Well-balancedness, Hamiltonian preserving, and beyond

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Outline

- Hyperbolic systems with singular coefficients
- Well-balancedness in shallow-water equations
- Hamiltonian preservation in singular Hamiltonian system
- High frequency waves through interfaces/barriers
- Quantum-classical coupling

Hyperbolic systems with singular coefficients

$$(2.1) \qquad \begin{cases} \partial_t u + \partial_x \left(c(x)u\right) = 0, & t > 0, x \in \mathbb{R}, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases}$$

with a piecewise constant coefficient

$$(2.2) \qquad c(x) = \begin{cases} c^- > 0, & x < 0, \\ c^+ > 0, & x > 0. \end{cases}$$

- Applications: wave propagation through interfaces

Renormalized solutions

- Discontinuous coefficients: DiPerna-Lions, Ambrosio, Perthame, Bouchut, James, Hauray, Jabin, …

Interface condition

- We take a different route– since these problems arise in wave propagation through interface, one physical condition—the interface condition—should be added to determine a unique solution

$$u(0^+, t) = \rho\, u(0^-, t)$$

$\rho = 1$ conservation of mass u

$\rho = c^- / c^+$ conservation of flux cu

Then the initial value problem is well-posed (method of characteristics)

The (generalized) method of characterisitcs

$$\frac{\partial x}{\partial t} = c(x)\,, \quad x(0) = x_0$$

- For $x_1<0$

$$x(t) = \begin{cases} x_0 + c_- t & \text{for} \quad t \le t_c = -x_0/c_- \\ x_1 + c_+ t & \text{for} \quad t > t_c \end{cases}$$

- x_1 cannot be determined unless one provides an interface condition at x=0
- If x is continuous then $x_1=0$, corresponds to $\rho=1$;
- How to define solution when $\rho \neq 1$?

Numerical discretization

- Immersed interface method

(Peskin, Mayo, LeVeque-Li, LeVeque-Zhang)

$$\partial_t U_j + \frac{1}{\Delta x}\left(c^-_{j+1/2}U^-_{j+1/2} - c^+_{j-1/2}U^+_{j-1/2}\right)$$

$$U^-_{j+1/2} = U_j, \qquad U^+_{j+1/2} = \rho_{j+1/2}U^-_{j+1/2}$$

$$\rho_{j+1/2} = \begin{cases} 1 & \text{if } j \neq 0 \\ \rho, & \text{if } j = 0 \end{cases}$$

If ρ=1 (no interface), this is just the upwind scheme

convergence and l^1 error estimate: Jin-Wen, Jin-Qi

Shallow-water equations

- h- height; v: mean velocity, g: gravitational constant, B(x): bottom topography (can be discontinous!)

$$\partial_t h + \partial_x (hv) = 0,$$
$$\partial_t (hv) + \partial_x \left(hv^2 + \frac{1}{2} g h^2 \right) = -gh\partial_x B$$

Steady-state

$$\partial_x(hv) = 0,$$
$$\partial_x\left(hv^2 + \frac{1}{2}gh^2\right) = -gh\partial_x B$$

- When B(x) is continuous, B'(x) is measure-valued, this system of ODEs has measure-valued right hand side. A condition needs to be provided to select the unique solution (Diperna-Lions theory for discontinuous or BV RHS does not apply here):

- $hv = C_1,$ Conservation of momentum
- $E(h,u,B) = \frac{1}{2}v^2 + gh + gB = C_2$ Conservation of energy

Well-balanced schemes

- Constructing numerical schemes to preserve these conservations:

  Roe, Bermudez-Vasquez, Greenberg-LeRoux, Gosse, LeVeque, Botchorishvili-Perthame-Vasseur, Perthame-Simeoni, Jin, Bouchut, Wen-Jin, Levy-Kurganov, Russo, Shu, Noelle, Karni, Pares…

  Presevation is either exact or at least second-order accuracy

The Perthame-Simeoni approach

- kinetic formulation of shallow-water equations

$$\partial_t M + \xi\,\partial_x M - g\,\partial_x B\,\partial_\xi M = Q(t,x,\xi) \tag{3.7}$$

where

$$M(t,x,\xi) = M(h,\xi-u) = \sqrt{h(t,x)}\,\chi\left(\frac{\xi-u(t,x)}{\sqrt{h(t,x)}}\right), \tag{3.8}$$

$$\chi(\omega) = \frac{\sqrt{2}}{\pi\sqrt{g}}\left(1-\frac{\omega^2}{2g}\right)_+^{1/2}, \tag{3.9}$$

for some collision term $Q(t,x,\xi)$ which satisfies, for almost every (t,x),

$$\int_R Q\,d\xi = 0\,, \qquad \int_R \xi Q\,d\xi = 0\,. \tag{3.10}$$

Furthermore, the χ chosen in (3.9) is the only function such that M defined in (3.8) satisfies the steady state equation

$$\xi\,\partial_x M - g\,\partial_x B\,\partial_\xi M = 0 \tag{3.11}$$

on all steady state given by a *lake at rest*:

$$u(t,x) = 0, \quad h(t,x) + B(x) = H\,, \quad \forall t \geq 0\,. \tag{3.12}$$

Moments:

The macroscopic quantities in the shallow water equations can be recovered from the kinetic variable M by taking the first three moments, defined by

$$h = \int_R M(h, \xi - u)\, d\xi\,, \tag{3.13}$$

$$hu = \int_R \xi M(h, \xi - u)\, d\xi\,, \tag{3.14}$$

$$hu^2 + \frac{1}{2}gh^2 = \int_R \xi^2 M(h, \xi - u)\, d\xi\,. \tag{3.15}$$

By multiplying the kinetic equation (3.7) with $(1, \xi)$ one obtains the shallow-water equations (2.1).

