H \cdot \nabla_{\mathbf{x}} f - \nabla_x H \cdot \nabla_\xi f = 0$$

- The PDE does not make sense for discontinuous H. What is a weak solution? (*DiPerna-Lions renormalized solution for discontinuous coefficients does not apply*)

$$d\mathbf{x}/dt = \nabla_\xi H$$
$$d\xi/dt = -\nabla_{\mathbf{x}} H$$

- How to define a solution of systems of ODEs when the RHS is discontinuous or/and measure-valued?

Numerical issues

- for $H=1/2|\xi|^2+V(x)$

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i |DV_i|}{\Delta \xi} \right] \leq 1.$$

- since $V'(x)= \infty$ at a discontinuity of V, this implies $\Delta t=0$
- one can smooth out V then Dv_i=O(1/Δx), thus

$\Delta t=O(\Delta x \Delta \xi)$

poor resoultion (for complete transmission)
wrong solution (for partial transmission)

II. Mathematical and Numerical Approaches (*with Wen*)

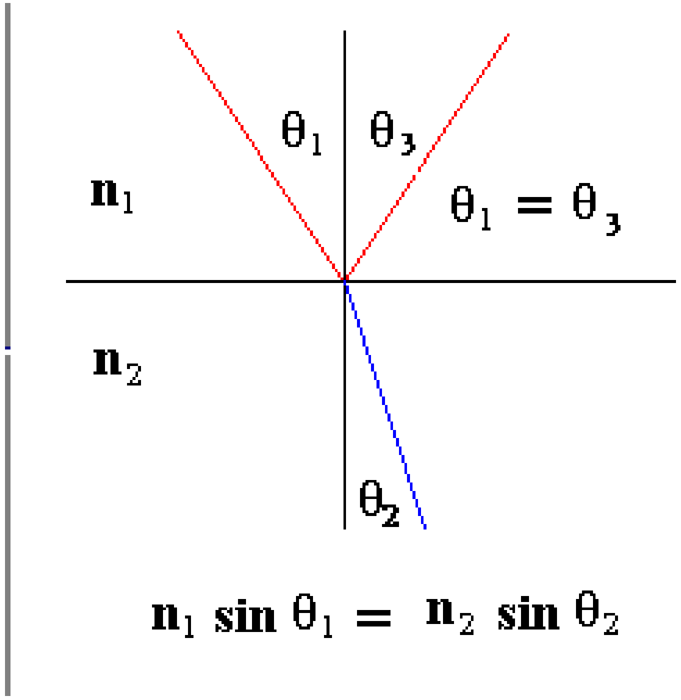
Q: what happens before we take the high frequency limit?

Snell-Decartes Law of refraction

- When a plane wave hits the interface,

  the angles of incident and transmitted waves satisfy ($n=c_0/c$)

  (*Miller, Bal-Keller-Papanicolaou-Ryzhik*)



An interface condition

- We use an interface condition for f that connects (the good) Liouville equations on both sides of the interface.

$$f(x^+, \xi^+)=\alpha_T f(x^-,\xi^-)+\alpha_R f(x^+, -\xi^+) \quad \text{for } \xi^+>0$$

$$H(x^+, \xi^+)=H(x^-,\xi^-)$$

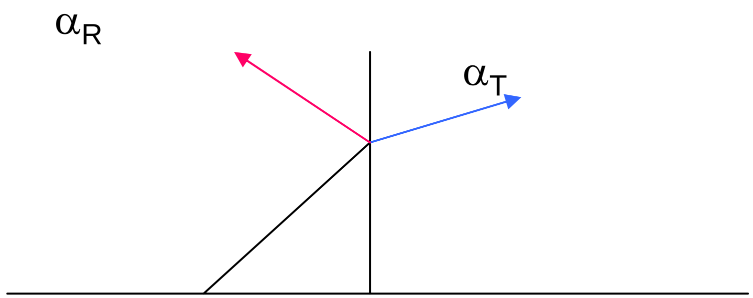
α_R: reflection rate α_T: transmission rate

$$\alpha_R+\alpha_T=1$$

- α_T, α_R defined from the original "microscopic" problems
- This gives a mathematically well-posed problem that is physically relavant
- We can show the interface condition is equivalent to Snell's law in geometrical optics
- A new method of characteristics (bifurcate at interfaces)

Solution to Hamiltonian System with discontinuous Hamiltonians

- This way of defining solutions also gives a definition to the solution of the underlying Hamiltonian system across the interface:



- Particles cross over or be reflected by the corresponding transmission or reflection coefficients (probability)
- Based on this definition we have also developed particle methods (both deterministic and Monte Carlo) methods

Key idea in numerical discretizations

- consider a standard finite difference approximation

$$\partial_t f_{ij} + \xi_j \frac{f^-_{i+\frac{1}{2},j} - f^+_{i-\frac{1}{2},j}}{\Delta x} - \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0,$$

V: piecewise linear approximation—allow good CFL

$f_{I,j+1/2}$, $f^-_{i+1/2,j}$ ---- upwind discretization

$f^+_{i+1/2,\, j}$ ---- incorporating the interface condition

(Perthame-Semioni)

Scheme I (finite difference formulation)

- If at $x_{i+1/2}$ V is continuous, then $f^+_{i+1/2,j} = f^-_{i+1/2,j};$
- Otherwise,

  For $\xi_j > 0$,

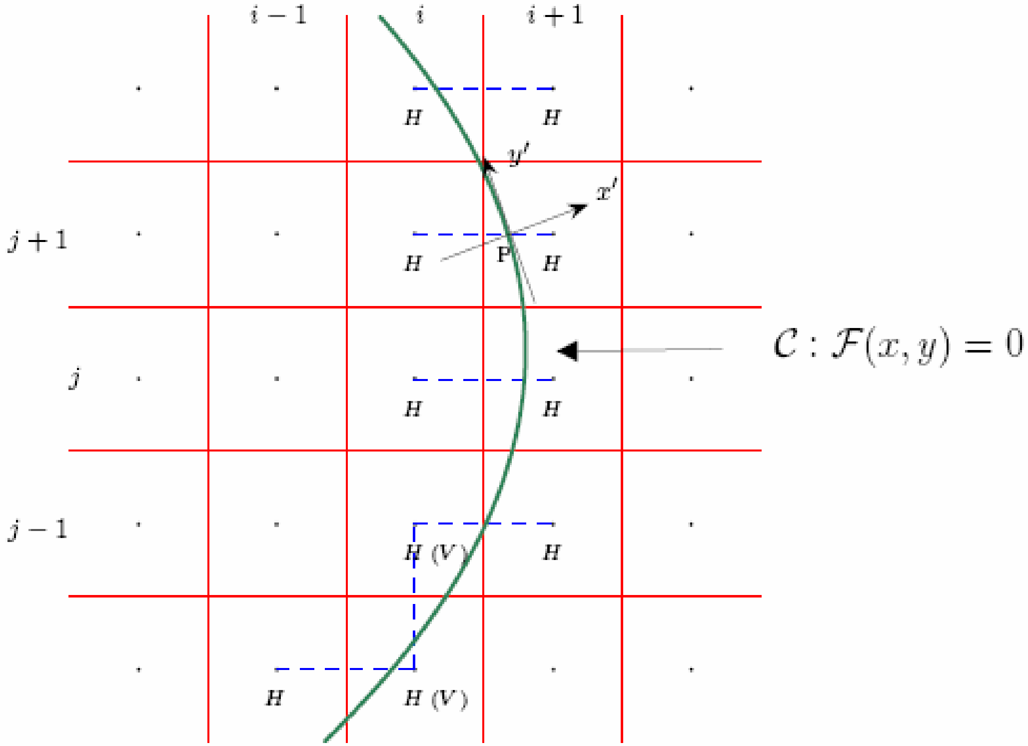
$$f^+_{i+1/2,j} = f(x^+_{i+1/2}, \xi^+)$$

$$= \alpha_T f^-(x^-_{i+1/2}, \xi^-) + \alpha_R f(x^+_{i+1/2}, -\xi^+)$$

$$= \alpha_T f_i(\xi^-) + \alpha_r f_{i+1}(-\xi^+)$$

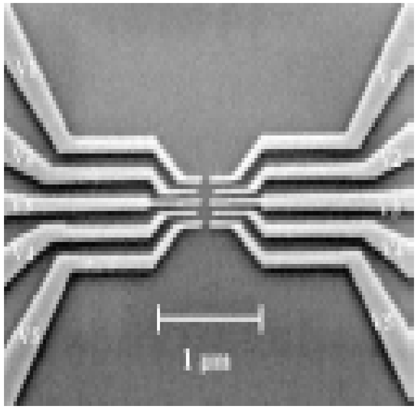
Stabilitly, convergence under the CFL condition

Curved interface



Quantum barrier

We want to study quantum scale phenomena using a largely classical scale model.

