A Semiclassical Transport Model for Quantum Barriers

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University of Wisconsin–Madison

IPAM: Quantum and Kinetic Transport
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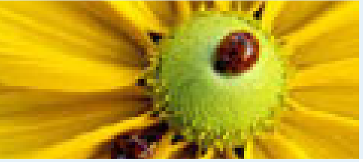


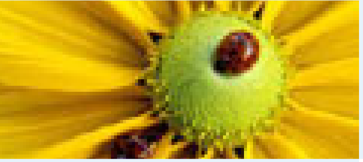
Overview

Background

Thin Barrier Model

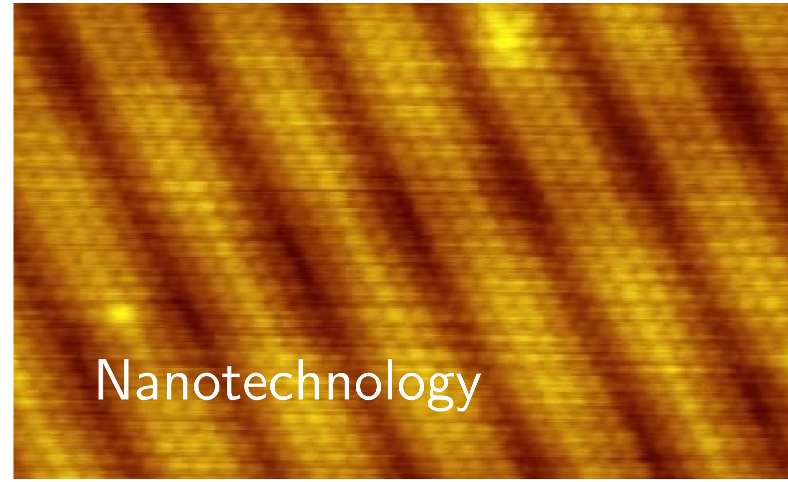
Two Dimensions

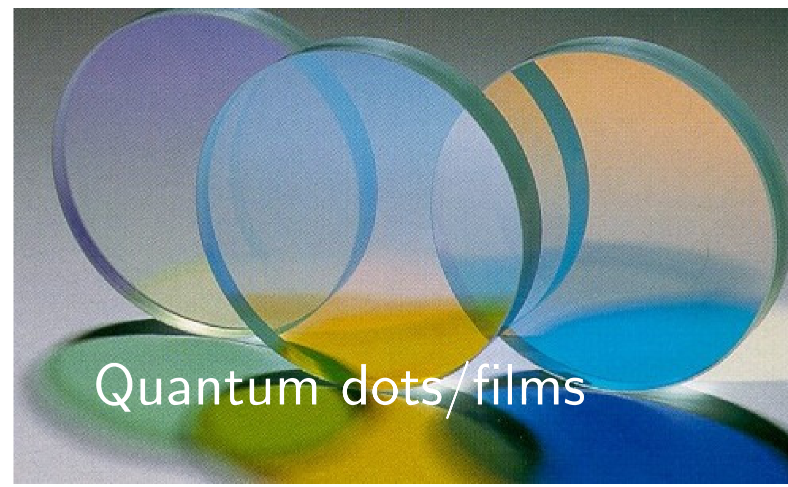
Coherent Model

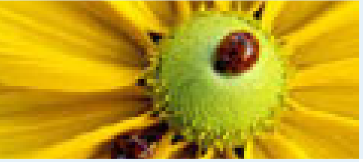


Background

Classical and Quantum Scales







Problem

Problem Model the dynamics of a particle in a largely classical potential field with local quantum discontinuities

- Classical model misses key features — wrong solution
- Numerical Schrödinger solution must resolve the de Broglie wavelength — inefficient over large domains/times
- Ben Abdallah, Gamba, Degond ['02] proposed a general classical-quantum coupling model — difficult to implement

