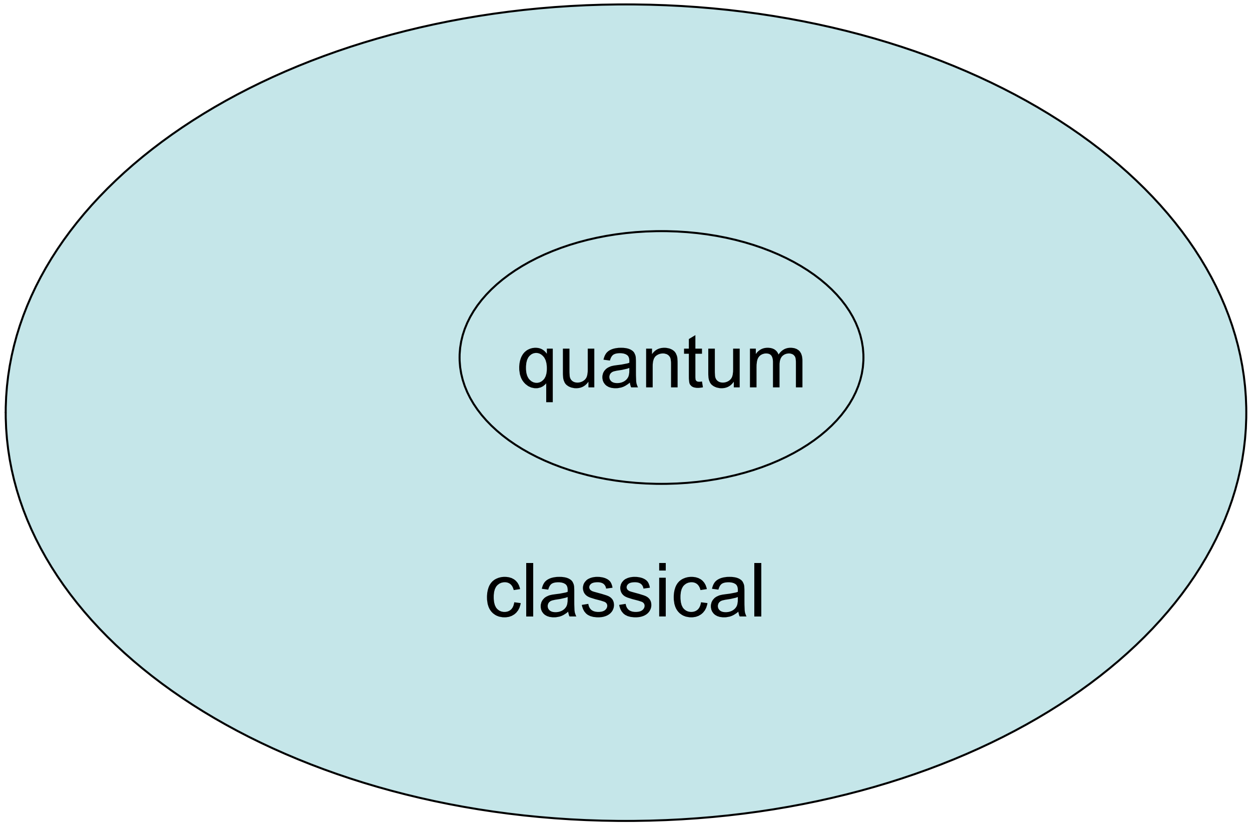
II. Quantum-classical coupling



Classical mechanics

- Hamiltonian equations

  $dx/dt = p = \nabla_x H$

  $dp/dt = -\nabla V = -\nabla_p H$

  Hamiltonian $H = ½ |p|^2 + V$

- Liouville equation for probability density distribution f(t,x,p):

  $\partial_t f + p¢ \nabla_x f - \nabla_x V¢ \nabla_p f = 0$

Quantum mechanics

Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi = \left(-\tfrac{1}{2}\hbar^2\Delta + V(x)\right)\psi$$

Density matrix

$$\hat{\rho}(x,x',t) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{f}(\tilde{x},\tilde{p})\psi(x,t;\tilde{x},\tilde{p})\overline{\psi}(x',t;\tilde{x},\tilde{p})\,d\tilde{x}\,d\tilde{p}$$

Von Neumann equation

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(x,x',t) = \left(-\tfrac{1}{2}\hbar^2[\Delta_x - \Delta_{x'}] + V(x) - V(x')\right)\hat{\rho}(x,x',t)$$

Semiclassical limit

If $V(x)$ is *sufficiently smooth*, [Lions and Paul '93; Gérard, Markowich, Mauser and Poupaud '97]

$$\Theta^{\varepsilon} W \to \nabla_x V \cdot \nabla_p W \text{ as } \varepsilon \to 0$$

Wigner equation $(\varepsilon \to 0)$

$$\frac{\partial}{\partial t} W + p \cdot \nabla_x W - \nabla_x V \cdot \nabla_p W = 0$$

Classical Liouville equation

$$\frac{\partial}{\partial t} f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = 0$$

A quantum-classical coupling model (*Jin-Novak*)

- Classical–quantum coupling [Ben Abdallah, Degond, Gamba '02]
- Hamiltonian-preserving scheme [Jin and Wen '05]

Idea

1. Solve the Liouville equation locally.
2. Use the weak form of the conservation of energy ($H =$ constant) to connect the local solutions together.
3. Use a physically relevant interface condition to choose correct solution.

Assumptions

1. Barrier width $O(\varepsilon)$.
2. Distance between neighboring barriers is $O(1)$.
3. $\nabla V(x)$ is $O(1)$ except at barrier.
4. Barriers are mutually independent.

Interface condition (one dimensional)

Push

$$f(x^-, p^-, t^-) = R(p^+) f(x^+, p^+, t^+) + T(q^+) f(x^+, q^+, t^+)$$
$$p^+ = -p^-$$
$$q^+ = p^- \sqrt{1 + 2(V(x^-) - V(x^+))/|p^-|^2}$$

- Lagrangian
- One-to-many function

Pull

$$f(x^+, p^+, t^+) = R(p^-) f(x^-, p^-, t^-) + T(q^-) f(x^-, q^-, t^-)$$
$$p^- = -p^+$$
$$q^- = p^+ \sqrt{1 + 2(V(x^+) - V(x^-))/|p^+|^2}$$

- Eulerian
- Many-to-one function

Liouville equation with singular coefficients

This interface condition allows us to solve Liouville equations with singular coefficients.

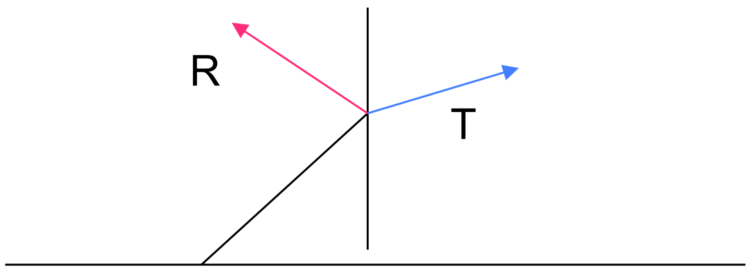
$$f_t + H_p f_p - H_x f_p = 0$$

- Weak solution not well-defined
- DiPerna-Lions renormalized solution for linear transport with discontinuous (BV) coefficients does not apply

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:

$$dx/dt = H_p, \quad dp/dt = -H_x$$



- 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

Implementation (one dimensional)

- Initialization
  - Solve time-independent Schrödinger equation for $E = \frac{1}{2}p^2$ (using transfer matrix method)
  - Calculate $T(p)$ and $R(p)$ to get interface condition
- Liouville Solver
  - Use finite volume method globally
  - Incorporate interface condition at quantum barrier