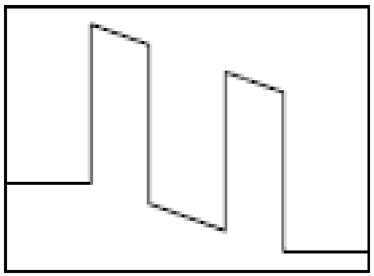


- Nanotechnology
- Electron transport in semiconductors
- Tunneling diodes
- Quantum dot structures
- Quantum computing

A semiclassical approach for thin barriers (with Kyle Novak--AFIT, SIAM Multiscale Model Simul & JCP 06)

- Barrier width in the order of De Broglie length, separated by order one distance
- Solve a time-independent Schrodinger equation for the local barrier/well to determine the scattering data
- Solve the classical liouville equation elsewhere, using the scattering data at the interface

Resonant tunnelling



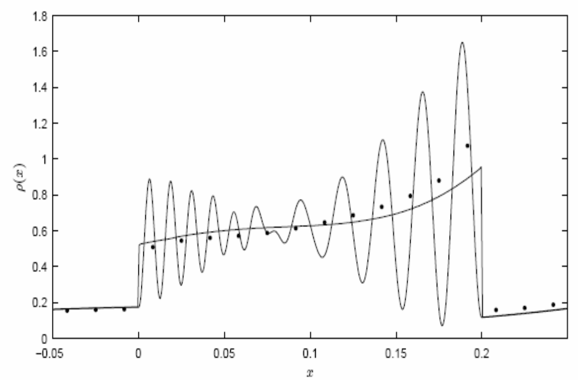


FIG. 5.4. *Detail of Fig. 5.3 showing position densities for the numerical semiclassical Liouville and von Neumann solutions. The • shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the "exact" Liouville solution and the von Neumann solution using* $\varepsilon = 0.002$.

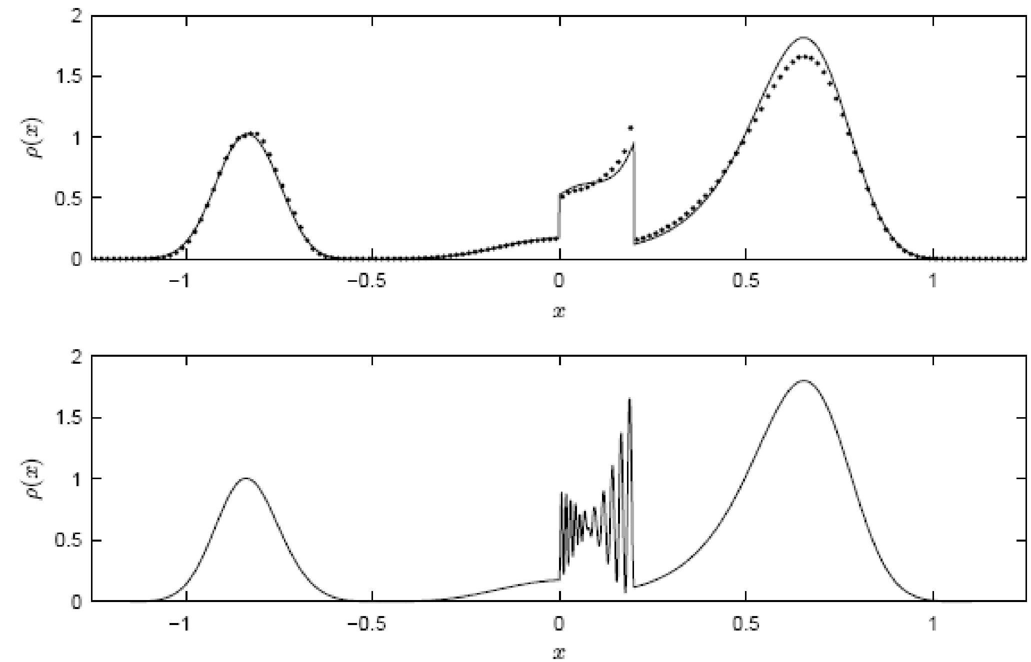
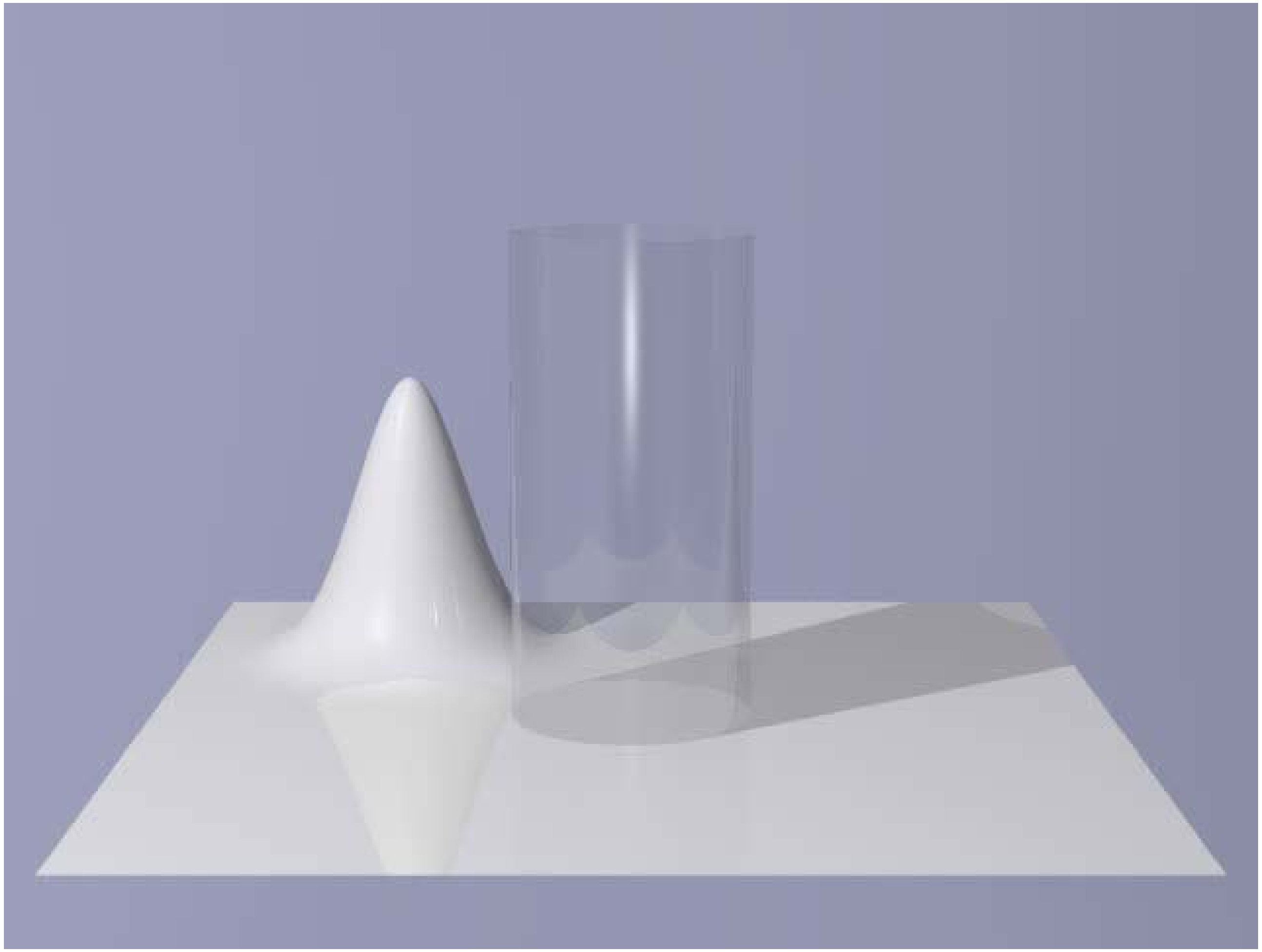
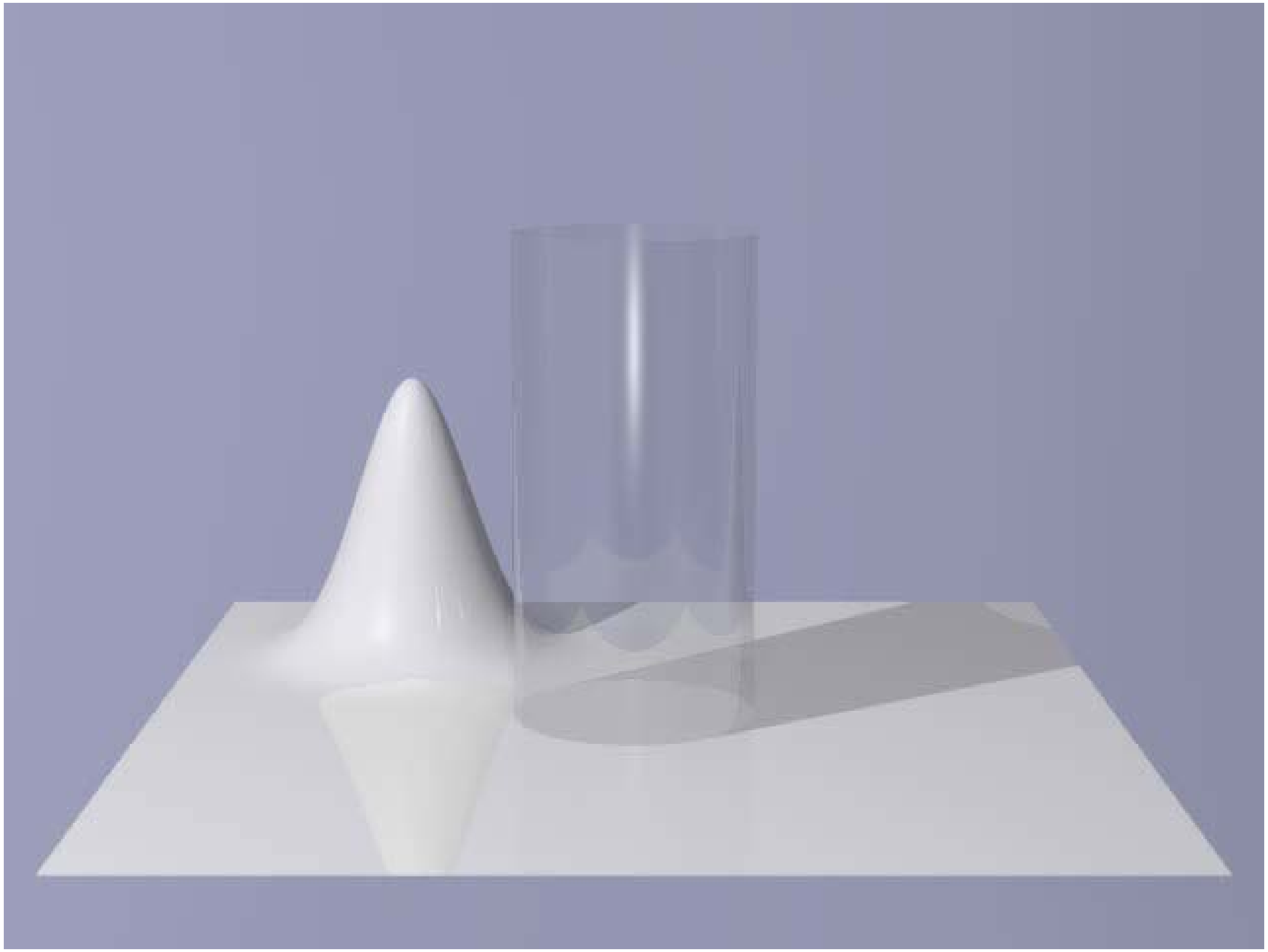