Approach A multiscale method for a thin quantum barrier

Step

$3\pi\varepsilon$

$(3 + \frac{1}{2})\pi\varepsilon$

Wide

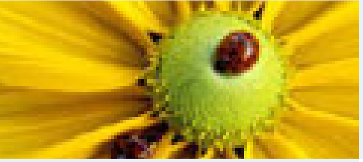
Thin Barriers

Step

$3\pi\varepsilon$

$(3 + \frac{1}{2})\pi\varepsilon$

Wide



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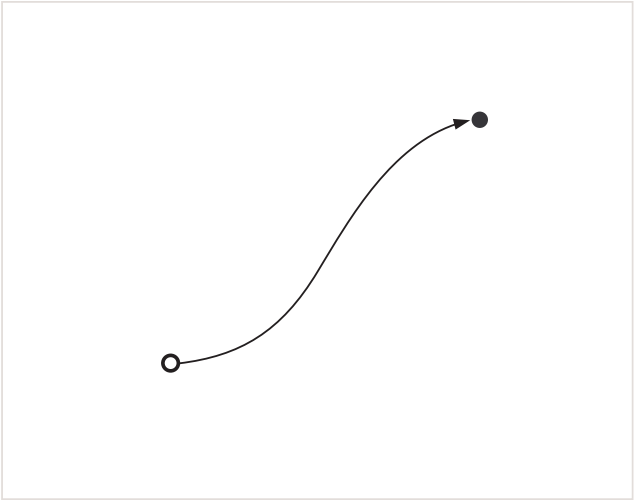
Hamilton's equations

$$\frac{dx}{dt} = p = \nabla_p H(x,p), \qquad \frac{dp}{dt} = -\nabla_x V = -\nabla_x H(x,p)$$

Conservation of energy

$$H(x,p) = \tfrac{1}{2}|p|^2 + V(x) = E$$



Classical Mechanics

Hamilton's equations

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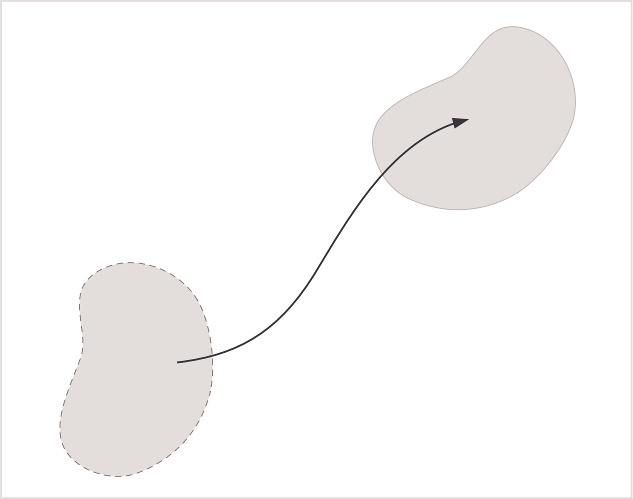
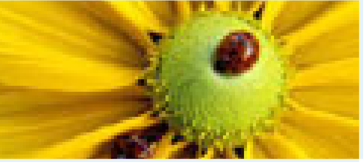
Probability distribution $f(x,p,t)$

$$\frac{d}{dt} f = 0$$





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Probability distribution $f(x,p,t)$

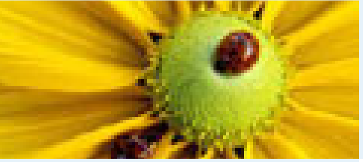
$$\frac{d}{dt}f = \frac{\partial}{\partial t}f + \frac{dx}{dt}\cdot\nabla_x f + \frac{dp}{dt}\cdot\nabla_p f = 0$$

Liouville equation

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

Dirac quantization

$$x \quad \rightarrow \quad x, \qquad p \quad \rightarrow \quad -i\hbar\nabla, \qquad \text{and} \qquad E \quad \rightarrow \quad i\hbar\frac{\partial}{\partial t}$$



Quantum Mechanics

Dirac quantization

$$x \quad \rightarrow \quad x, \qquad p \quad \rightarrow \quad -i\hbar\nabla, \qquad \text{and} \qquad E \quad \rightarrow \quad i\hbar\frac{\partial}{\partial t}$$

Conservation of energy

$$E = H(x,p) = \tfrac{1}{2}|p|^2 + V(x)$$

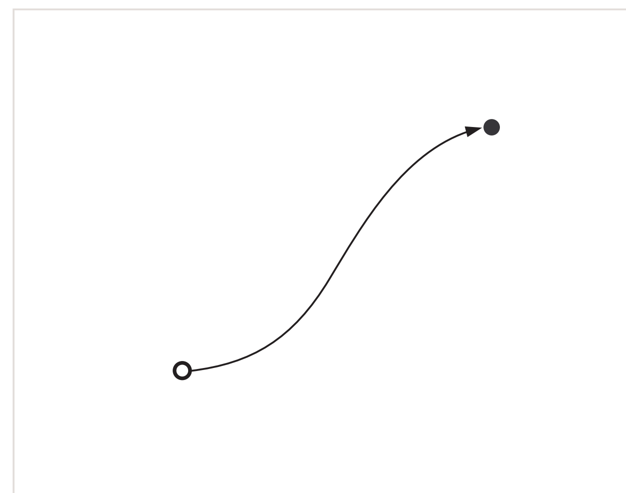
Quantum Mechanics

Dirac quantization

$$x \to x, \quad p \to -i\hbar\nabla, \quad \text{and} \quad E \to i\hbar\frac{\partial}{\partial t}$$