Transfer matrix method

$$-\varepsilon^2\psi''(x) + 2V(x)\psi(x) = p^2\psi(x)$$

$$\psi(x) = \begin{cases} a_1 e^{ix\sqrt{p^2-2V_1}/\varepsilon} + b_1 e^{-ix\sqrt{p^2-2V_1}/\varepsilon}, & x \in \mathcal{C}_1 \\ a_2 e^{ix\sqrt{p^2-2V_2}/\varepsilon} + b_2 e^{-ix\sqrt{p^2-2V_2}/\varepsilon}, & x \in \mathcal{C}_2 \end{cases}$$

Transfer matrix M

$$\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \mathsf{M} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$$

$$\mathsf{M} = \mathsf{M}_n \cdots \mathsf{M}_2 \mathsf{M}_1$$

Scattering matrix S

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \mathsf{S} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r_1 & t_2 \\ t_1 & r_2 \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} -m_{21}/m_{22} & 1/m_{22} \\ \det \mathsf{M}/m_{22} & m_{12}/m_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}$$

Scattering coefficients

Transmission and reflection coefficients

$$T = \frac{\text{transmitted current density}}{\text{incident current density}} \quad R = \frac{\text{reflected current density}}{\text{incident current density}}$$

Continuity equation

$$\frac{\partial}{\partial t}\rho + \nabla \cdot J = 0 \quad \text{where} \quad J(x) = \varepsilon \mathrm{Im}\left(\overline{\psi}\nabla\psi\right)$$

Wave incident from the left ($a_1 = 1$, $b_1 = r_1$, $a_2 = t_1$ and $b_2 = 0$)

$$J(x) = \begin{cases} \kappa_1\left(1 - |r_1|^2\right), & x \in \mathcal{C}_1 \\ \kappa_2\left(|t_2|^2\right), & x \in \mathcal{C}_2 \end{cases}$$

$$R = |r_1|^2 \quad \text{and} \quad T = \sqrt{\frac{p^2 - 2V_2}{p^2 - 2V_1}}|t_1|^2$$

Liouville solver

Liouville Equation

$$\frac{\partial f}{\partial t} = -p\frac{\partial f}{\partial x} + \frac{dV}{dx}\frac{\partial f}{\partial x}$$

Finite volume discretization of Liouville equation

$$\frac{f_{ij}^{n+1} - f_{ij}^{n}}{\Delta t} = -p_j \partial_x f_{ij}^{n} + \partial_x V_i \partial_p f_{ij}^{n}$$

where the cell average

$$f_{ij}^{n} = \frac{1}{\Delta x \Delta p} \iint_{C_{ij}} f(x, p, t_n)\, dx\, dp$$

Interface condition built into the numerical flux

Pull interface condition

$$f^+_{Z+1/2,j} = R(q_j)f^+_{Z+1/2,-j} + T(q_j)f(x^-_{Z+1/2}, q_j) \qquad \text{for } j > 0$$
$$f^-_{Z+1/2,j} = R(q_j)f^-_{Z+1/2,-j} + T(q_j)f(x^+_{Z+1/2}, q_j) \qquad \text{for } j < 0$$

where the incident $q_j = p_j\sqrt{1 + 2(V^+_{Z+1/2} - V^-_{Z+1/2})/p_j|p_j|}$.

We define $f(x^-_{Z+1/2}, q_j)$ as the cell average

$$f(x^-_{Z+1/2}, q_j) = \frac{1}{p_j \Delta p}\int_{q_{j-1/2}}^{q_{j+1/2}} p f(x^-_{Z+1/2}, p)\, dp$$

where $q_{j\pm1/2} = \sqrt{p^2_{j\pm1/2} + 2(V^+_{Z+1/2} - V^-_{Z+1/2})}$. The integral is approximated by a composite mid-point rule.

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

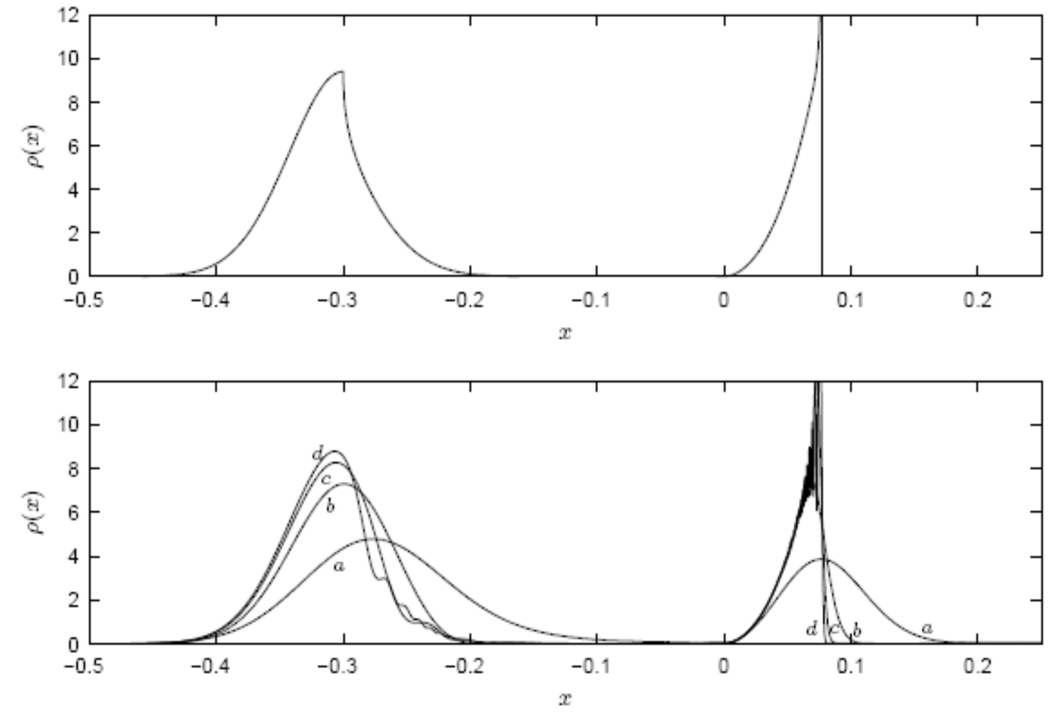
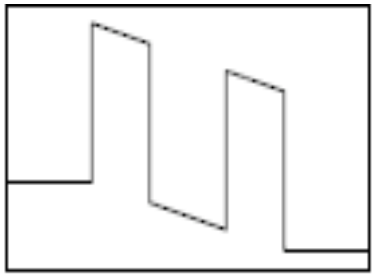


FIG. 5.1. *Position densities for the semiclassical Liouville (top) and Schrödinger (bottom) solutions of Example 5.1. The Schrödinger solution shows* $\varepsilon =$ *(a)* 200^{-1}, *(b)* 800^{-1}, *(c)* 3200^{-1} *and (d)* 12800^{-1}. *The position density of Liouville solution exhibits a caustic near*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



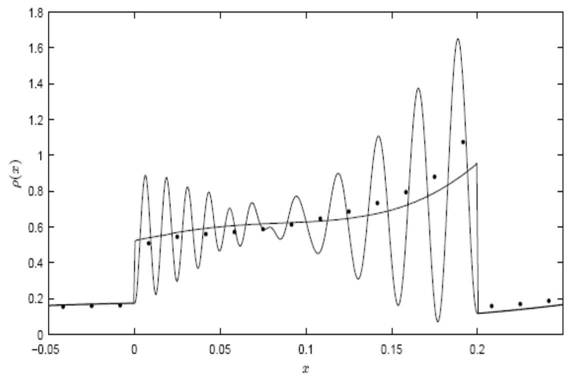


FIG. 5.4. *Detail of Fig. 5.3 showing position densities for the numerical semiclassical Liouville and von Neumann solutions. The* • *shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the "exact" Liouville solution and the von Neumann solution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