The numerical approximation

- Building in particle transmission/reflection:

$$\partial_t f_i(\xi) + \frac{1}{\Delta x}\xi\left(M^-_{i+1/2} - M^+_{i-1/2}(\xi)\right) = 0\,;$$

$$(3.17) \qquad M^-_{i+1/2}(\xi) = M_i(\xi)\,\mathbf{I}_{\xi\geq 0} + M_{i+1/2}(\xi)\,\mathbf{I}_{\xi\leq 0}$$

$$(3.18) \qquad M^+_{i-1/2}(\xi) = M_{i-1/2}(\xi)\,\mathbf{I}_{\xi\geq 0} + M_i(\xi)\,\mathbf{I}_{\xi\leq 0}$$

where $\mathbf{I}_A$ is the characteristic function with support at set A, and

$$(3.19) \qquad M_{i+1/2}(\xi) = M_i(-\xi)\,\mathbf{I}_{|\xi|^2\leq 2g\Delta B_{i+1/2}}$$

$$(3.20) \qquad +M_{i+1}\left(-\sqrt{|\xi|^2 - 2g\Delta B_{i+1/2}}\right)\,\mathbf{I}_{|\xi|^2\geq 2g\Delta B_{i+1/2}}\,,$$

$$(3.21) \qquad M_{i-1/2}(\xi) = M_i(-\xi)\,\mathbf{I}_{|\xi|^2\leq 2g\Delta B_{i+1/2}}$$

$$(3.22) \qquad +M_{i-1}\left(-\sqrt{|\xi|^2 - 2g\Delta B_{i-1/2}}\right)\,\mathbf{I}_{|\xi|^2\geq 2g\Delta B_{i-1/2}}\,,$$

with $\Delta B_{i+1/2} = B^+_{i+1/2} - B^- i + 1/2$. An important feature of this scheme is that *it builds the microscopic physical of particle collisions with barriers (either transmission and reflection) into the numerical flux.*

- One take the moments of these schemes to get a WB scheme for shallow-water equations

Fugure illustration

- Classical particle transmission and reflection

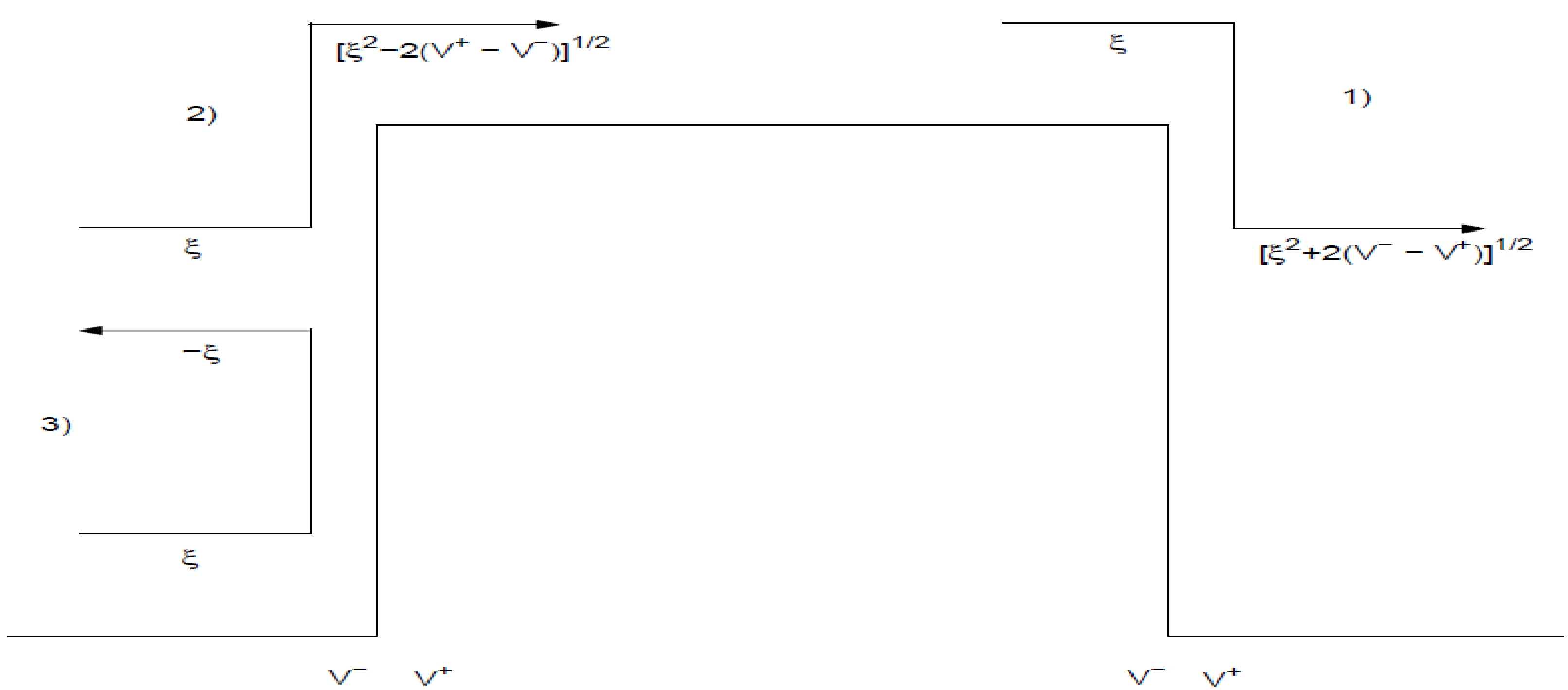


FIG. 2.1. *Change of particle momentum across a potential barrier for the case when* $\xi^- > 0$.

Hamiltonian system in Classical Mechanics

- a Hamiltonian system:

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

$H=H(x, \xi)$ is the Hamiltonian

Classical mechanics: $H=1/2\,|\xi|^2+V(\mathbf{x})$ (=> Newton's second law)
Geometrical optics: $H = c(\mathbf{x})\,|\xi|$

computational method based on solving the Hamiltonian system is referred to as the particle method, of a Lagrangian method

- Phase space representation:

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

$f(t, x, \xi)$ is the density distribution of a classical particle at position x, time t, with momentum ξ

The Liouville equation can be solved by method of characteristics if H is smooth

Discontinuous Hamiltonians

- $H=1/2|\xi|^2+V(x)$: $V(x)$ 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, wave propagation through interfaces between different materials or media, 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?