Schrödinger equation

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



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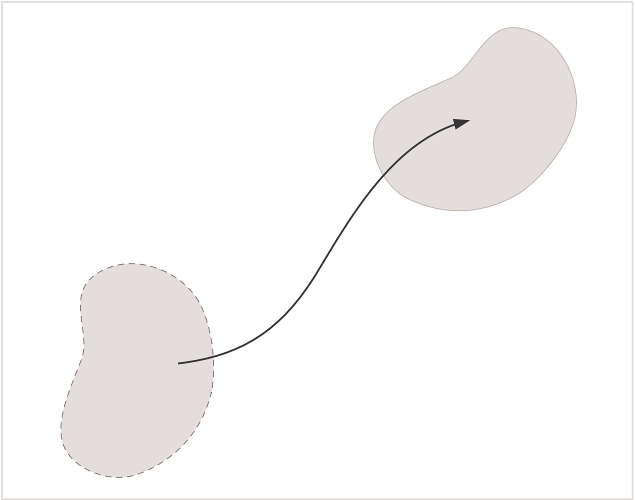
Macroscopic distribution $\tilde{f}(x,p)$



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

Density matrix

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

Dirac quantization

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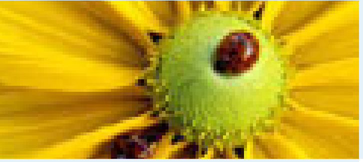
Von Neumann equation

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



Physical Observable—Position Density

Liouville equation | zeroth moment

$$\rho(x,t) = \int_{\mathbb{R}^d} f(x,p,t)\,dp$$

von Neumann equation | diagonal of density matrix

$$\rho(x,t) = \hat{\rho}(x,x,t) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{f}(\tilde{x},\tilde{p})|\psi(x,t;\tilde{x},\tilde{p})|^2\,d\tilde{x}\,d\tilde{p}$$

Schrödinger | $\tilde{f}(\tilde{x},\tilde{p}) = \delta(\tilde{x}-x_0)\delta(\tilde{p}-p_0)$

$$\rho(x,t) = |\psi(x,t)|^2$$

Characteristic length and time scale:

$$L\delta x \text{ and } L\delta t \text{ (where } \delta x = \lambda = \hbar/p_0\text{)}$$

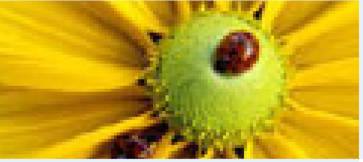
Rescale x, x', and t

$$x \mapsto x/L\delta x, \quad x' \mapsto x'/L\delta x, \quad t \mapsto t/L\delta t$$

then

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

where $\varepsilon = \hbar/[L(\delta x)^2/\delta t]$



Scaled Equations

Characteristic length and time scale:

$$L\delta x \text{ and } L\delta t \text{ (where } \delta x = \lambda = \hbar/p_0\text{)}$$

Rescale x, x', and t

$$x \mapsto x/L\delta x, \quad x' \mapsto x'/L\delta x, \quad t \mapsto t/L\delta t$$

then

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

where $\varepsilon = \hbar/[L(\delta x)^2/\delta t]$

! What's the behavior of physical observables as $\varepsilon \to 0$?

Wigner Equation

von Neumann equation

$$i\varepsilon \frac{\partial}{\partial t}\hat{\rho} - \left(-\tfrac{1}{2}\varepsilon^2[\Delta_x - \Delta_{x'}] + V(x) - V(x')\right)\hat{\rho} = 0$$

Wigner transform

$$W(x,p,t) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \hat{\rho}(x + \tfrac{1}{2}\varepsilon y, x - \tfrac{1}{2}\varepsilon y, t)e^{-ip\cdot y}\,dy$$

Wigner Equation

von Neumann equation

$$i\varepsilon\frac{\partial}{\partial t}\hat{\rho} - \left(-\tfrac{1}{2}\varepsilon^2[\Delta_x - \Delta_{x'}] + V(x) - V(x')\right)\hat{\rho} = 0$$

Wigner transform

$$W(x,p,t) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \hat{\rho}(x + \tfrac{1}{2}\varepsilon y, x - \tfrac{1}{2}\varepsilon y, t)e^{-ip\cdot y}\,dy$$

Wigner equation

$$\frac{\partial}{\partial t}W + p\cdot\nabla_x W - \Theta^\varepsilon W = 0$$

where

$$\Theta^\varepsilon W = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \frac{i}{\varepsilon}\left[V(x + \tfrac{1}{2}\varepsilon y) - V(x - \tfrac{1}{2}\varepsilon y)\right]\widehat{W}(x,y,t)e^{-ip\cdot y}\,dy$$

Semiclassical Limit

Background
Applications
Problem
Thin Barriers
Classical Mechanics
Quantum Mechanics
Position Density
Scaled Equations
Wigner Equation
Semiclassical Limit
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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

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

Semiclassical Limit

What if $V(x)$ is only *piecewise* continuous (as $\varepsilon \rightarrow 0$)?