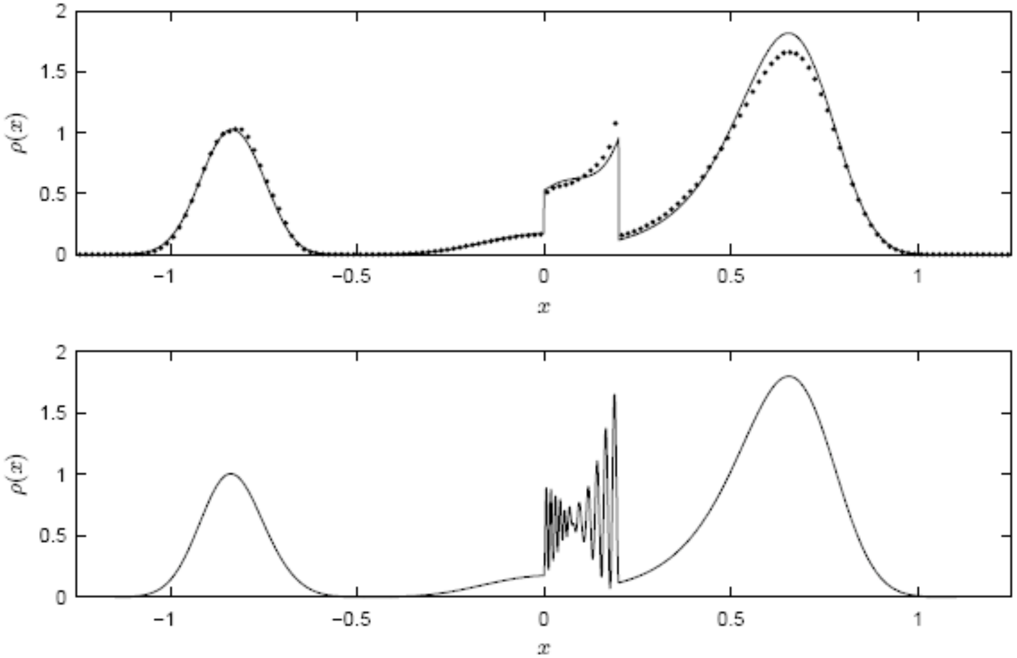


FIG. 5.3. *Position densities for the numerical semiclassical Liouville (top) and von Neumann (bottom) solutions of Example 5.3. The* • *in the Liouville plot shows the numerical solution for with 150 grid points over the domain* $[-1.25, 1.25]$. *The solid line shows the numerical solution for 3200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

2D interface condition

Pull interface condition

$$f(\mathbf{x}_{\text{out}}, p_{\text{out}}, \theta_{\text{out}}) = \int_{-\pi/2}^{\pi/2} R(\theta_{\text{in}}; p_{\text{in}}, \theta_{\text{out}}) f(\mathbf{x}_{\text{in}}, p_{\text{in}}, \theta_{\text{in}})\, d\theta_{\text{in}} + \int_{-\pi/2}^{\pi/2} T(\theta_{\text{in}}; q_{\text{in}}, \theta_{\text{out}}) f(\mathbf{x}_{\text{in}}, q_{\text{in}}, \theta_{\text{in}})\, d\theta_{\text{in}}$$

Push interface condition

$$f(\mathbf{x}_{\text{in}}, p_{\text{in}}, \theta_{\text{in}}) = \int_{-\pi/2}^{\pi/2} R(\theta_{\text{out}}; p_{\text{out}}, \theta_{\text{in}}) f(\mathbf{x}_{\text{out}}, p_{\text{out}}, \theta_{\text{out}})\, d\theta_{\text{out}} + \int_{-\pi/2}^{\pi/2} T(\theta_{\text{out}}; q_{\text{out}}, \theta_{\text{in}}) f(\mathbf{x}_{\text{out}}, q_{\text{out}}, \theta_{\text{out}})\, d\theta_{\text{out}}$$

(with $q^2 = p^2 + 2\Delta V$)

Implementation

- Initialization
  - Solving time-independent Schrödinger equation for each $E = \frac{1}{2}p^2$ and θ_{in}.
  - Calculate $T(\theta_{\text{out}}; p, \theta_{\text{in}})$ and $R(\theta_{\text{out}}; p, \theta_{\text{in}})$.
- Liouville Solver:
  - Particle method
  - Push interface condition

Scattering probabilities

$$S(\theta; p, \theta_{\text{in}}) = \frac{\theta\text{-component to flux scattered across interface}}{\text{incident flux}}$$

Current density: $J(x,y) = \text{Im}\left(\overline{\psi}(x,y)\nabla\psi(x,y)\right)$

Solution in $\mathcal{C}_j$ for constant V_j

$$\psi_j(x,y) = \int_{-\pi}^{\pi} a_j(\theta) e^{ip_j(x\cos\theta + y\sin\theta)}\, d\theta, \qquad j = 1, 2.$$

Flux

$$\int_{-\infty}^{\infty} J(x,y)\, dy = \int_{-\pi}^{\pi} p|a(\theta)|^2 (\cos\theta, \sin\theta)\, d\theta$$

Scattering probabilities

For particle incident from left at angle θ_{in}:

$$\psi_1(x,y) = e^{ip_1(x\cos\theta_{\mathsf{in}} + y\sin\theta_{\mathsf{in}})} + \int_{-\pi/2}^{\pi/2} r(\theta) e^{-ip_1(x\cos\theta + y\sin\theta)}\, d\theta$$

$$\psi_2(x,y) = \int_{-\pi/2}^{\pi/2} t(\theta) e^{ip_2(x\cos\theta + y\sin\theta)}\, d\theta$$

$$R(\theta; p_1, \theta_{\mathsf{in}}) = |r(\theta)|^2 \frac{\cos\theta}{\cos\theta_{\mathsf{in}}} \quad \text{and} \quad T(\theta; p_1, \theta_{\mathsf{in}}) = |t(\theta)|^2 \frac{p_2\cos\theta}{p_1\cos\theta_{\mathsf{in}}}$$

! Find $r(\theta)$ and $t(\theta)$ by solving Schrödinger equation in Q.

Quantum transmitting boundary method

Solve the Schrödinger equation

$$-\frac{\partial^2}{\partial x^2}\psi_{\mathcal{Q}}(x,y)-\frac{\partial^2}{\partial y^2}\psi_{\mathcal{Q}}(x,y)+2V_{\mathcal{Q}}(x,y)\psi_{\mathcal{Q}}(x,y)=p^2$$

in $\mathcal{Q}$ with matching conditions

$$\psi_{\mathcal{Q}}(x_j,y)=\psi_j(x_j,y)$$
$$\frac{\partial}{\partial x}\psi_{\mathcal{Q}}(x_j,y)=\frac{\partial}{\partial x}\psi_j(x_j,y),\qquad j=1,2$$

! We must eliminate unknowns $r(\theta)$ and $t(\theta)$ from boundary conditions. But $r(\theta)$ and $t(\theta)$ are coupled by the integral.

Quantum transmitting boundary method

Fourier transform of ψ into momentum space ($y \mapsto \xi$)

$$\frac{\partial^2}{\partial x^2}\hat{\psi}_{\mathcal{Q}}(x,\xi)+\eta_1^2(\xi)\hat{\psi}_{\mathcal{Q}}(x,\xi)-2\int_{-\infty}^{\infty} V_{\mathcal{Q}}(x,y)\psi(x,y)e^{-i\xi y}\,dy=0$$

in $\mathcal{Q}$ with matching conditions

$$\hat{\psi}_{\mathcal{Q}}(x_j,\xi)=\hat{\psi}_j(x_j,\xi)$$
$$\frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}}(x_j,\xi)=\frac{\partial}{\partial x}\hat{\psi}_j(x_j,\xi), \qquad j=1,2$$

where $\eta_1^2(\xi)=p^2-\xi^2$

Quantum transmitting boundary method

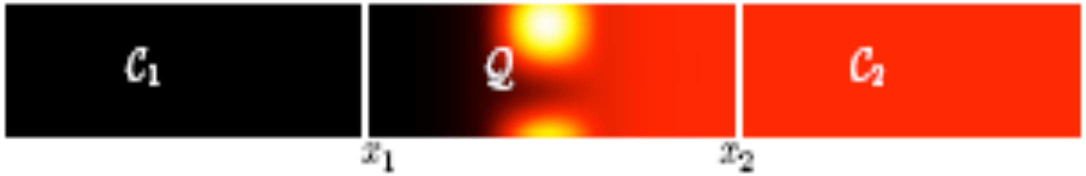
In $\mathcal{C}_1$ and $\mathcal{C}_2$

$$\hat{\psi}_1(x,\xi) = \delta(\xi - \xi_{\text{in}})e^{i\eta_1(\xi)(x-x_1)} + s_1(\xi)e^{-i\eta_1(\xi)(x-x_1)}$$
$$\hat{\psi}_2(x,\xi) = s_2(\xi)e^{i\eta_2(\xi)(x-x_2)}$$