FIG. 5.3. *Position densities for the numerical semiclassical Liouville (top) and von Neumann (bottom) solutions of Example 5.3. The • in the Liouville plot shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the numerical solution for 3200 grid points. The von Neumann solution is for* $\varepsilon = 0.002$.

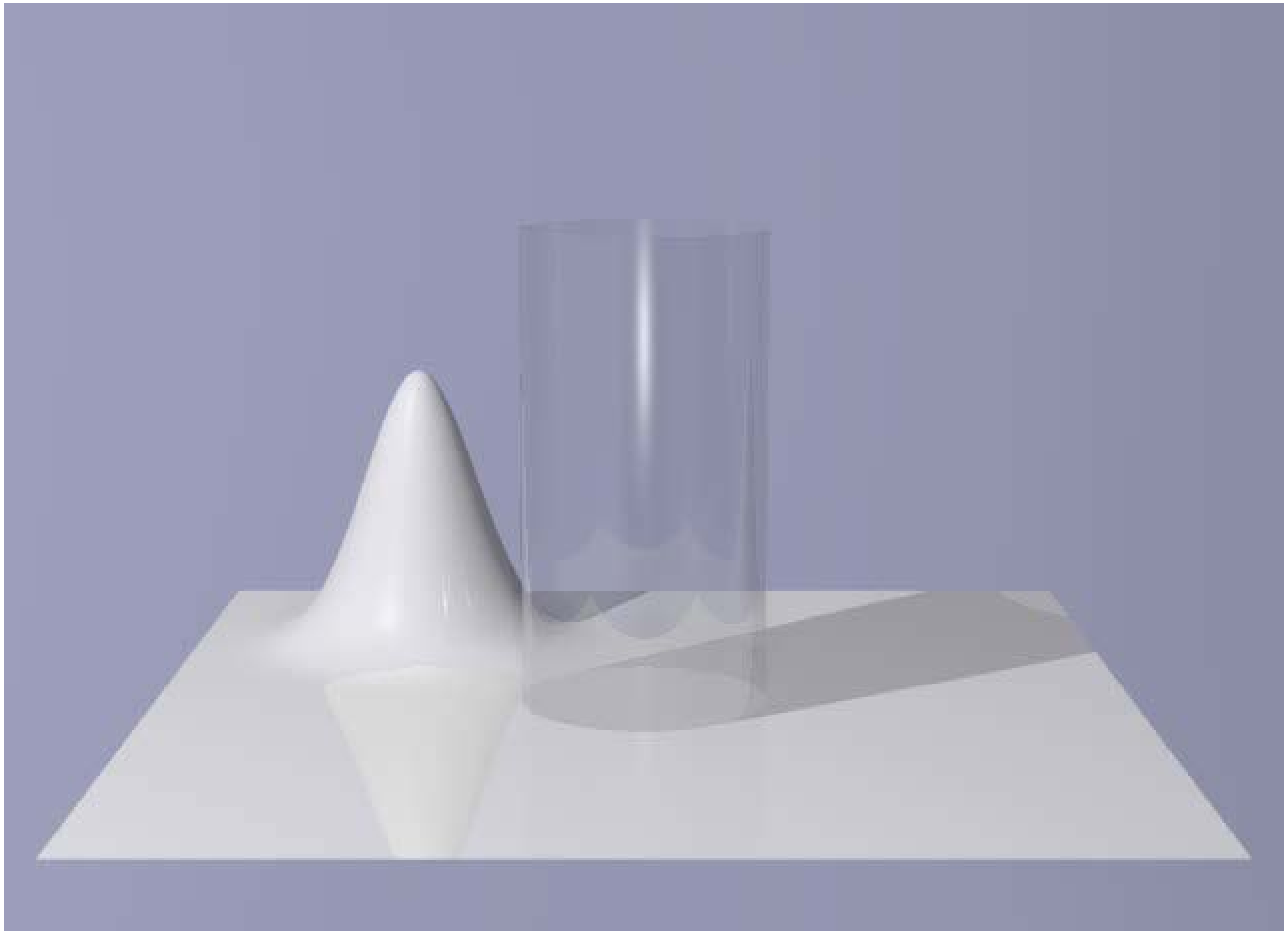
Circular barrier (Schrodinger with ε=1/400)



Circular barrier (semiclassical model)

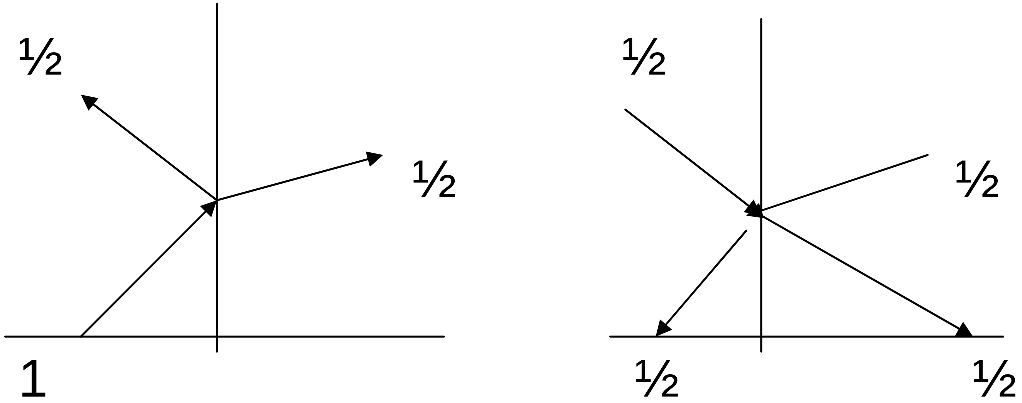


Circular barrier (classical model)



Entropy

- The semiclassical model is time-irreversible.