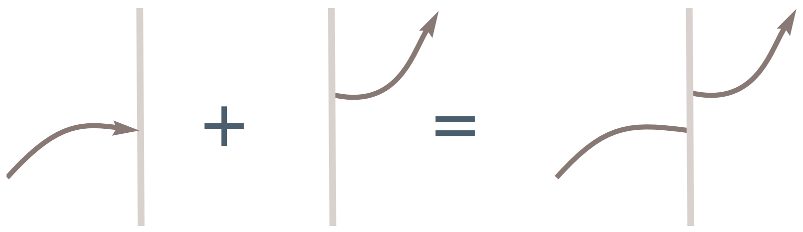
Thin Barrier Model

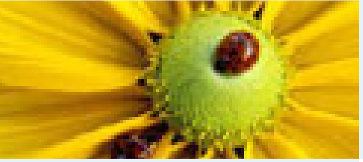
Idea

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

Approach

1. Solve the Liouville equation locally.
2. Use the weak form of the conservation of energy ($H =$ constant) to piece the local solutions together.
3. Use the steady-state Schrödinger equation to choose the unique solution.





Semiclassical Thin Barrier Model

Idea

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

Approach

1. Solve the Liouville equation locally.
2. Use the weak form of the conservation of energy ($H =$ constant) to piece the local solutions together.
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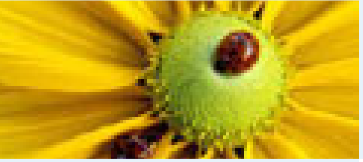
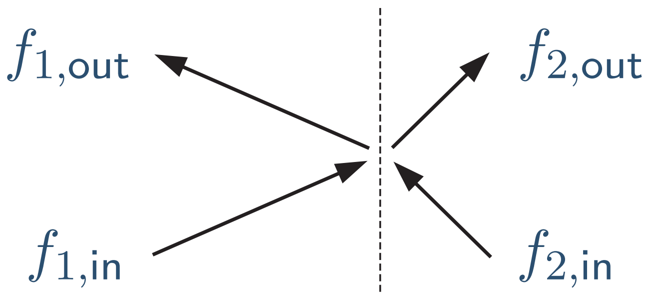
Assumptions

1. Potential is sufficiently smooth away from the barrier.
2. Barrier width $O(\varepsilon)$.
3. Barrier interactions are mutually independent.



Approach

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - \frac{dV}{dx}\frac{\partial f}{\partial p} = 0$$

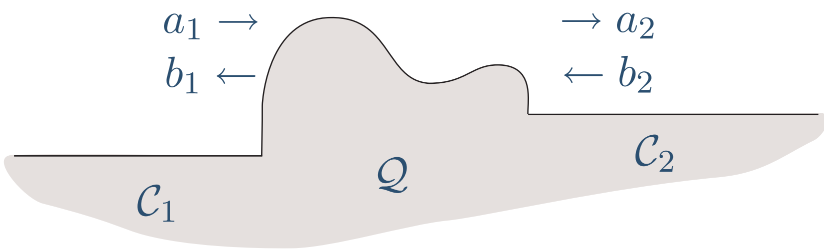


$$f_{1,\text{out}} + f_{2,\text{out}} = f_{1,\text{in}} + f_{2,\text{in}}$$

$$f_{1,\text{out}} = Rf_{1,\text{in}} + Tf_{2,\text{in}}$$
$$f_{2,\text{out}} = Tf_{1,\text{in}} + Rf_{2,\text{in}}$$