Eliminating the unknowns $s_1(\xi)$ and $s_2(\xi)$ gives the mixed boundary conditions

$$i\eta_1(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 2i\eta_1(\xi)\delta(\xi - \xi_{\text{in}}) \qquad \text{at } x = x_1$$
$$i\eta_2(\xi)\hat{\psi}_{\mathcal{Q}} - \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 0 \qquad \text{at } x = x_2$$

Quantum transmitting boundary method



After solving Schrödinger equation

$$r(\theta; p, \theta_{\text{in}}) = \hat{\psi}_Q(x_1, p\sin\theta) - 1_{\theta=\theta_{\text{in}}}$$
$$t(\theta; p, \theta_{\text{in}}) = \hat{\psi}_Q(x_2, p_2(p)\sin\theta)$$

! We need to do this for every incident p and θ_{in}.

Particle method

- Initial conditions

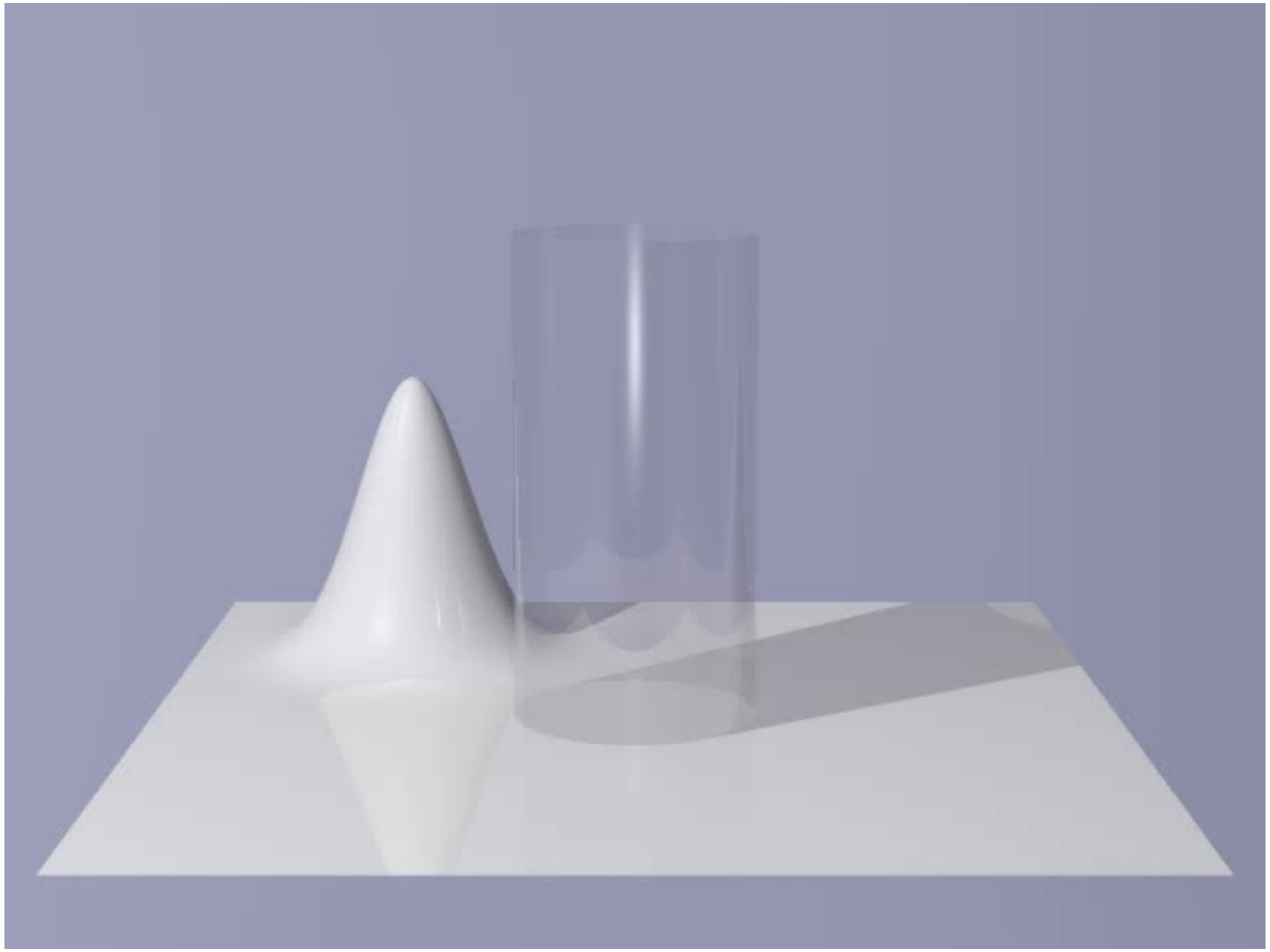
$$f_0(r) = \int_\Omega f_0(\tilde{r})\delta(r-\tilde{r})\,d\tilde{r} \quad \longrightarrow \quad f_0^h = \sum_{j=1}^{N} w_j \delta^h(r-r_j)$$

- Solve $\quad \dfrac{dx}{dt} = p, \quad \dfrac{dp}{dt} = -\nabla_x V$
- Push interface condition is one-to-many

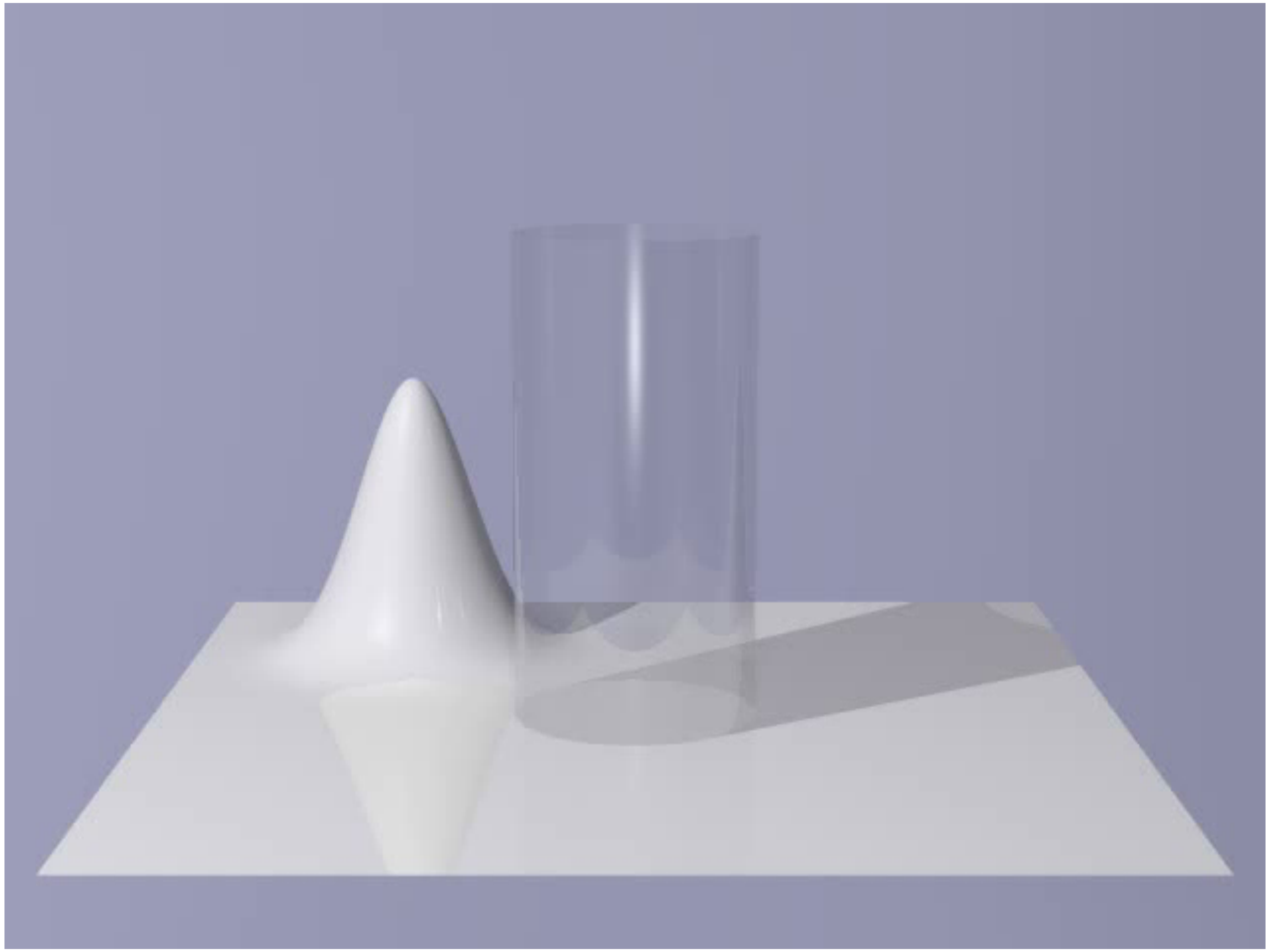
  Monte Carlo take a path randomly from $S(\theta_{\text{out}}; p, \theta_{\text{in}})$