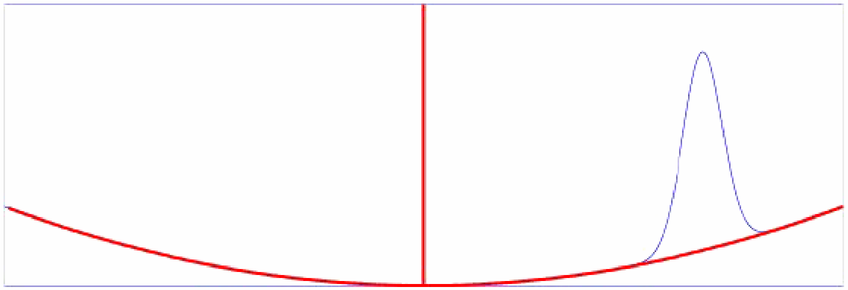
Loss of the phase information

cannot deal with interference

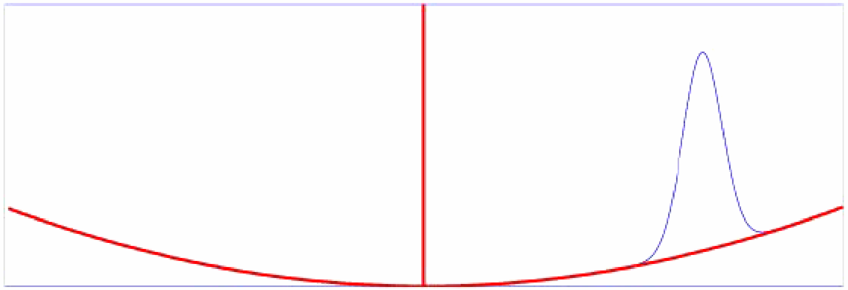
decoherence

$V(x) = \delta(x) + x^2/2$

Quantum



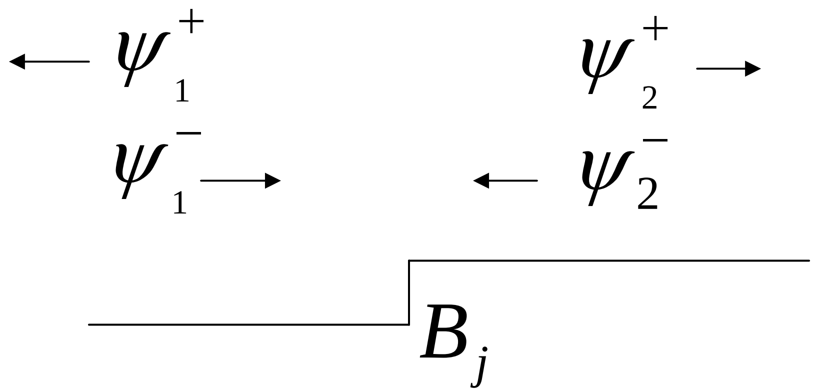
semiclassical



A Coherent Semiclassical Model

Initialization:

- Divide barrier into several thin barriers $B_1, B_2, \ldots, B_n$
- Solve stationary Schrödinger equation



- Matching conditions

$$\begin{pmatrix} \psi_1^+ \\ \psi_2^+ \end{pmatrix} = \begin{pmatrix} r_1 & t_2 \\ t_1 & r_2 \end{pmatrix} \begin{pmatrix} \psi_1^- \\ \psi_2^- \end{pmatrix} = S_j \begin{pmatrix} \psi_1^- \\ \psi_2^- \end{pmatrix}$$

A coherent model

- Initial conditions $\Phi(x,p,0)=\sqrt{f(x,p,0)}$
- Solve Liouville equation

$$\frac{d\Phi}{dt}=\frac{\partial\Phi}{dt}+p\frac{\partial\Phi}{dx}-\frac{dV}{dx}\frac{\partial\Phi}{dp}=0$$

- Interface condition

$$\begin{pmatrix}\Phi^{+}_{j-1}\\ \Phi^{+}_{j}\end{pmatrix}=S_j\begin{pmatrix}\Phi^{-}_{j-1}\\ \Phi^{-}_{j}\end{pmatrix}$$

- Solution $f(x,p,t)=\left|\Phi(x,p,t)\right|^2$

Interference

Define the semiclassical probability amplitude as

$$\Phi(x,p,t) = \sqrt{f(x,p,t)}e^{i\theta(x,p)}$$

where $\theta(x,p)$ is the phase offset from the initial conditions $\Phi(x,p,0) = \sqrt{f(x,p,0)}$.

Hence, if $\Phi(x,p,t)$ is a solution to the Liouville equation for initial condition $\Phi(x,p,0)$, then $f_{\mathrm{coh}}(x,p,t)$ is a solution to the Liouville equation for initial condition $f_{\mathrm{coh}}(x,p,0)$. Furthermore, for two solutions Φ_1 and Φ_2 with $f_1 = |\Phi_1|^2$ and $f_2 = |\Phi_2|^2$,

$$|\Phi_1 + \Phi_2|^2 = f_1 + f_2 + 2\sqrt{f_1 f_2}\cos(\theta_1 - \theta_2). \tag{10}$$

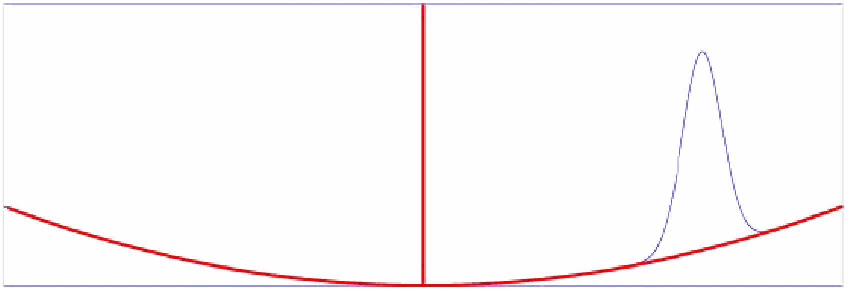
For any two probability densities ψ_1 and ψ_2 with with $\rho_1 = \int f_1\, dp = |\psi_1|^2$ and $\rho_2 = \int f_2\, dp = |\psi_2|^2$,

$$|\psi_1 + \psi_2|^2 = \rho_1 + \rho_2 + 2\sqrt{\rho_1 \rho_2}\cos(\theta_1 - \theta_2). \tag{11}$$