with $R + T = 1$

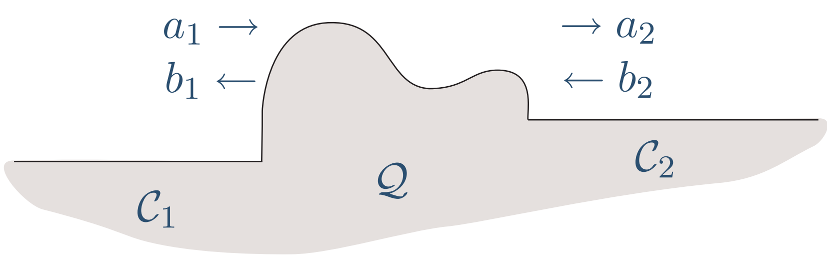
Transfer Matrix



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

$$\psi(x) = \begin{cases} a_1 e^{ixp_1/\varepsilon} + b_1 e^{-ixp_1/\varepsilon}, & x \in \mathcal{C}_1 \\ a_2 e^{ixp_2/\varepsilon} + b_2 e^{-ixp_2/\varepsilon}, & x \in \mathcal{C}_2 \end{cases}$$

with $p_1 = \sqrt{2(E - V_1)}$ and $p_2 = \sqrt{2(E - V_2)}$



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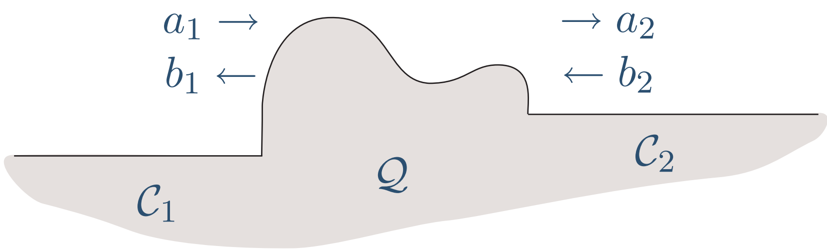
Transfer matrix M

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

Transfer Matrix



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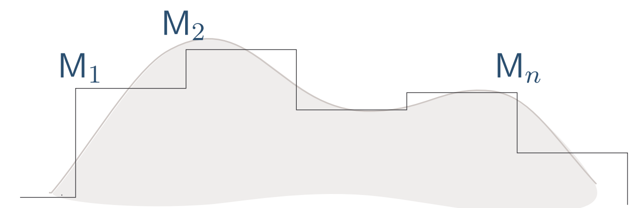
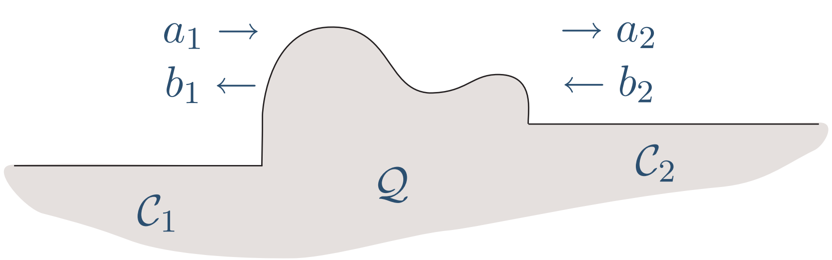


$$\mathsf{M} = \mathsf{M}_n \cdots \mathsf{M}_2 \mathsf{M}_1$$



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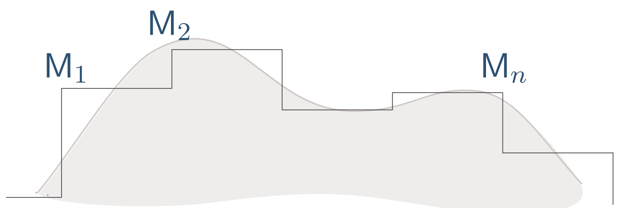
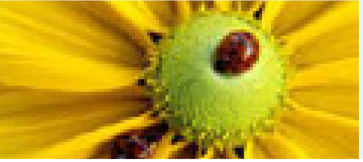


$$\mathsf{M} = \mathsf{M}_n \cdots \mathsf{M}_2 \mathsf{M}_1$$

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 probabilities

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

Continuity equation

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

Scattering coefficients

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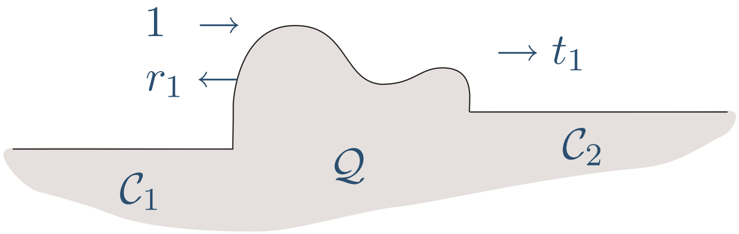
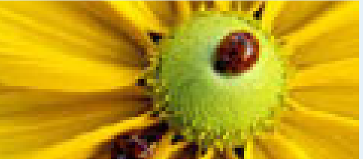
Wave incident from the left ($a_1 = 1$, $b_2 = 0$, $b_1 = r_1$ and $a_2 = t_1$)