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

- How to define a solution of systems of ODEs when the RHS is discontinuous or/and measure-valued? (DiPerna-Lions renormalized solution does not apply here)

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, one can smooth out V then $Dv\_i=O(1/\Delta x)$, thus

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

poor resoultion (for complete transmission)

wrong solution (for partial transmission)

Mathematical and Numerical Approaches

- Liouville equation is the semiclassical limit of the (quantum) Schrodinger equation

  Lions-Paul, Gerard-Markowich-Mauser-Poupaud

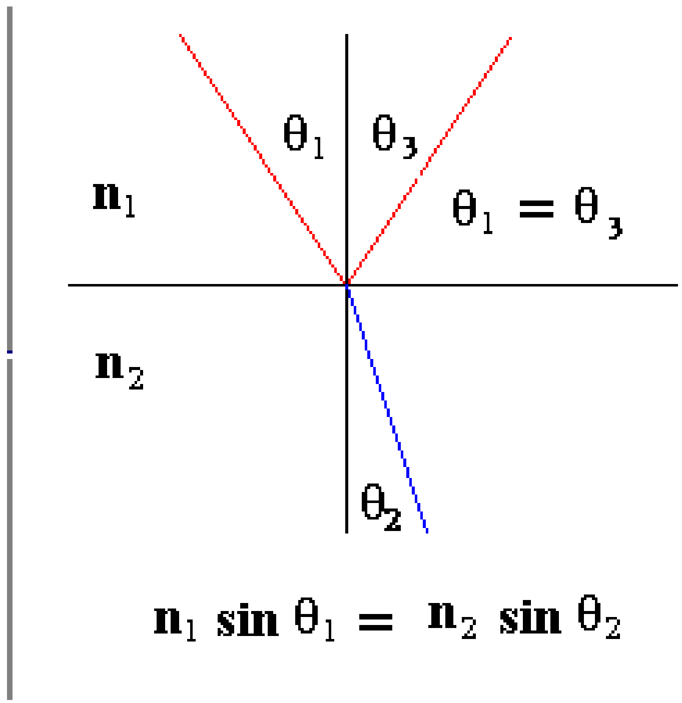
- High frequency limit needs to take into consideration of wave transmissions and reflections

  L. Miller, Bal-Keller-Papanicolaou-Ryzhik

Snell-Decartes Law of refraction

- When a plane wave hits the interface,

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



An interface condition

an interface condition for f should be used to connect
(the good) Liouville equations on both sides of the interface.

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

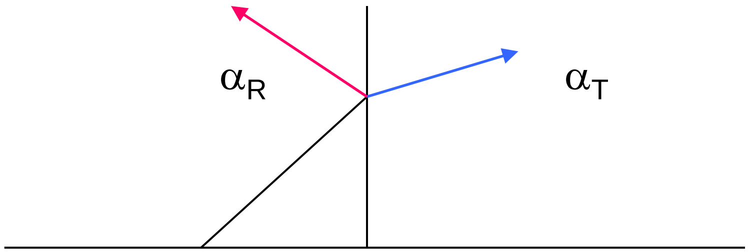
$$H(x^+, \xi^+) = H(x^-, \xi^-)$$

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 relevant
- We can show the interface condition is equivalent to Snell's law in geometrical optics

Solution to Hamiltonian System with discontinuous Hamiltonians



- 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

Numerical discreitzation

- One can use the Perthame-Semioni method to discretize this equation: interface condition can be built into the numerical flux
- Stability is a hyperbolic CFL condition

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|}{\Delta \xi} \right] \leq 1.$$

- Note the discrete derivative of V is defined only on **continuous** points of V, thus

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

Positivity, stability, l^1-convergence

- for first order scheme (forward Euler in time + upwind in space), under the “good” CFL condition

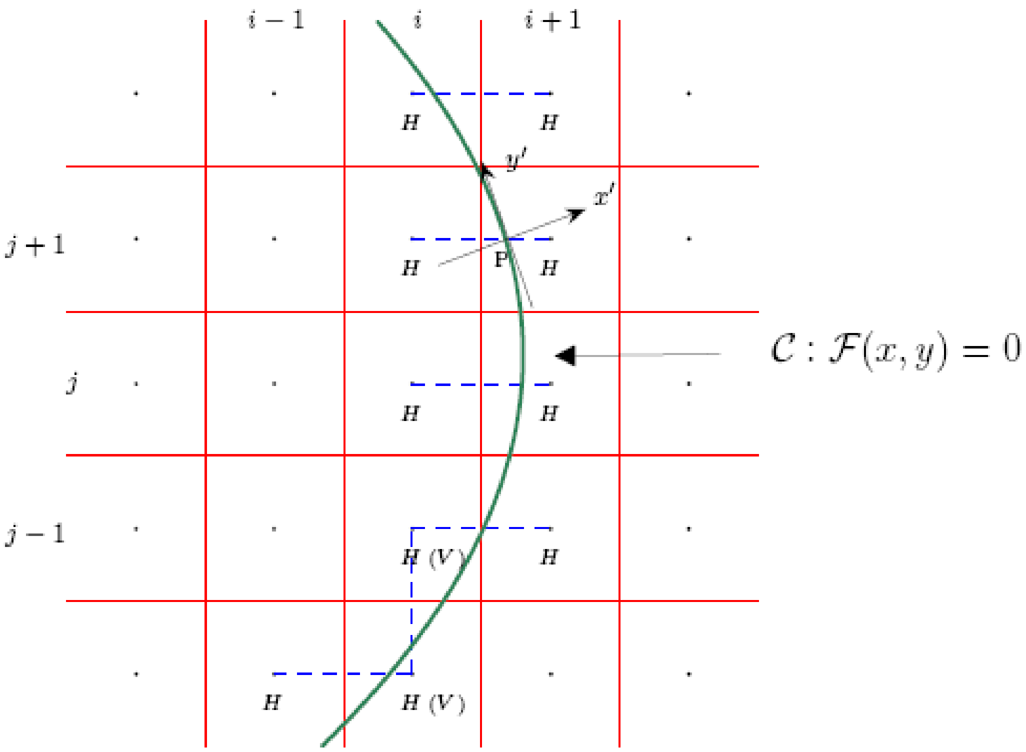
if $f^n > 0$, then $f^{n+1} > 0$;

$\| f^{n+1} \|_{l^\infty (x, \xi)} \leq \| f^n \|_{l^\infty (x, \xi)}$

$\| f^n \|_1 \leq C \| f^0 \|_1$ (except for measure-valued initial data)

l^1-convergence

Curved interface



Geometrical optics

- The same idea has also been extended to geometric optics

  $H = c(x)\,|\xi|$

  with partial transmission and reflection

  We build in Snell's Law into the flux

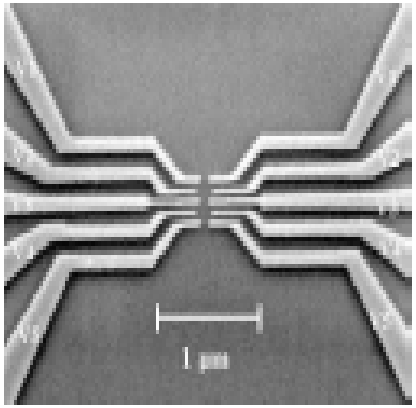
References:

J-Wen, semiclassical limit of Schrodiger, *Comm Math Sci* '05

J-Wen, geometrical optics, *JCP* 06, *SINUM*

Quantum barrier: a multiscale approach (with *K. Novak*, MMS, JCP)

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 quantum-classical coupling approach for thin barriers

- 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

A step potential (V(x)=1/2 H(x))

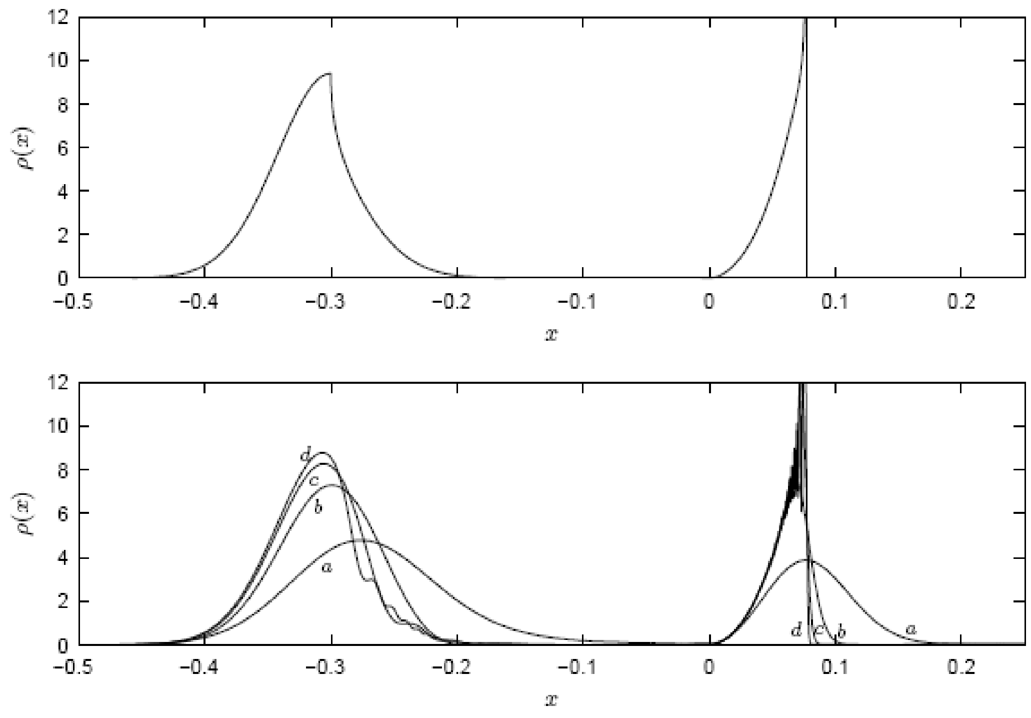
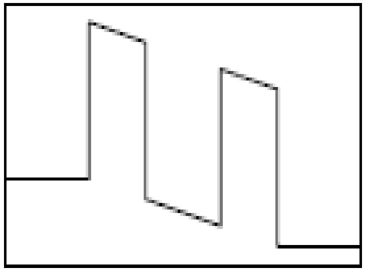


FIG. 5.1. *Position densities for the semiclassical Liouville (top) and Schrödinger (bottom) solutions of Example 5.1. The Schrödinger solution shows* $\varepsilon =$ *(a)* 200^{-1}, *(b)* 800^{-1}, *(c)* 3200^{-1} *and (d)* 12800^{-1}. *The position density of Liouville solution exhibits a caustic near* $x = 0.08$ *and the peak is unbounded. For the Schrödinger solution the peak reaches a height of 19 for the* $\varepsilon = 12800^{-1}$. *The plots are truncated for clarity.*

Resonant tunnelling



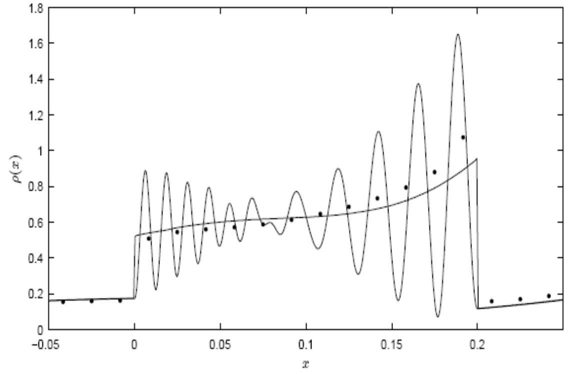


FIG. 5.4. *Detail of Fig. 5.3 showing position densities for the numerical semiclassical Liouville and von Neumann solutions. The* • *shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the "exact" Liouville solution and the von Neumann solution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