  Deterministic take all paths (binary tree)
- Reconstruct density distribution with bicubic cutoff function

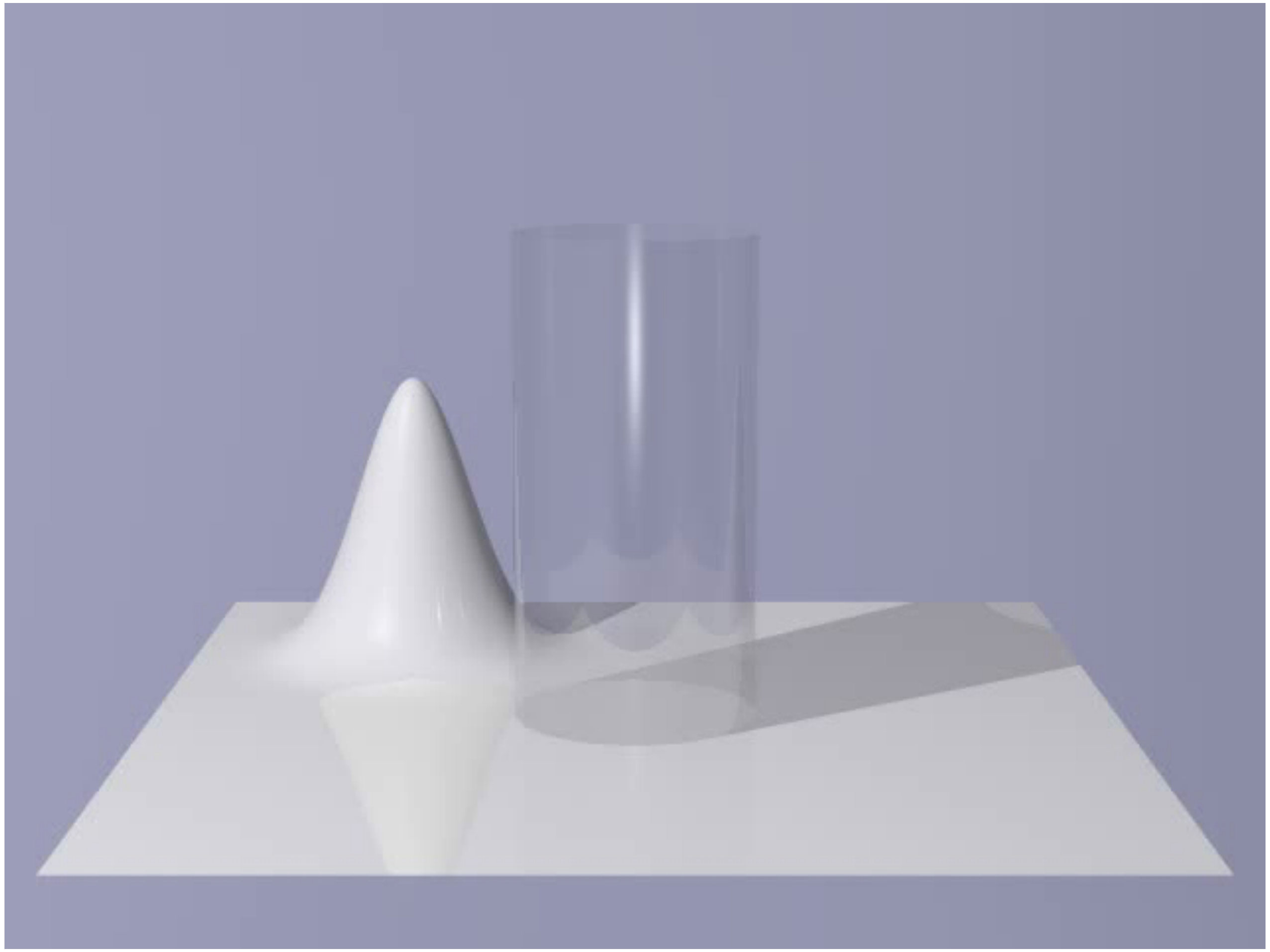
Circular barrier (Schrodinger with ε=1/400)



Circular barrier (semiclassical model)

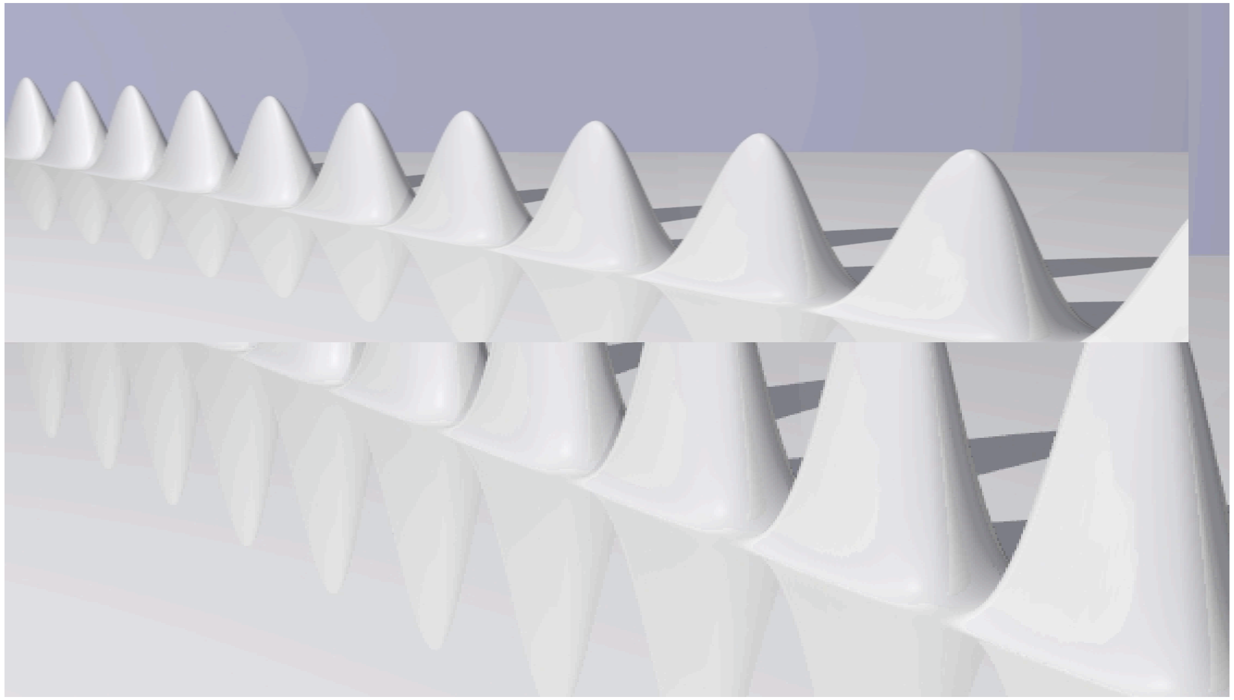


Circular barrier (classical model)