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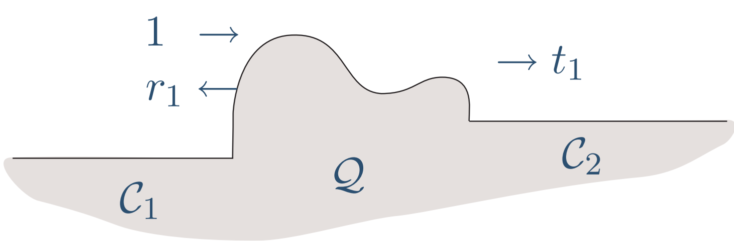
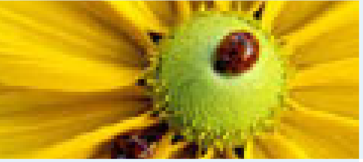


$$J(x) = \begin{cases} p_1\left(1 - |r_1|^2\right), & x \in \mathcal{C}_1 \\ p_2\left(|t_2|^2\right), & x \in \mathcal{C}_2 \end{cases}$$

$$R = |r_1|^2 \qquad \text{and} \qquad T = \tfrac{p_2}{p_1}|t_1|^2$$



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

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

Liouville Solver

The discrete operators $\partial_x f_{ij}$, $\partial_p f_{ij}$ and $\partial_x V_i$ are

$$\partial_x f_{ij} = (f^-_{i+1/2,j} - f^+_{i-1/2,j})/\Delta x,$$
$$\partial_p f_{ij} = (f_{i,j+1/2} - f_{i,j-1/2})/\Delta p,$$
$$\partial_x V_i = (V^-_{i+1/2} - V^+_{i-1/2})/\Delta x$$

with

$$f^\pm_{i+1/2,j} = \lim_{x \to x^\pm_{i+1/2}} \frac{1}{\Delta p} \int_{p_{j-1/2}}^{p_{j+1/2}} f(x,p)\,dp,$$
$$f_{i,j+1/2} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} f(x,p_{j+1/2})\,dx, \text{ and}$$

$$V^\pm_{i+1/2} = \lim_{x \to x^\pm_{i+1/2}} V(x).$$

Interface Condition

Interface condition

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

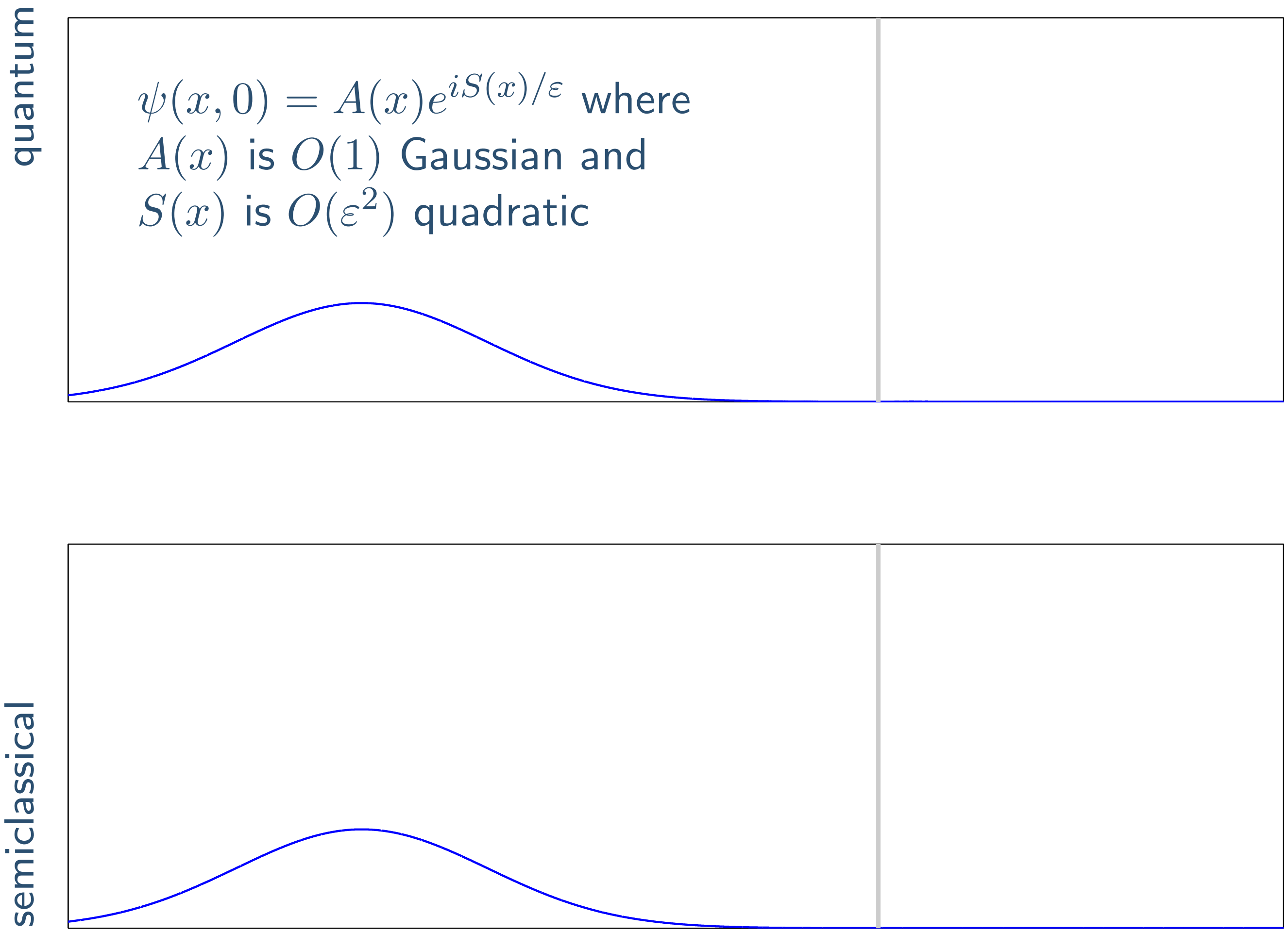
where the incident $q_j = p_j \sqrt{1 + 2(V^+_{Z+1/2} - V^-_{Z+1/2})/p_j|p_j|}$.