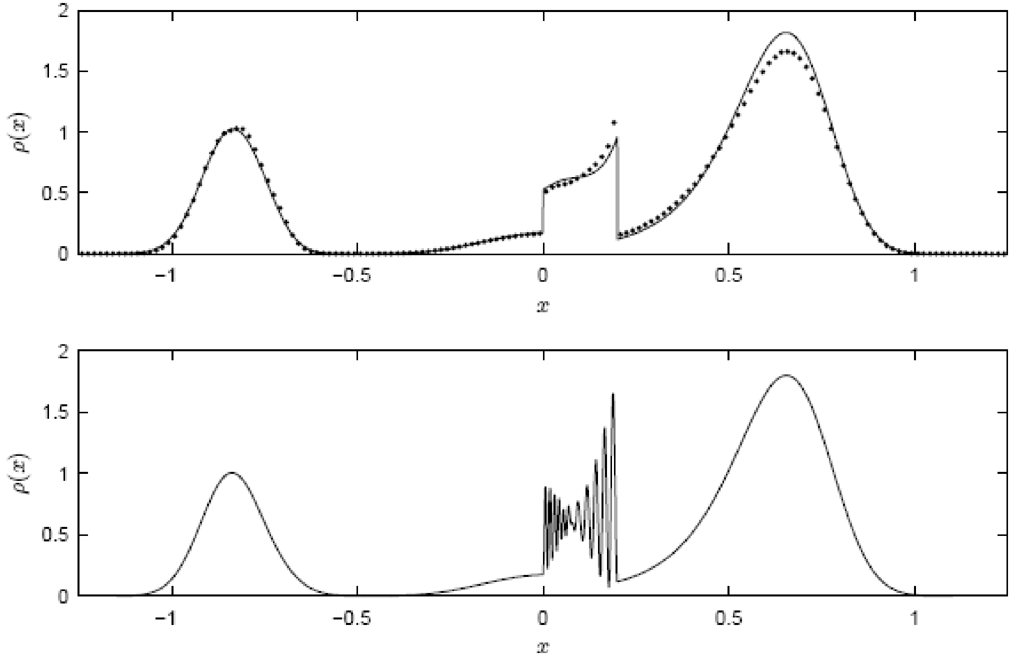
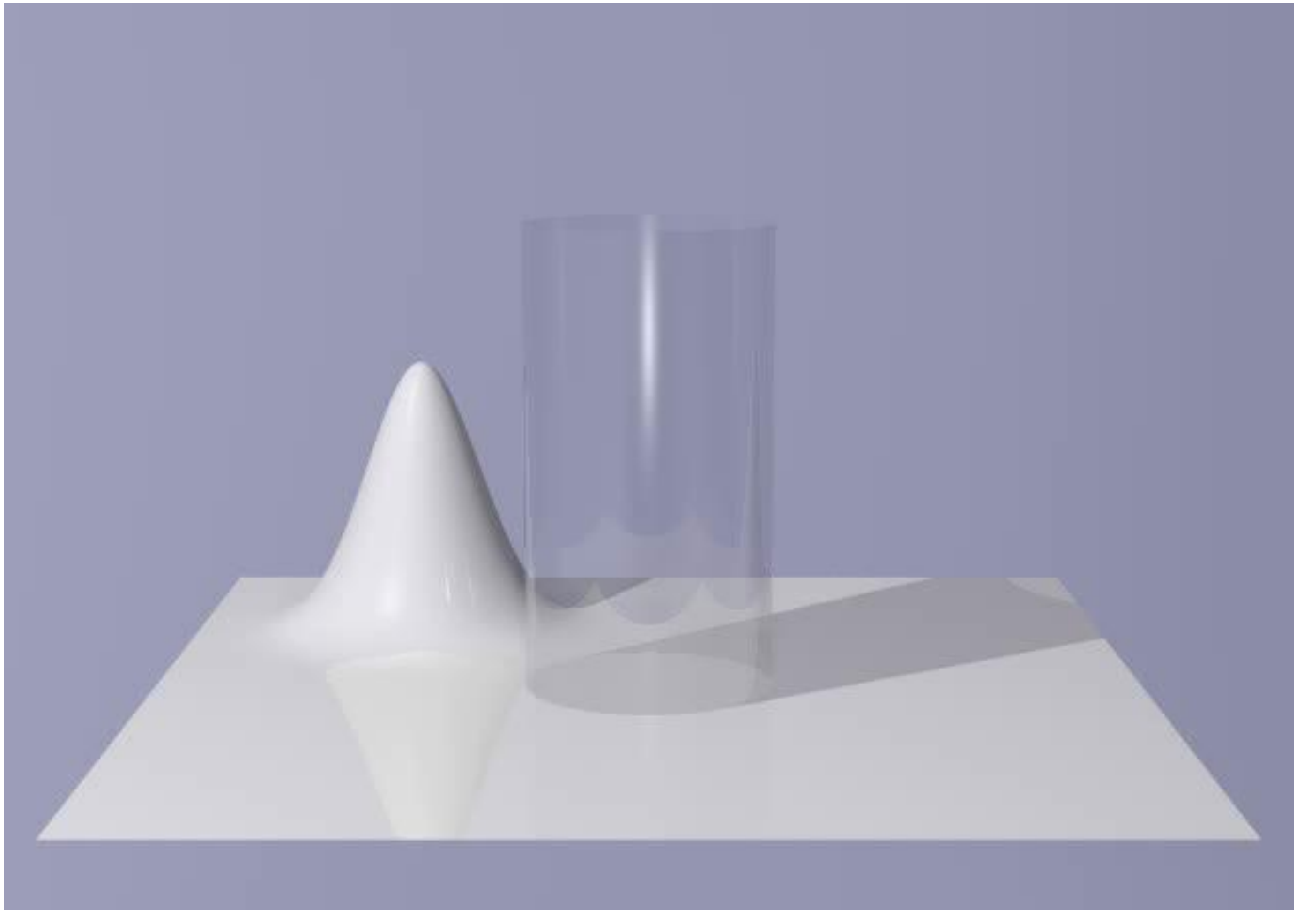
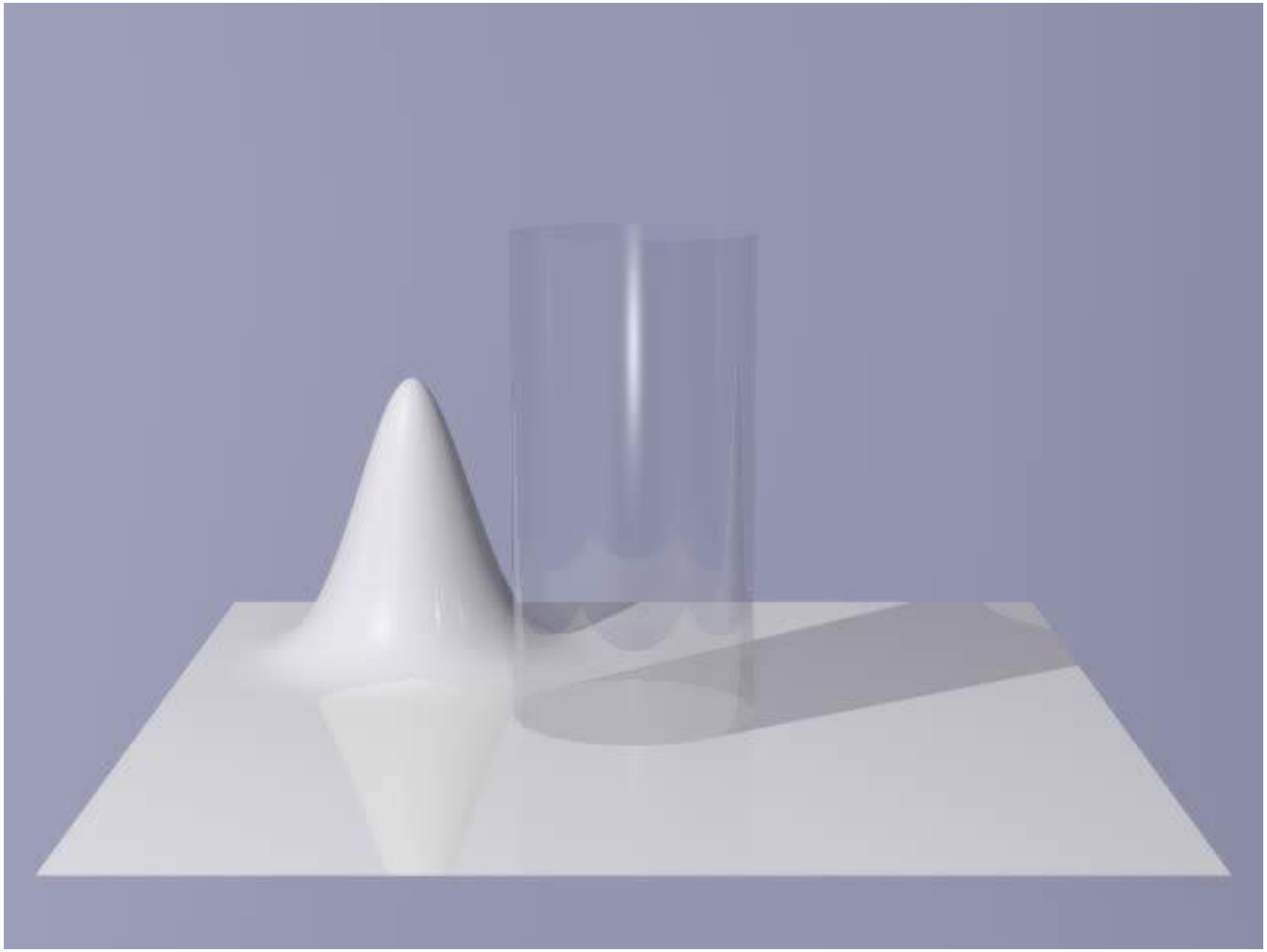