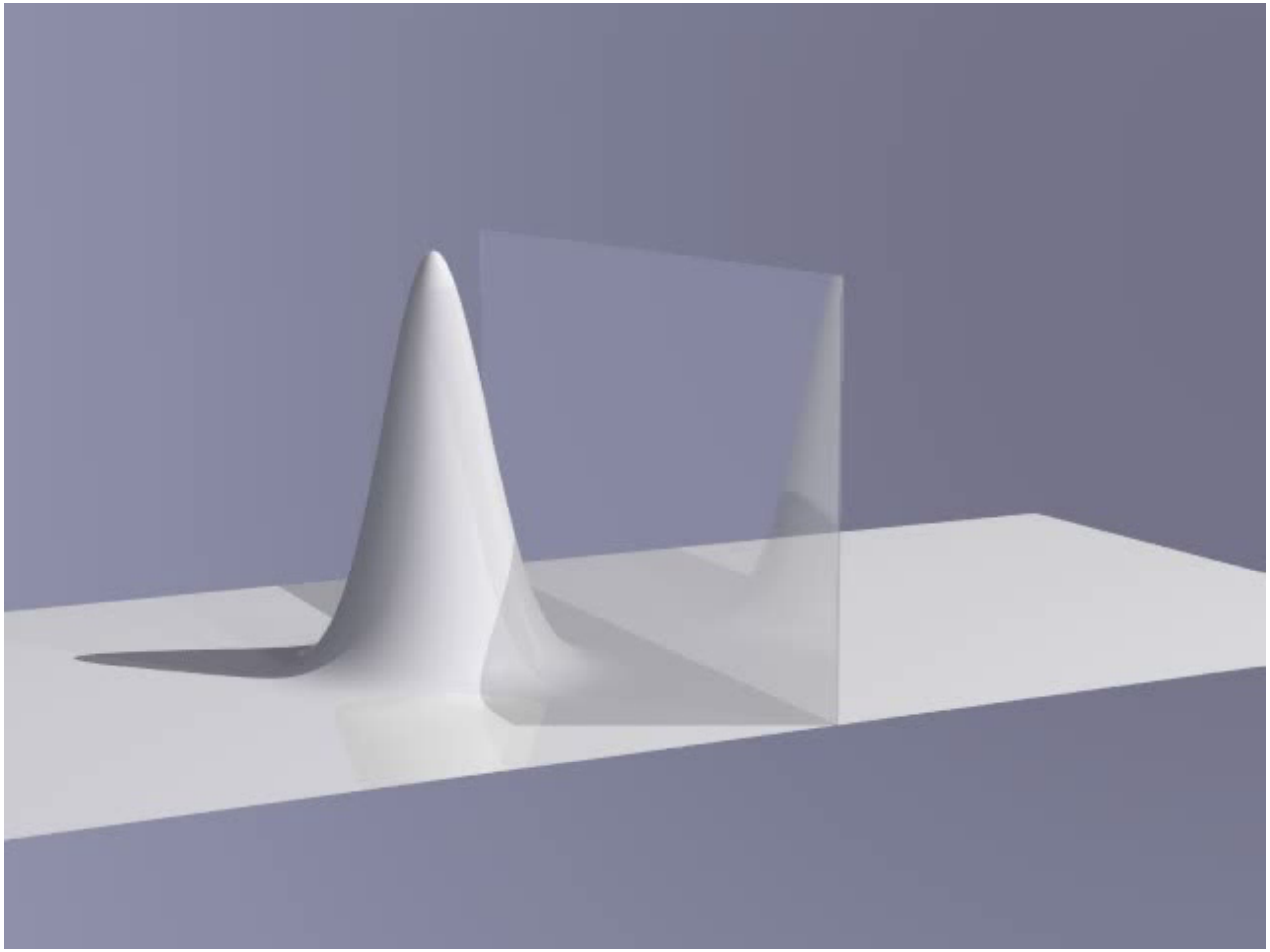


Diffraction grating:

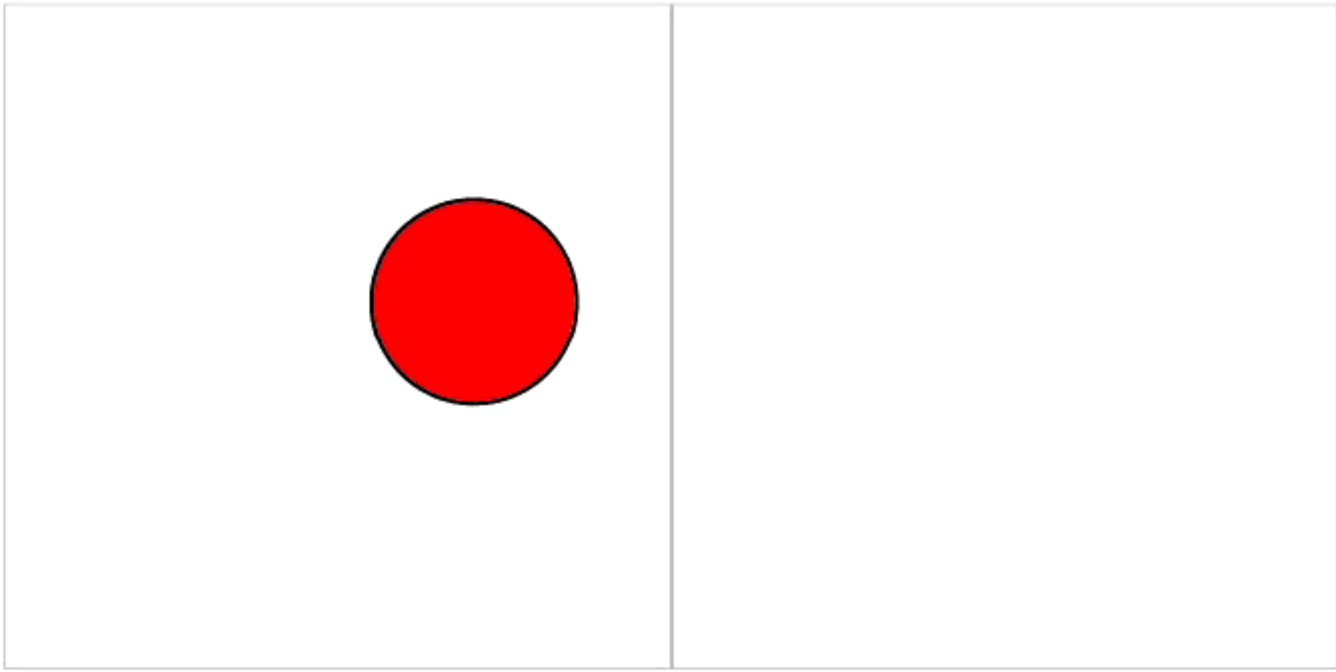
$$V(x,y) = \begin{cases} 2\cos^2(\pi x/2\varepsilon)\cos^2(y/4\varepsilon), & x \in (-\varepsilon, \varepsilon) \\ 0, & \text{otherwise} \end{cases}$$