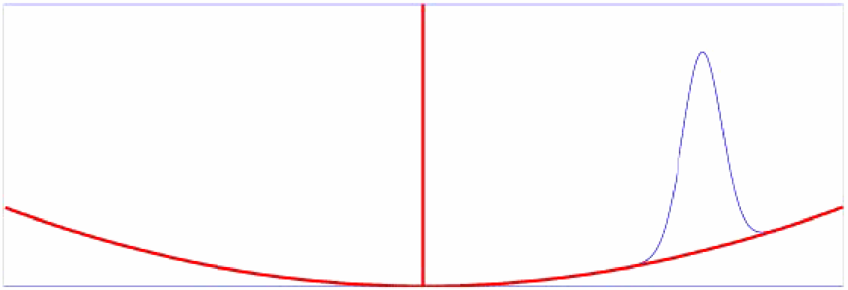
The coherent model

- $V(x) = \delta(x) + x^2/2$

Quantum



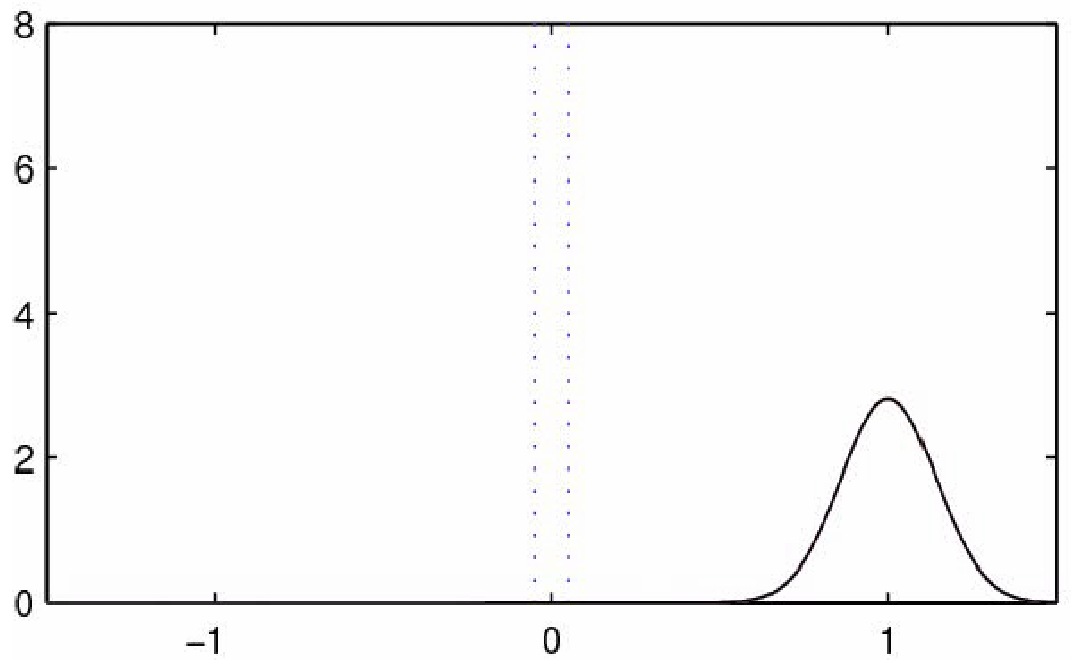
semiclassical



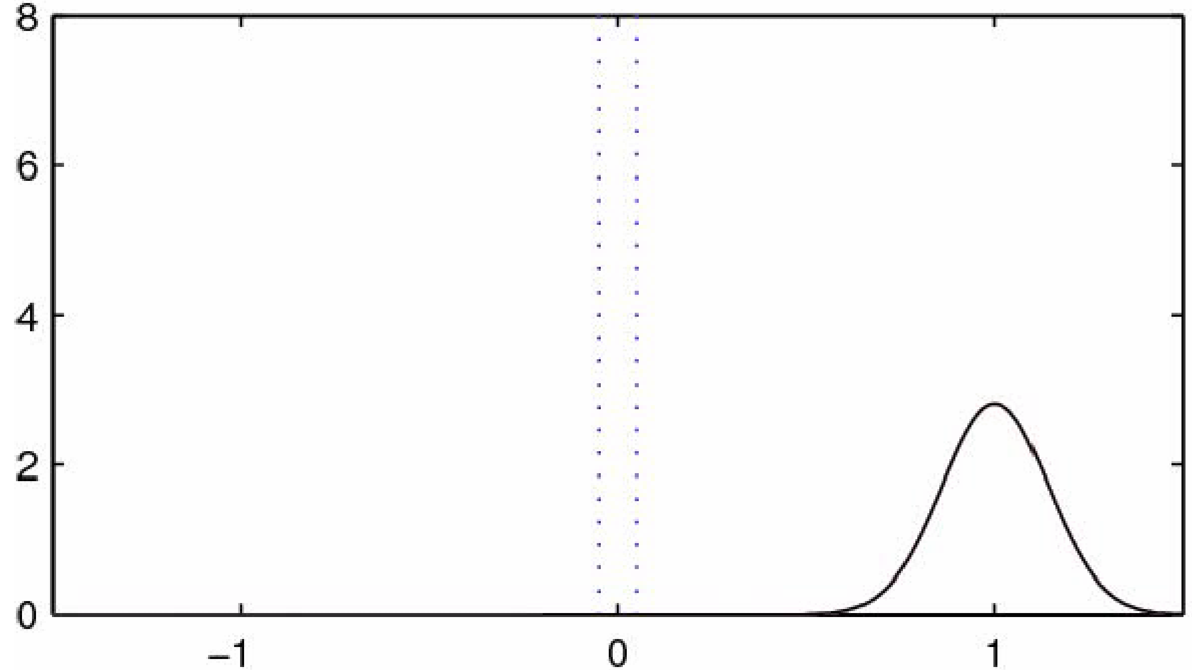
Another example

- $V(x) = \alpha\,[\,\delta(-l/2)+\delta(l/2)\,]$
  α=-1.5 ε, l=10 ε,
  ε=0.01

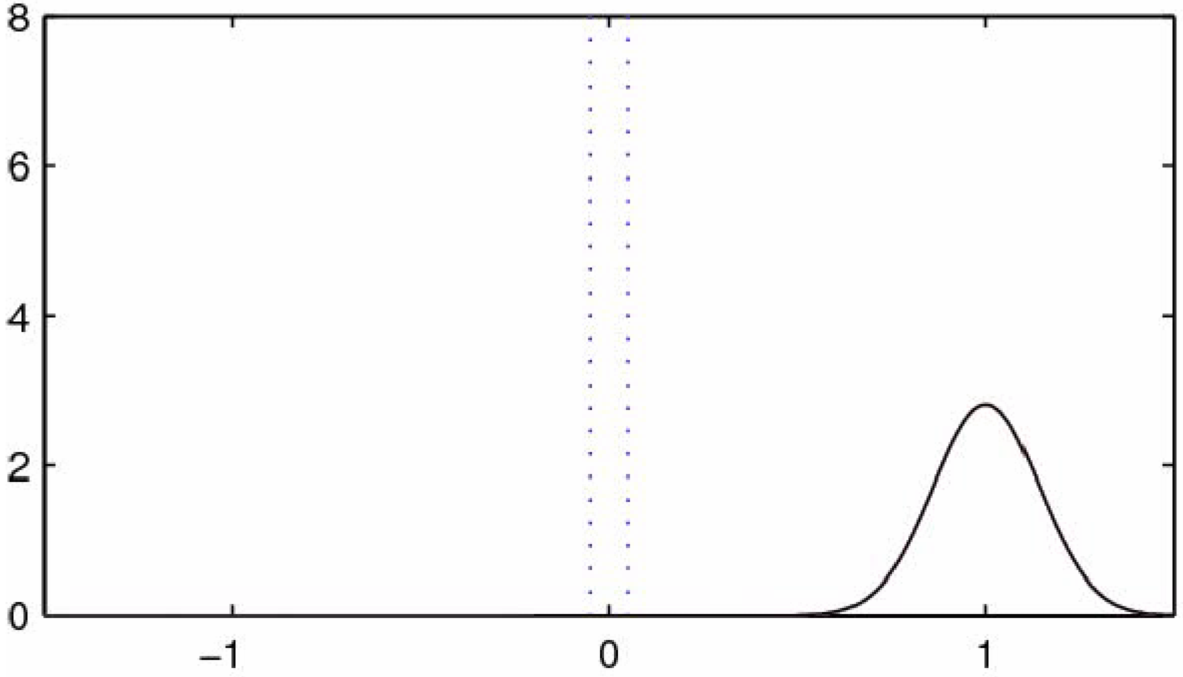
thin single
barrier
model



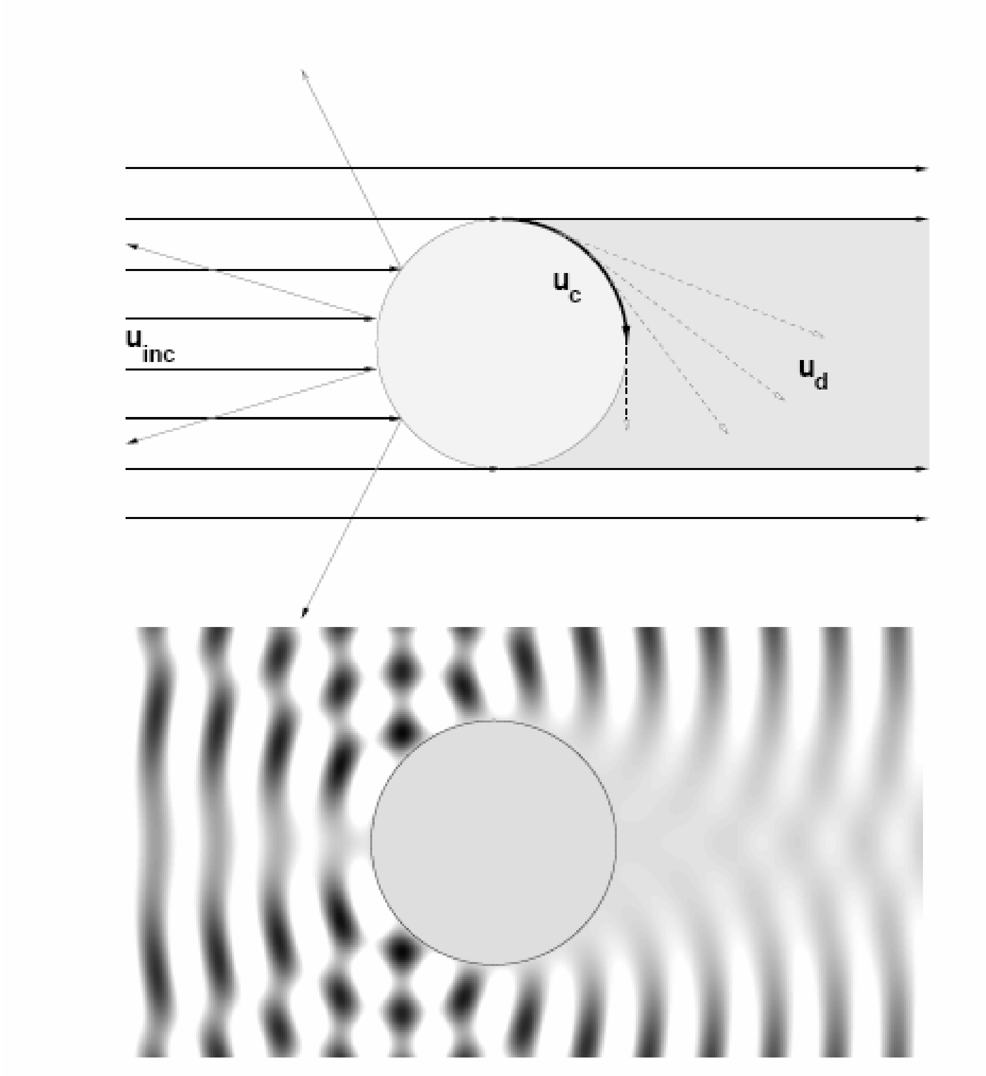
The decoherent model (two thinn barriers)