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 $q_{j\pm1/2} = \sqrt{p^2_{j\pm1/2} + 2(V^+_{Z+1/2} - V^-_{Z+1/2})}$.

Example: Step potential

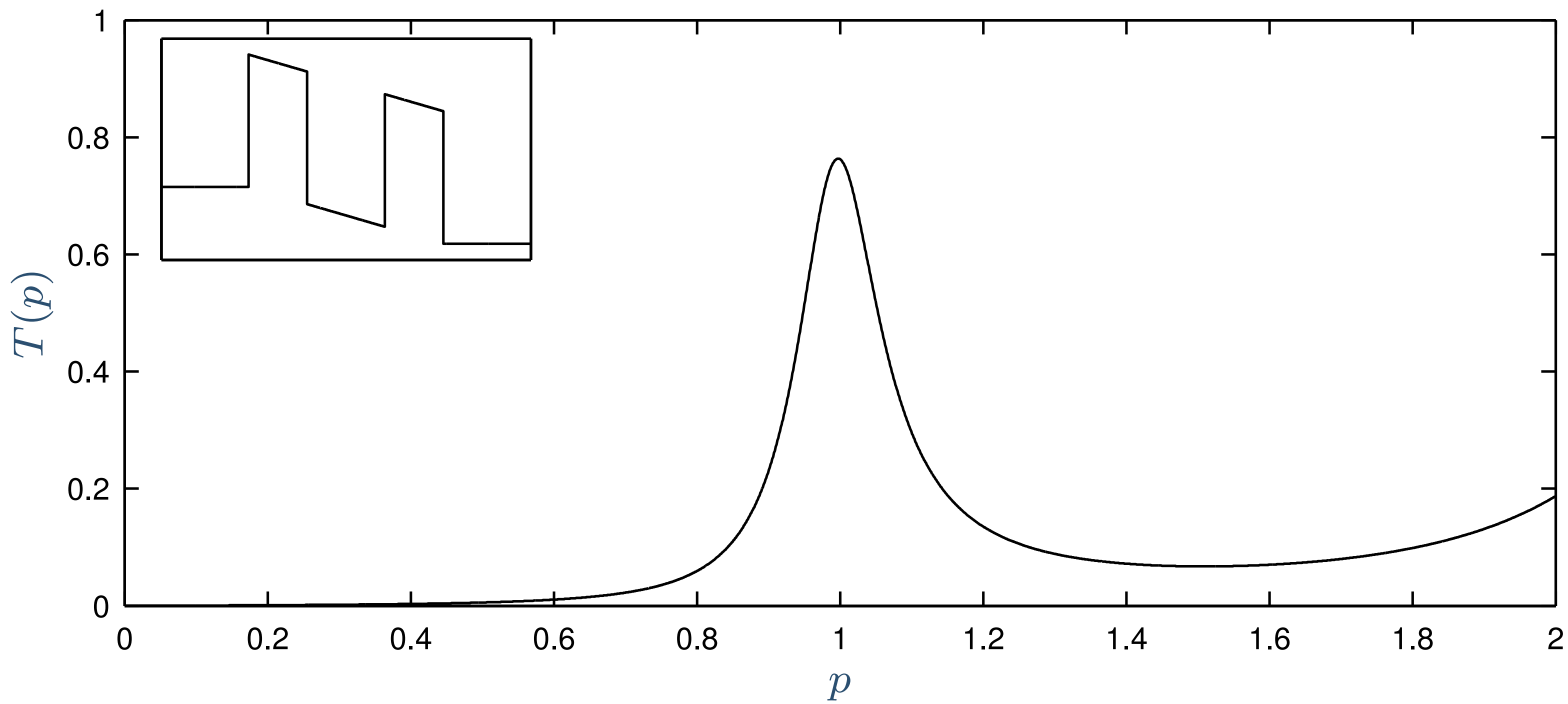