Semiclassical

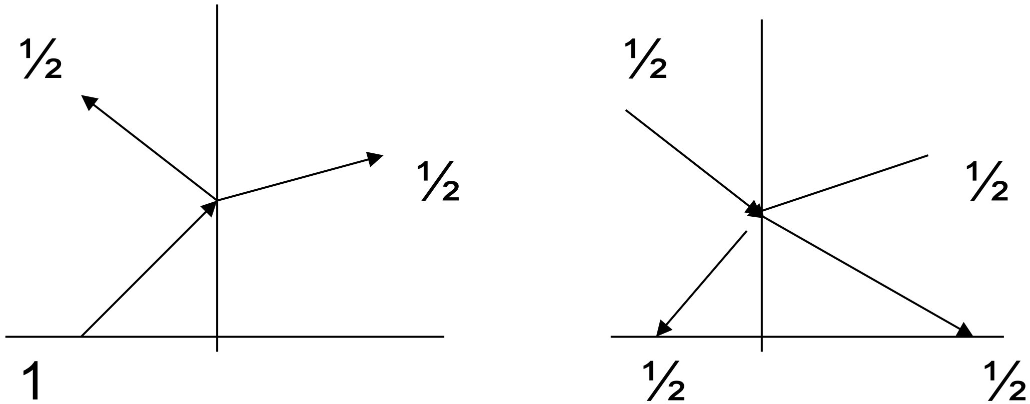


Semiclasical vs Schrodinger (ε=1/800)



Entropy

- The semiclassical model is time-irreversible.



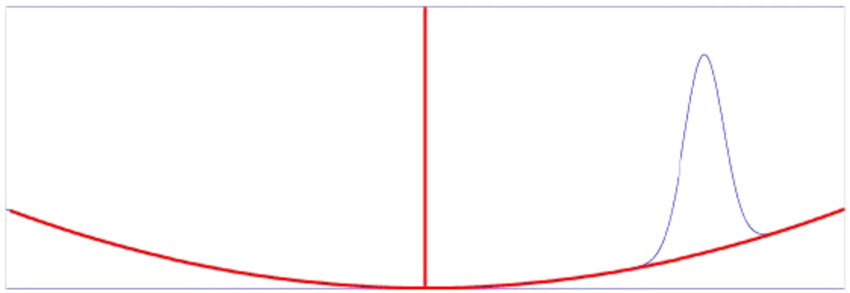
Loss of the phase information

cannot deal with interference

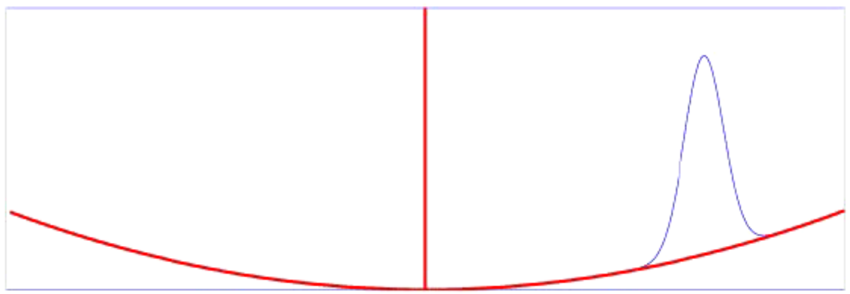
decoherence

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

Quantum



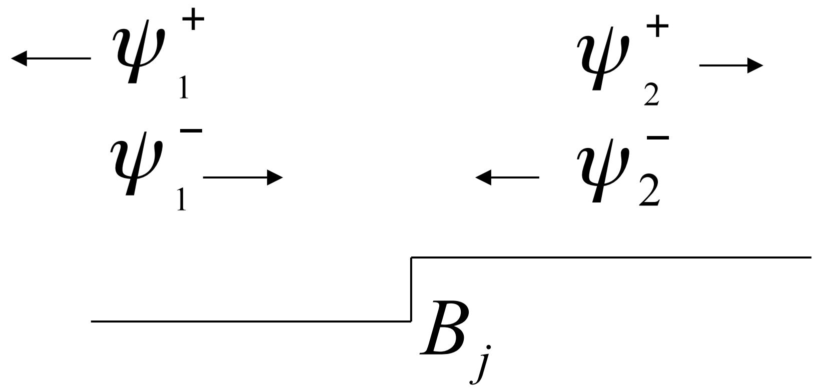
semiclassical



A Coherent Semiclassical Model

Initialization:

- Divide barrier into several thin barriers $B_1, B_2, \dots, B_n$
- 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 $f_{\text{coh}}(x,p,t)$ is a solution to the Liouville equation for initial condition $f_{\text{coh}}(x,p,0)$. Furthermore, for two solutions Φ_1 and Φ_2 with $f_1 = |\Phi_1|^2$ and $f_2 = |\Phi_2|^2$,

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

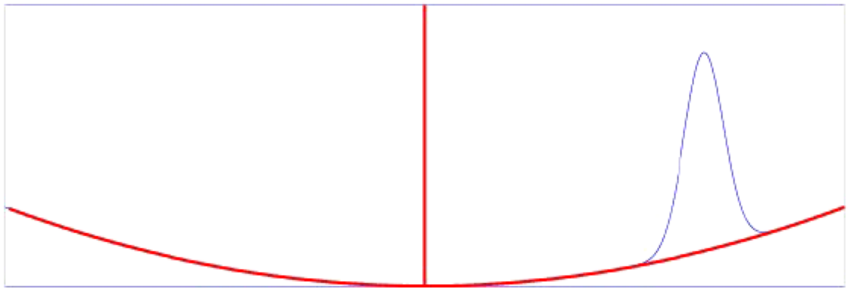
For any two probability densities ψ_1 and ψ_2 with with $\rho_1 = \int f_1\,dp = |\psi_1|^2$ and $\rho_2 = \int f_2\,dp = |\psi_2|^2$,