FIG. 5.3. *Position densities for the numerical semiclassical Liouville (top) and von Neumann (bottom) solutions of Example 5.3. The* • *in the Liouville plot shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the numerical solution for 3200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

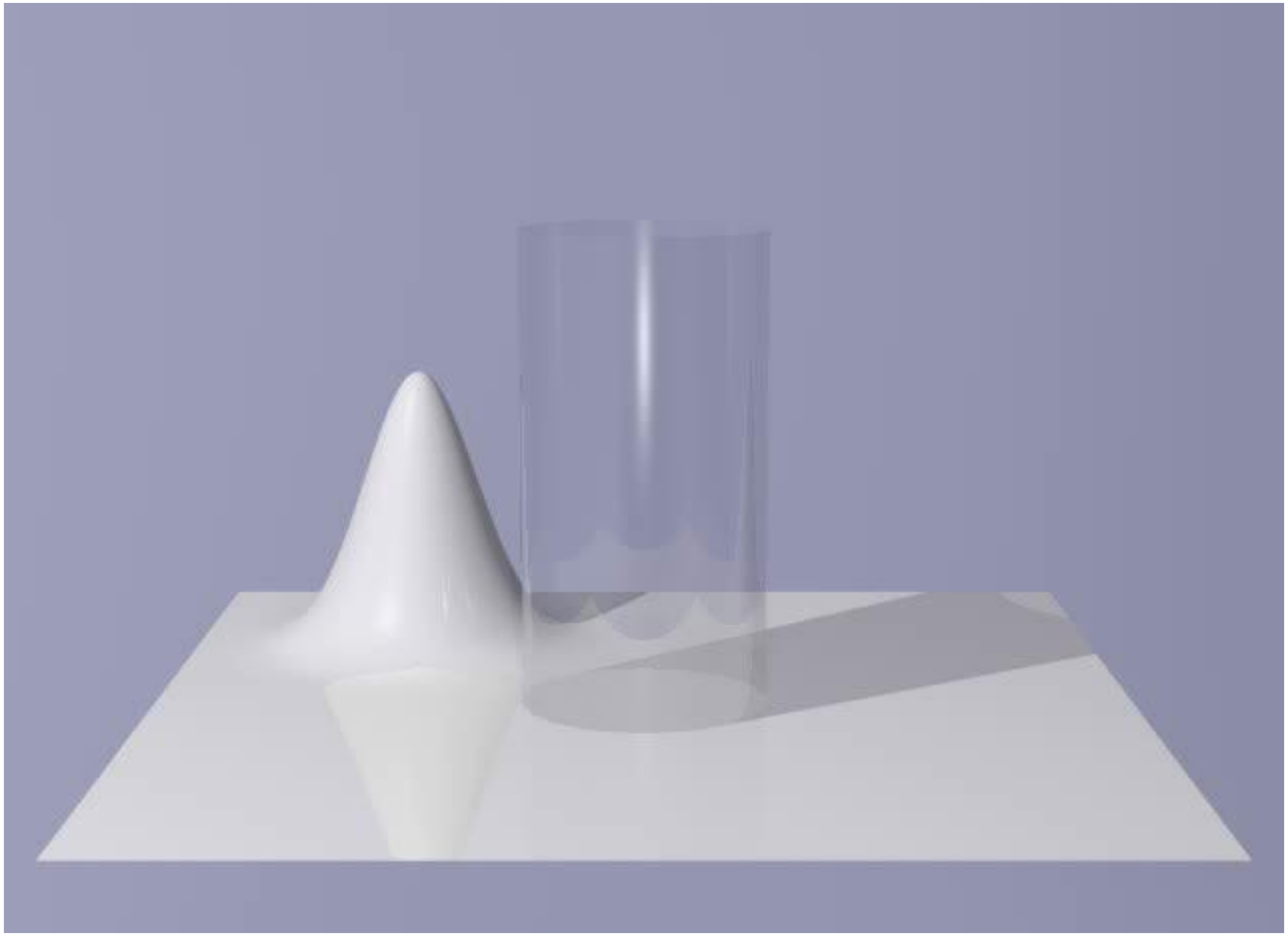
Circular barrier (Schrodinger with ε=1/400)



Circular barrier (semiclassical model)



Circular barrier (classical model)



Other applications/extensions

- Elastic waves (with X. Liao, JHDE)