The coherent model (two thin barriers)



VI. Computation of diffraction (with *Dongsheng Yin*)



Transmissions, reflections and diffractions (Type A interface)

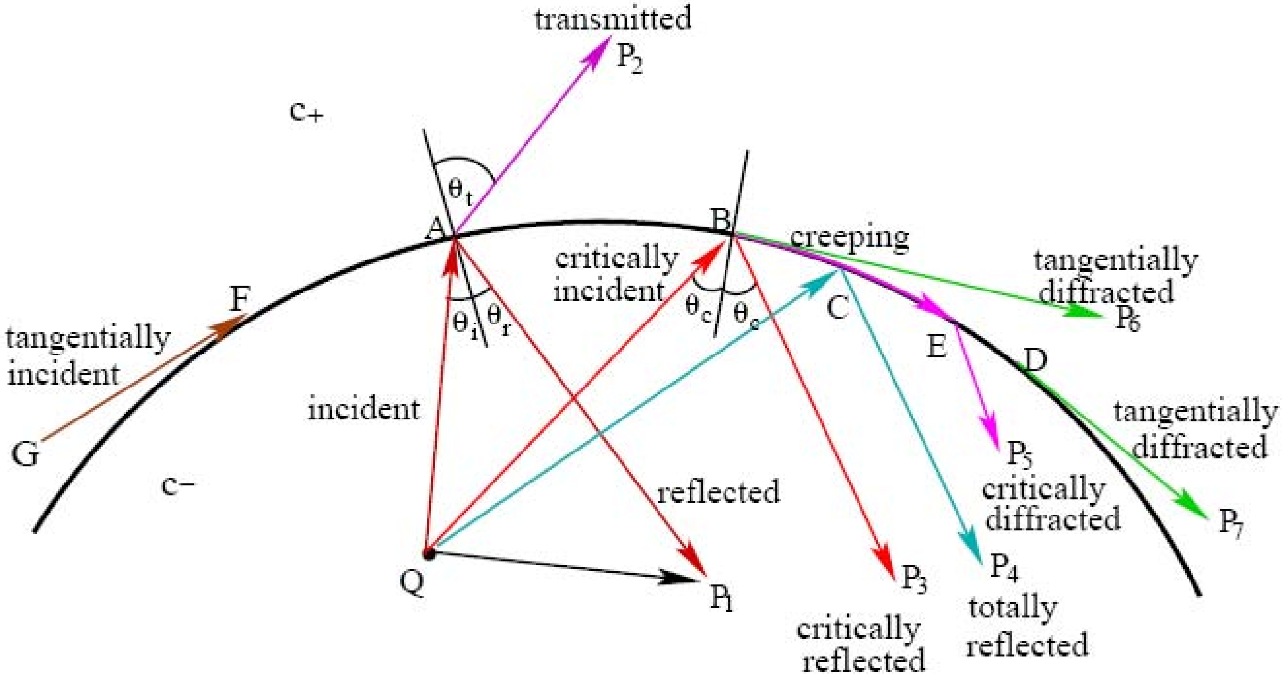


Figure 1: wave reflection, transmission and diffraction at a Type A interface

Type B interface

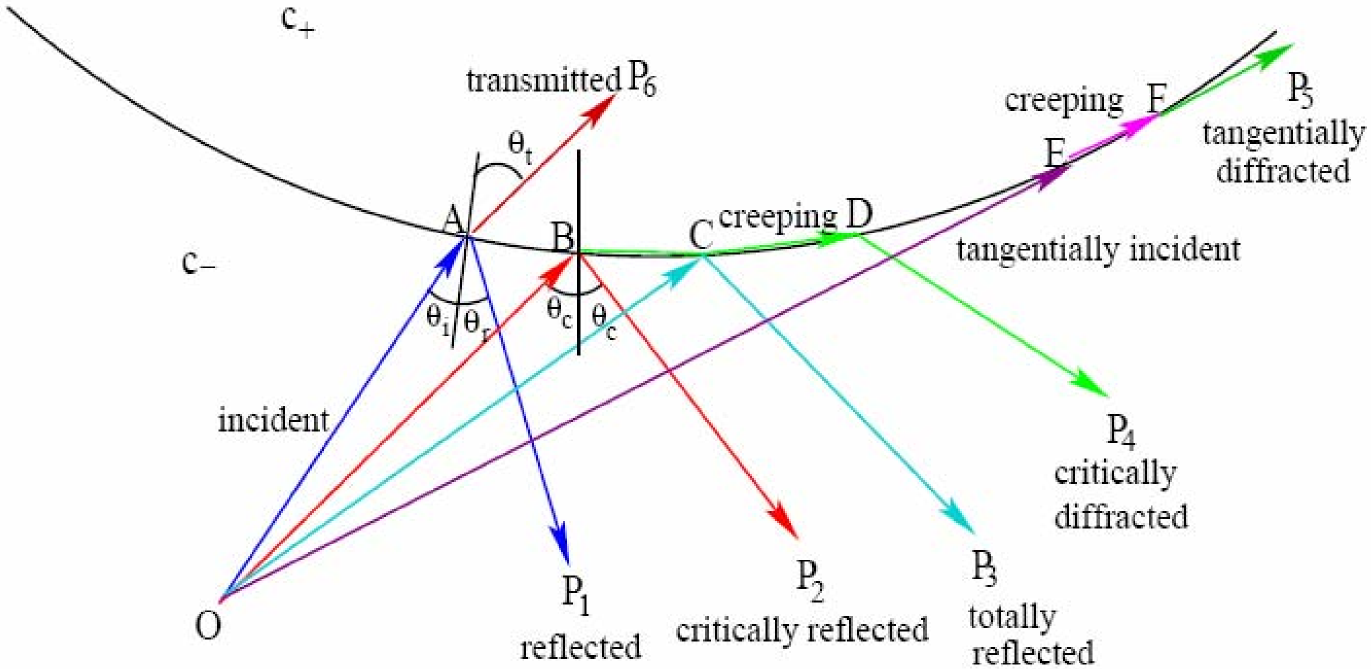


Figure 2: wave reflection, transmission and diffraction at a Type B interface

Hamiltonian preserving+Geometric Theory of Diffraction

- We uncorporate Keller's GTD theory into the interface condition:

Next, we consider a **Type A** interface. If $\xi^{-\prime} < 0$,

$$f(t,\mathbf{x}^-,\xi^{-\prime},\eta^{-\prime}) = \begin{cases} \alpha^D_{A_3,-}(\mathbf{x}) \sum_{q,l,m} \alpha^D_{A_3,-}(\mathbf{x}_q) e^{-\int_{s_q}^{s} \beta_{A_3,-}(z)dz} f(t-\bar{t}_q, \mathbf{x}_q^-, \xi_l^{-\prime}, \eta_m^{-\prime}) \\ +\left(1-\alpha^D_{A_3,-}(\mathbf{x})\right) f(t,\mathbf{x}^-,-\xi^{-\prime},\eta^{-\prime}), \qquad \textbf{(case II)} \\ \qquad \text{if } \left(\frac{c^-}{c^+}\right)^2 (\xi^{-\prime})^2 + \left[\left(\frac{c^-}{c^+}\right)^2 - 1\right](\eta^{-\prime})^2 = 0, \\ \alpha^R_- f(t,\mathbf{x}^-,-\xi^{-\prime},\eta^{-\prime}) + \alpha^T_- f(t,\mathbf{x}^+,\xi^{+\prime},\eta^{+\prime}), \\ \qquad \text{if } \left(\frac{c^-}{c^+}\right)^2 (\xi^{-\prime})^2 + \left[\left(\frac{c^-}{c^+}\right)^2 - 1\right](\eta^{-\prime})^2 > 0. \end{cases}$$

For ${\xi^+}' = 0$ (**case I**),

$$f_+(t, \mathbf{x}^+, {\xi^+}', {\eta^+}') = \alpha^D_{A_1,+}(\mathbf{x}) \sum_{q,l,m} \alpha^D_{A_1,+}(\mathbf{x}_q) e^{-\int_{s_q}^{s} \beta_{A_1,+}(z)dz} f_-(t - \bar{t}_q, \mathbf{x}^+_q, {\xi^+_l}', {\eta^+_m}')$$
$$+ \alpha^D_{A_2,+}(\mathbf{x}) \sum_{q_1,l_1,m_1} \alpha^D_{A_2,+}(\mathbf{x}_p) e^{-\int_{s_{q_1}}^{s} \beta_{A_2,+}(z)dz} f(t - \bar{t}_{q_1}, \mathbf{x}^-_{q_1}, {\xi^-_{l_1}}', {\eta^-_{m_1}}'),$$

and correspondingly for ${\xi^-}' = \sqrt{[(c^+/c^-)^2 - 1](\eta')^2}$,

$$f(t, \mathbf{x}^-, {\xi^-}', {\eta^-}') = (1 - \alpha^D_{A_1,+}) f_-(t, \mathbf{x}^+, {\xi^+}', {\eta^+}'),$$

A type B interface

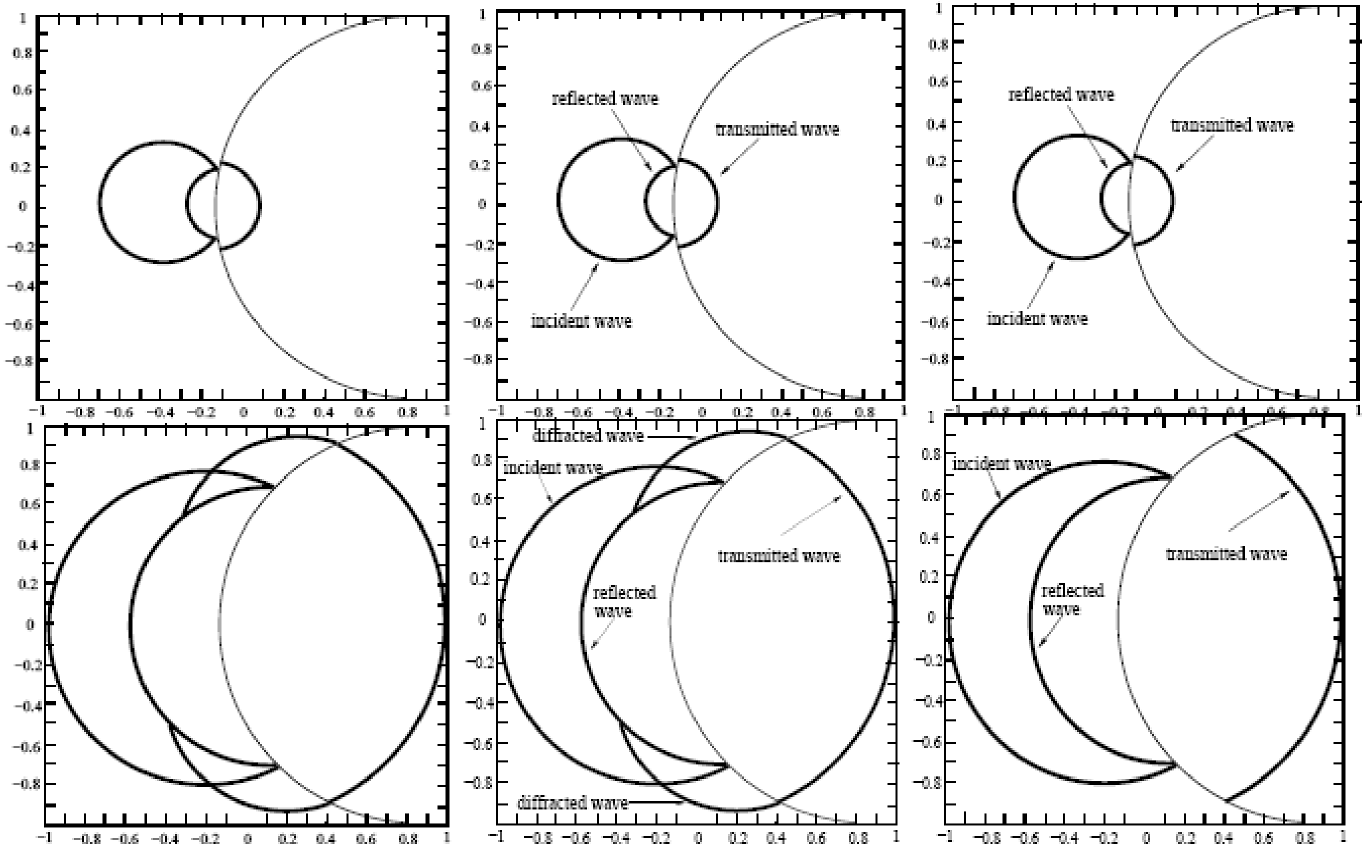


Figure 4: Example 5.1, wavefront of energy density $\mathcal{E}$ and $\mathcal{E}^{(0)}$ at $t = 0.1$ (top) and 0.4 (bottom). Left: $\mathcal{E}$; middle: $\mathcal{E}^{(0)}$ by GTD; right: $\mathcal{E}^{(0)}$ by GO.