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

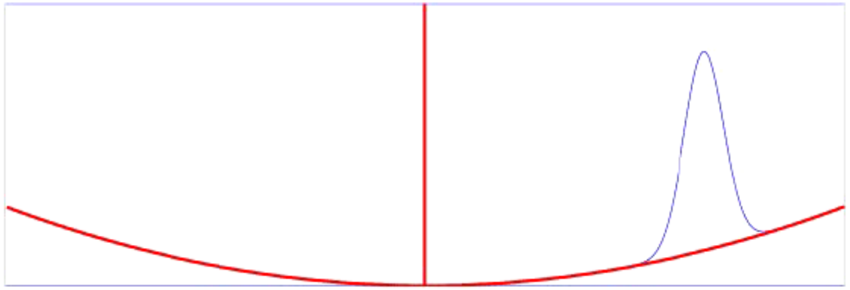
The coherent model

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

Quantum

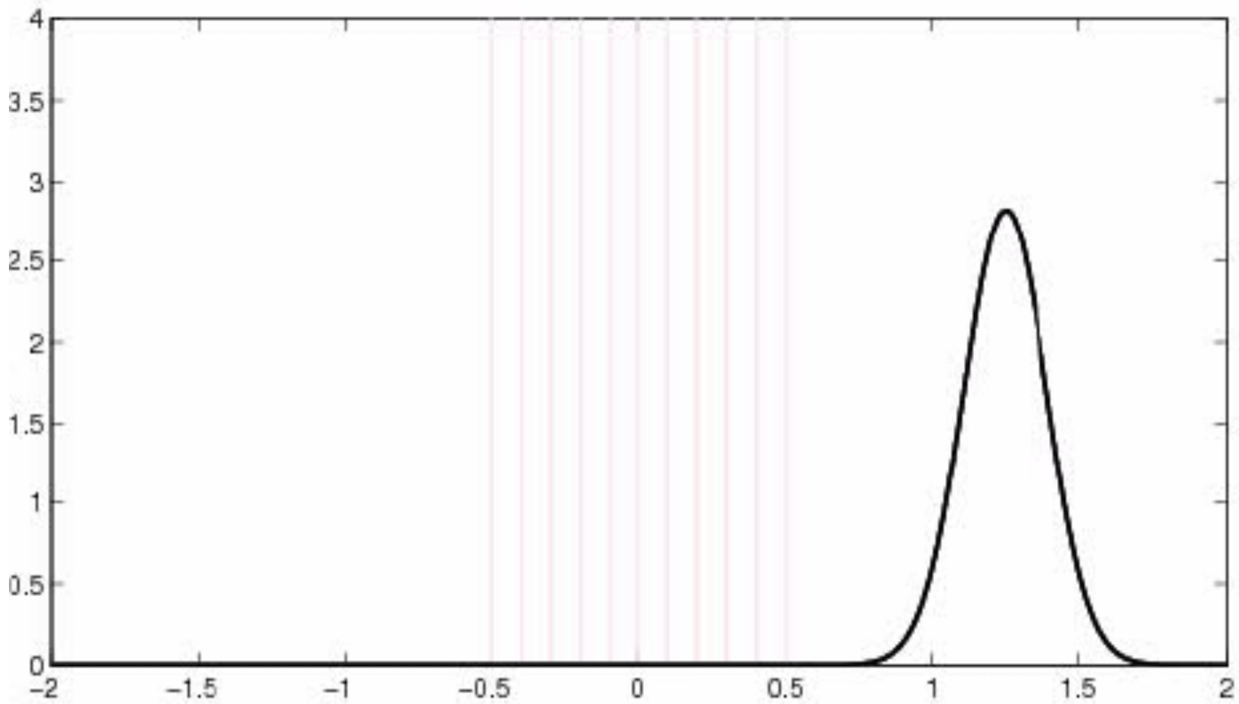


semiclassical

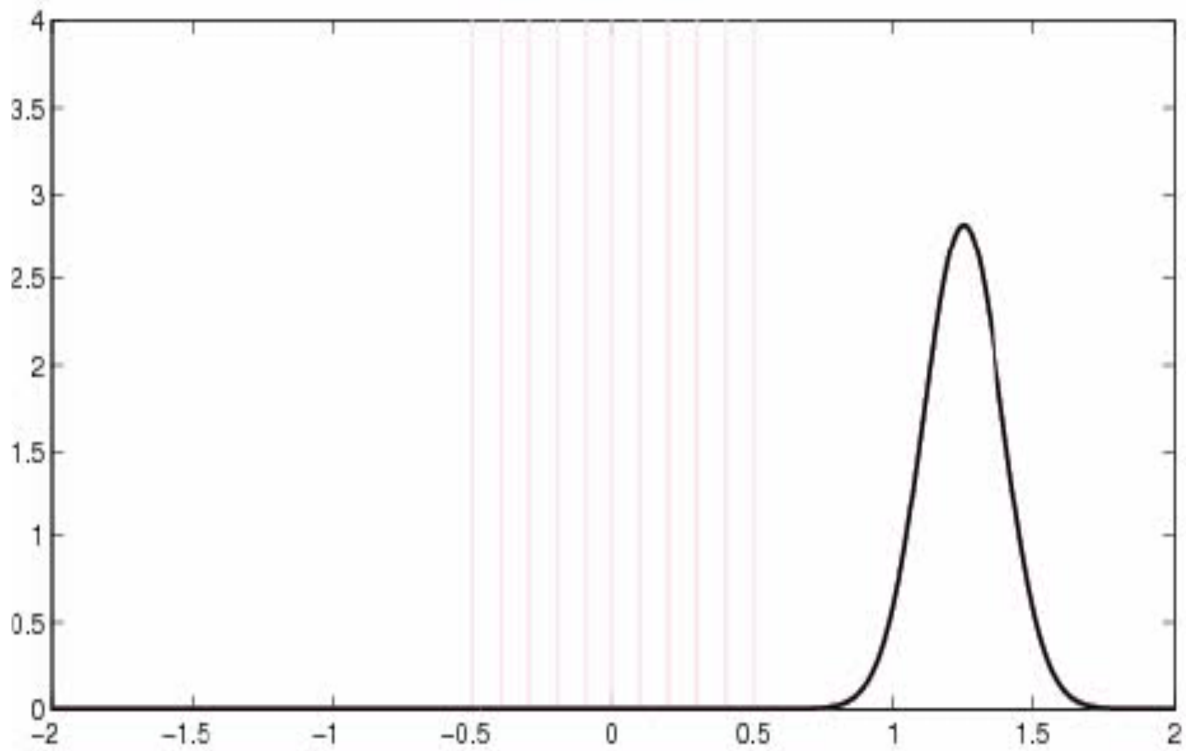


multiple delta barrier (Kronig-Penney)

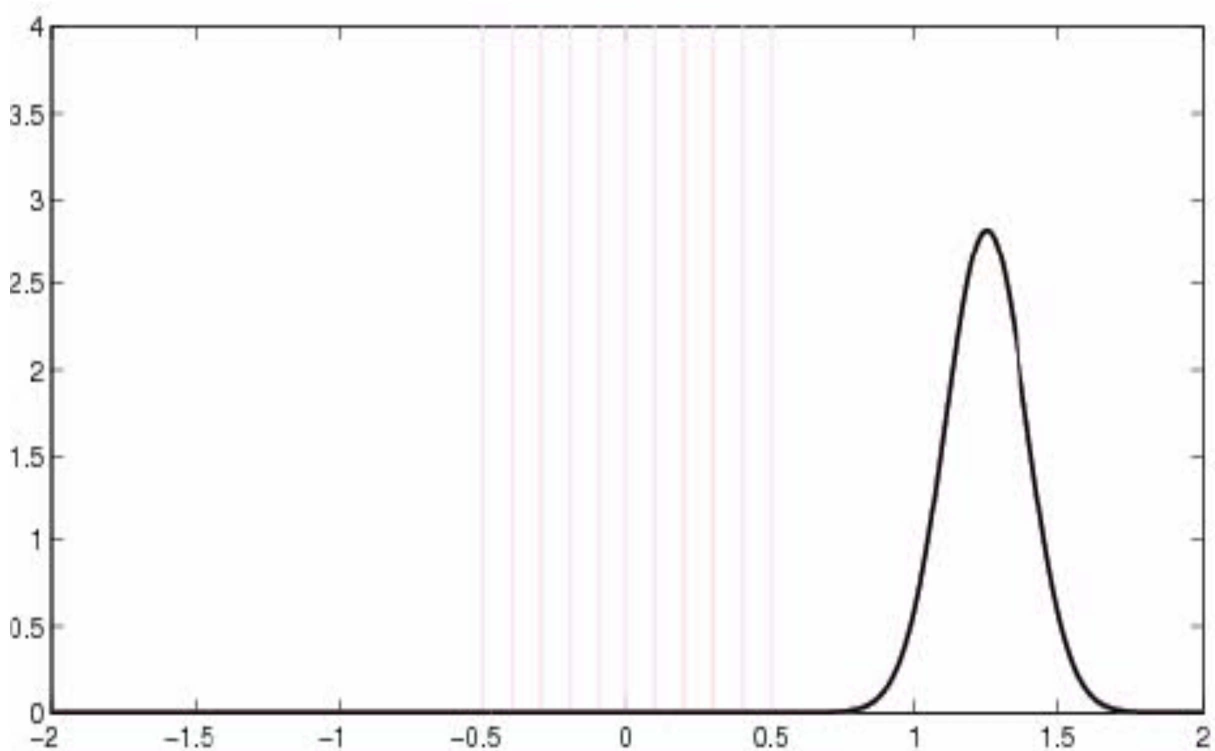
decoherent model vs Schrodinger



multiple delta barrier (Kronig-Penney) coherent model vs Schrodinger



multiple delta barrier (Kronig-Penney)
average soln of coherent model vs Schrodinger



Conclusions

- semiclassical de-coherent and a coherent model for quantum barriers; Computational cost is at the level of classical mechanics (does not numerically resolve the small De Broglie length)
- Compute correctly partial transmission, partial reflection, and phase information at the quantum barriers
- theoretical justification (*Miller, Bal-Keller-Papanicolaou-Ryzhik*) ; More general (wide) barriers
- How to deal with (nonlinear) mean field models: Hartree, Hartree-Fock, Density function theory