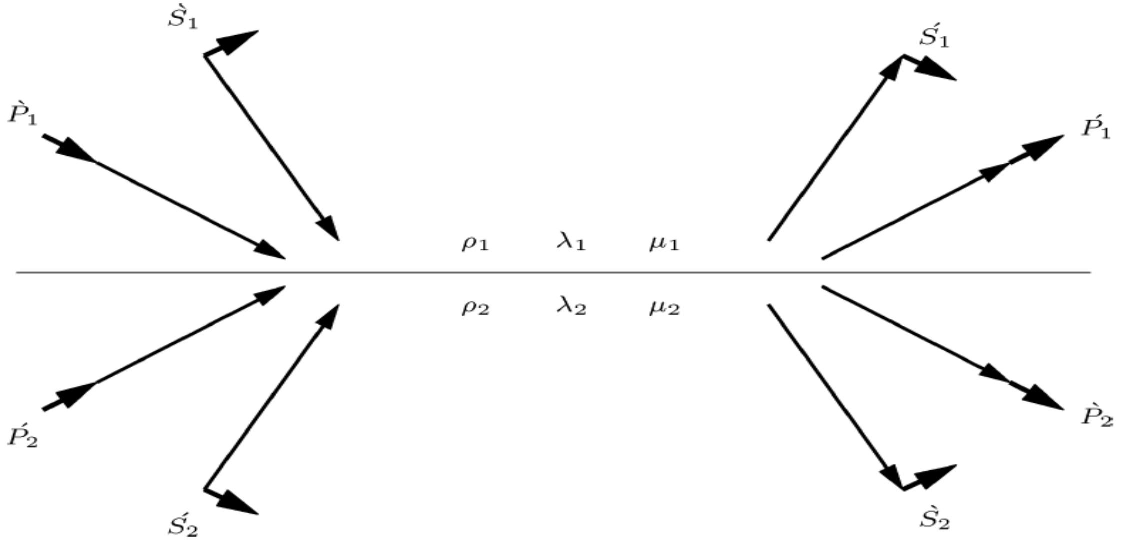
  high frequency limit (Bal-Keller-Papanicolaou-Ryzhik)

$$\frac{\partial a^p}{\partial t} + \nabla_{\mathbf{k}} H_p \cdot \nabla_{\mathbf{x}} a^p - \nabla_{\mathbf{x}} H_p \cdot \nabla_{\mathbf{k}} a^p = 0 \qquad \text{p-wave}$$

$$\frac{\partial a^s}{\partial t} + \nabla_{\mathbf{k}} H_s \cdot \nabla_{\mathbf{x}} a^s - \nabla_{\mathbf{x}} H_s \cdot \nabla_{\mathbf{k}} a^s = 0, \qquad \text{s-wave}$$

$$H_p(\mathbf{x}, \mathbf{k}) = c^p(\mathbf{x})|\mathbf{k}|, \qquad H_s(\mathbf{x}, \mathbf{k}) = c^s(\mathbf{x})|\mathbf{k}|$$

Interface scattering

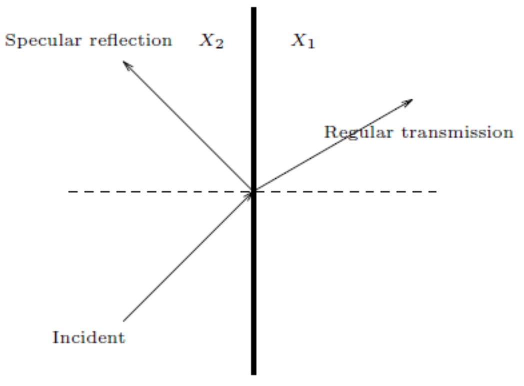


$$a^p(t, \mathbf{x}^+, \mathbf{k}^+) = \beta_R^{PP} \cdot a^p(t, \mathbf{x}^+, \mathbf{k}_{p_1}) + \beta_R^{SP} \cdot a^s(t, \mathbf{x}^+, \mathbf{k}_{p_2}) + \beta_T^{PP} \cdot a^p(t, \mathbf{x}^-, \mathbf{k}_{p_3}) + \beta_T^{SP} \cdot a^s(t, \mathbf{x}^-, \mathbf{k}_{p_4})$$

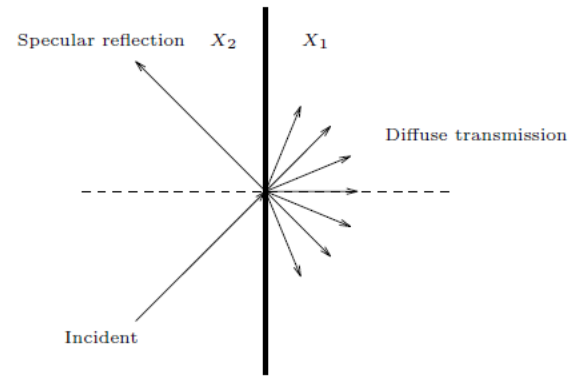
$$a^s(t, \mathbf{x}^+, \mathbf{k}^+) = \beta_R^{PS} \cdot a^p(t, \mathbf{x}^+, \mathbf{k}_{s_1}) + \beta_R^{SS} \cdot a^s(t, \mathbf{x}^+, \mathbf{k}_{s_2}) + \beta_T^{PS} \cdot a^p(t, \mathbf{x}^-, \mathbf{k}_{s_3}) + \beta_T^{SS} \cdot a^s(t, \mathbf{x}^-, \mathbf{k}_{s_4})$$

Radiative transfer through rough interfaces (with X. Liao and X. Yang)

- High frequency limit of acoustic wave in random media through a rough interface
- Specular/diffusive scattering
- Bal-Ryzhik