Another type B interface

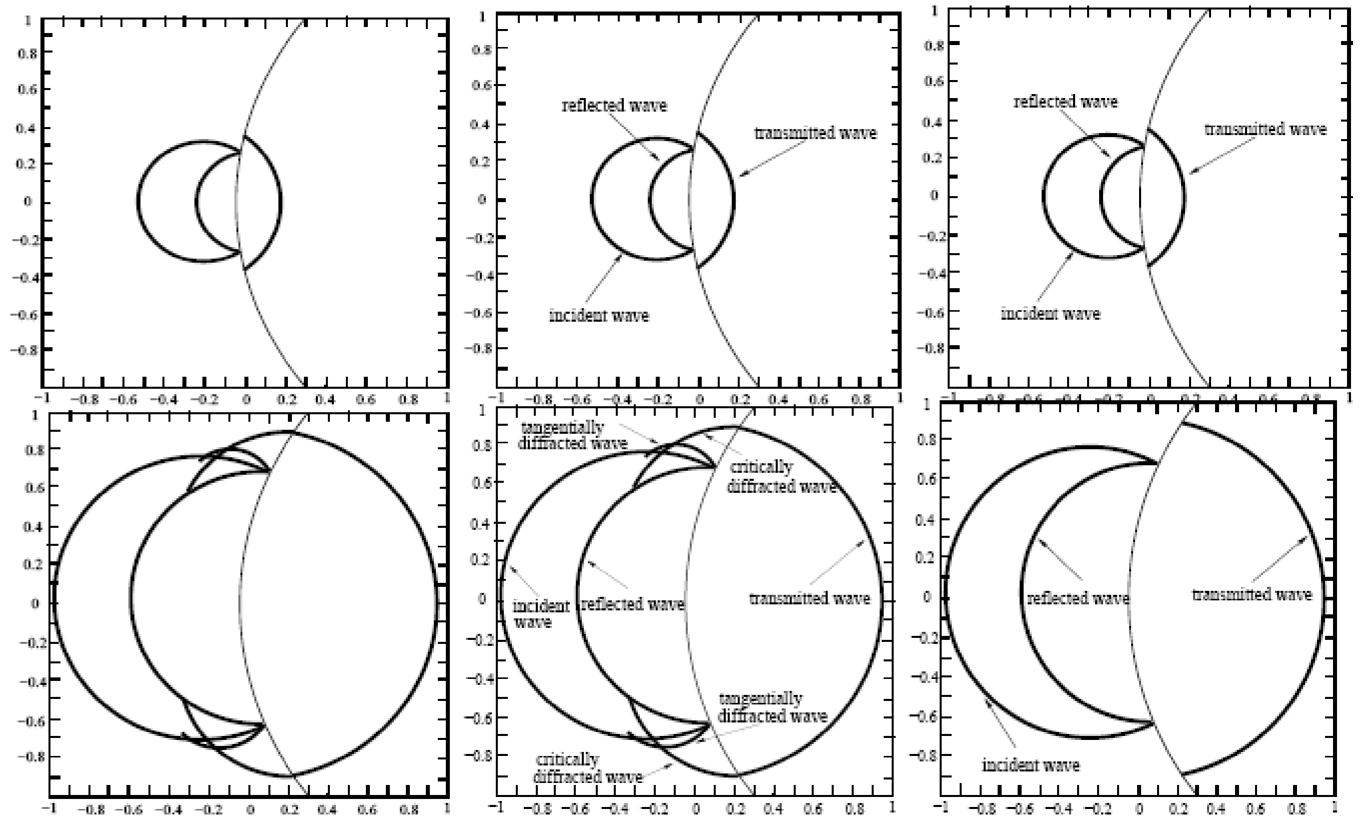


Figure 6: Example 5.2, wavefront of energy density $\mathcal{E}$ and $\mathcal{E}^{(0)}$ at $t = 0.15$ (top) and 0.5 (bottom). Left: $\mathcal{E}$; middle: $\mathcal{E}^{(0)}$ by GTD; right: $\mathcal{E}^{(0)}$ by GO.

A type A interface

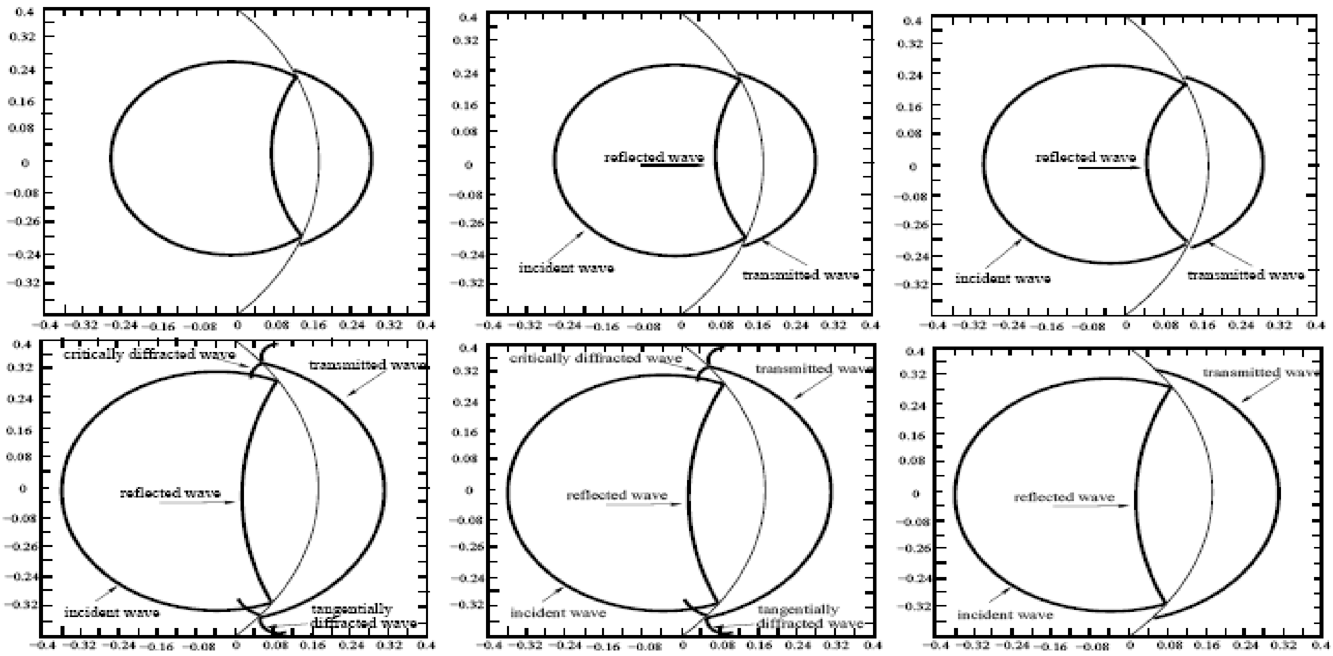


Figure 8: Example 5.3, wavefront of energy density $\mathcal{E}$ and $\mathcal{E}^{(0)}$ at $t = 0.1$ (top) and 0.2 (bottom). Left: $\mathcal{E}$; middle: $\mathcal{E}^{(0)}$ by GTD; right: $\mathcal{E}^{(0)}$ by GO.

Half plane

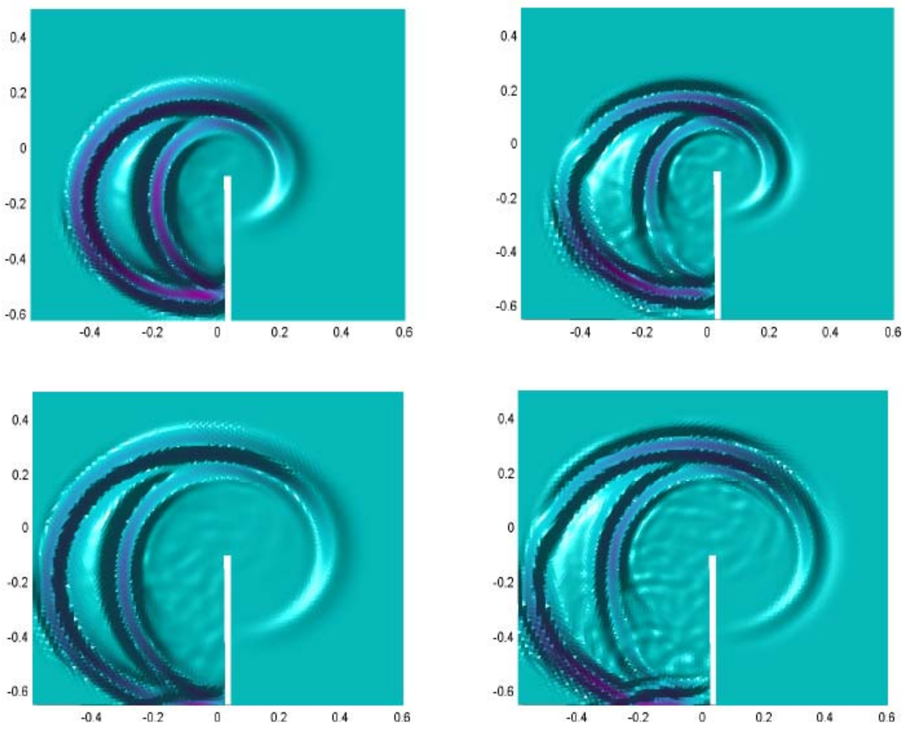


Figure 4: Example 5.1, energy density $\mathcal{E}^{(0)}$ and $\mathcal{E}$ at $t = 0.2$ (top) and 0.3 (bottom). Left: $\mathcal{E}^{(0)}$ by GTD; right: $\mathcal{E}$.

Computational cost ($\varepsilon=10^{-6}$)

- Full simulation of original problem for

$$\Delta x \sim \Delta t \sim O(\varepsilon)=O(10^{-6})$$

Dimension	total cost
2d,	$O(10^{18})$
3d	$O(10^{24})$

- Liouville based solver for diffraction

$$\Delta x \sim \Delta t \sim O(\varepsilon^{1/3}) = O(10^{-2})$$

Dimension	total cost
2d,	$O(10^{10})$
3d	$O(10^{14})$

Can be less with local mesh refinement

Other applications and ongoing projects

The wigner tranform works for any linear symmetric hyperbolic systems: elastic waves, electromagneticwaves, etc.

- Elastic waves (with *Xiaomei Liao, J. Hyp. Diff Eq. 06*)
- High frequency waves in random media with interfaces (with *X. Liao, X. Yang*)

Summary

- Developed finite difference, finite element, and particle (both Monte Carlo and deterministic) methods

- Able to compute (partial) transmission, reflection, and diffraction for many high frequency waves (geometrical optics, semiclassical limit of Schrodinger, elastic wave, thin quantum barrier, high frequency waves in random media, diffractions, etc.) without fully resolving the high frequency:

  only use Liouville equation + interface condition

- wide quantum barriers (under development)
- Mathematical theory: singular Hamiltonian systems—use (classical) particles to do (quantum) waves