(a) Interface condition I



(b) Interface condition II

Radiative transfer, nonlocal interface condition

$$\frac{\partial a}{\partial t} + v\hat{\mathbf{k}} \cdot \nabla_{\mathbf{x}} a = \int \sigma(\mathbf{x}, \mathbf{k}, \mathbf{k}')\delta(v|\mathbf{k}| - v|\mathbf{k}'|)(a(t, \mathbf{x}, \mathbf{k}') - a(t, \mathbf{x}, \mathbf{k}))\, d\mathbf{k}'$$

$$a_i(0, \mu)|_{\Gamma^i_-} = \sum_{j=1}^{2} R^{ij} \left(a_j(0, \cdot)|_{\Gamma^j_+} \right) (\mu).$$

$$R^{11}(a)(\mu_1) = \mathcal{F}^{11}(\mu_1)a(-\mu_1), \qquad R^{12}(a)(\mu_1) = 2\int_0^1 \mu_1 \frac{\mu_1 v_2}{\mu_2 v_1} \mathcal{F}^{12}(\mu_2)a(\mu_2)\, d\mu_1,$$

$$R^{22}(a)(-\mu_2) = \mathcal{F}^{22}(\mu_2)a(\mu_2), \qquad R^{21}(a)(-\mu_2) = 2\int_0^1 \mu_2 \frac{\mu_2 v_1}{\mu_1 v_2} \mathcal{F}^{21}(\mu_1)a(-\mu_1)\, d\mu_2. \tag{3.13}$$

Diffraction (with D. Yin)

- Have to incorporate geometric theory of diffraction (J. Keller) into the interface condition—it depends on geometry
- Have done: curved interface, half plane, rectangular wedge

Surface hopping (with P. Qi and Z. Zhang, MMS)

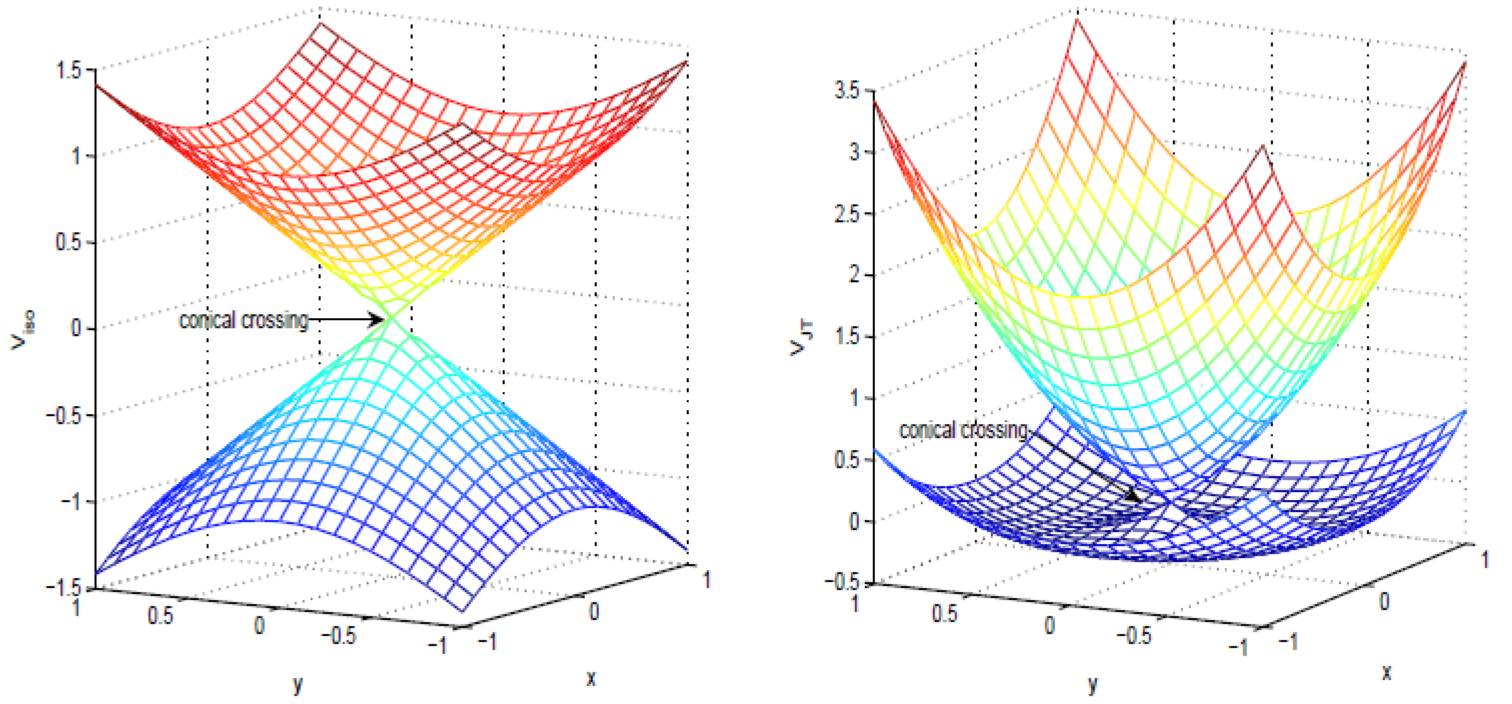
- Arising in Bohn-Oppenheimer approximation of N-body Schrodinger equation
- Classical trajectory for each potential electronic energy level + quantum hopping at conical crossing (Tully):

$$\partial_t u_\tau + \nabla_{\mathbf{k}} \lambda_\tau \cdot \nabla_{\mathbf{x}} u_\tau - \nabla_{\mathbf{x}} \lambda_\tau \cdot \nabla_{\mathbf{k}} u_\tau = 0, \quad (t, \mathbf{x}, \mathbf{k}) \in R^+ \times \Omega, \quad \tau = 1, 2\,,$$

$$j_\tau(\mathbf{x}, \mathbf{k}) = (\nabla_{\mathbf{k}} \lambda_\tau, -\nabla_{\mathbf{x}} \lambda_\tau)\, u_\tau(\mathbf{x}, \mathbf{k}), \quad \tau = 1, 2\,.$$

$$\begin{pmatrix} j_1(\mathbf{x}_0^+, \mathbf{k}_0^+) \\ j_2(\mathbf{x}_0^+, \mathbf{k}_0^+) \end{pmatrix} = \begin{pmatrix} 1 - T(\mathbf{x}_0, \mathbf{k}_0) & T(\mathbf{x}_0, \mathbf{k}_0) \\ T(\mathbf{x}_0, \mathbf{k}_0) & 1 - T(\mathbf{x}_0, \mathbf{k}_0) \end{pmatrix} \begin{pmatrix} j_1(\mathbf{x}_0^-, \mathbf{k}_0^-) \\ j_2(\mathbf{x}_0^-, \mathbf{k}_0^-) \end{pmatrix}$$

Conical crossing



Summary

Well-balanced scheme for shallow water equations

→ Hamiltonian preserving for Hamiltonian systems

→ high frequency waves through interfaces

→ quantum-classical couping