Example: Step potential

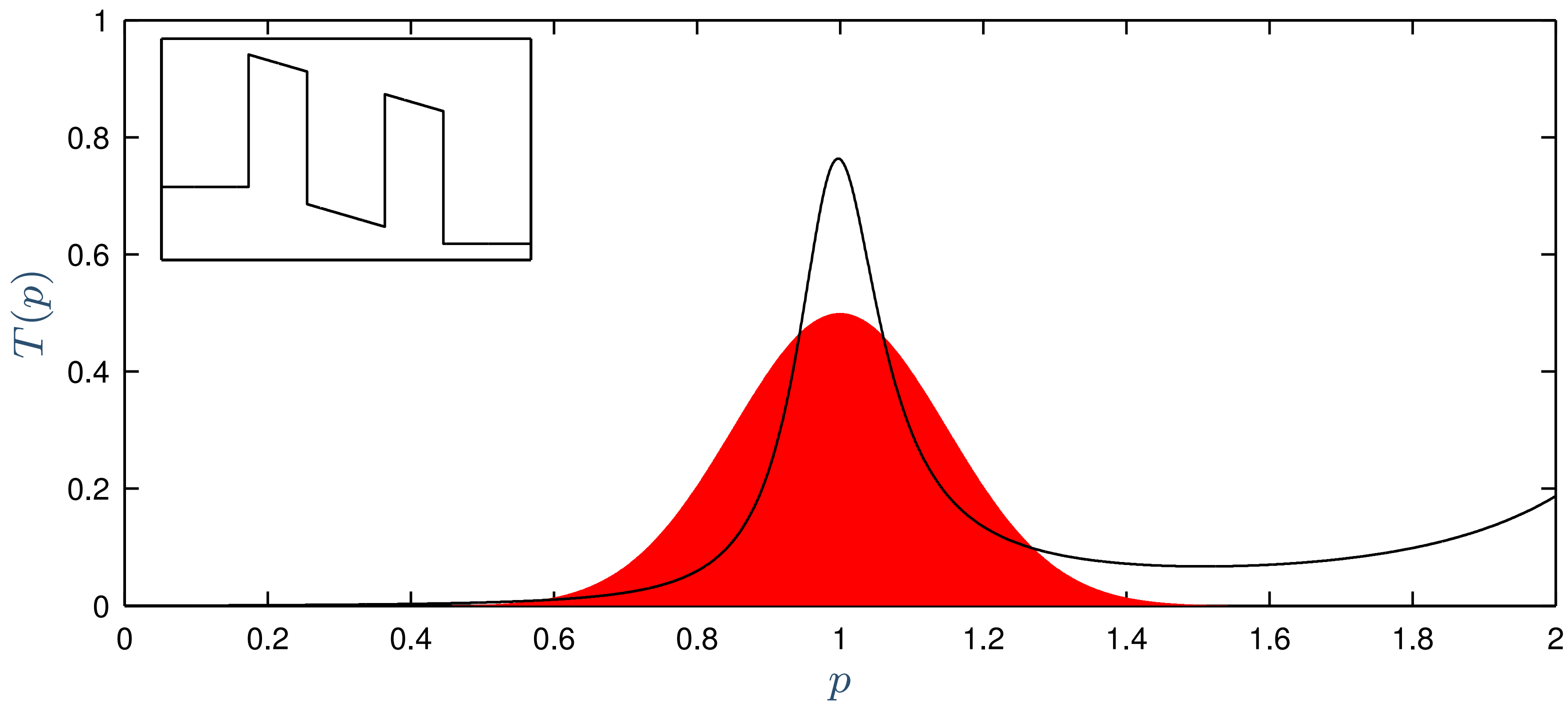
quantum

semiclassical

Resonant Tunneling Diode (RTD): Double-barrier quantum well

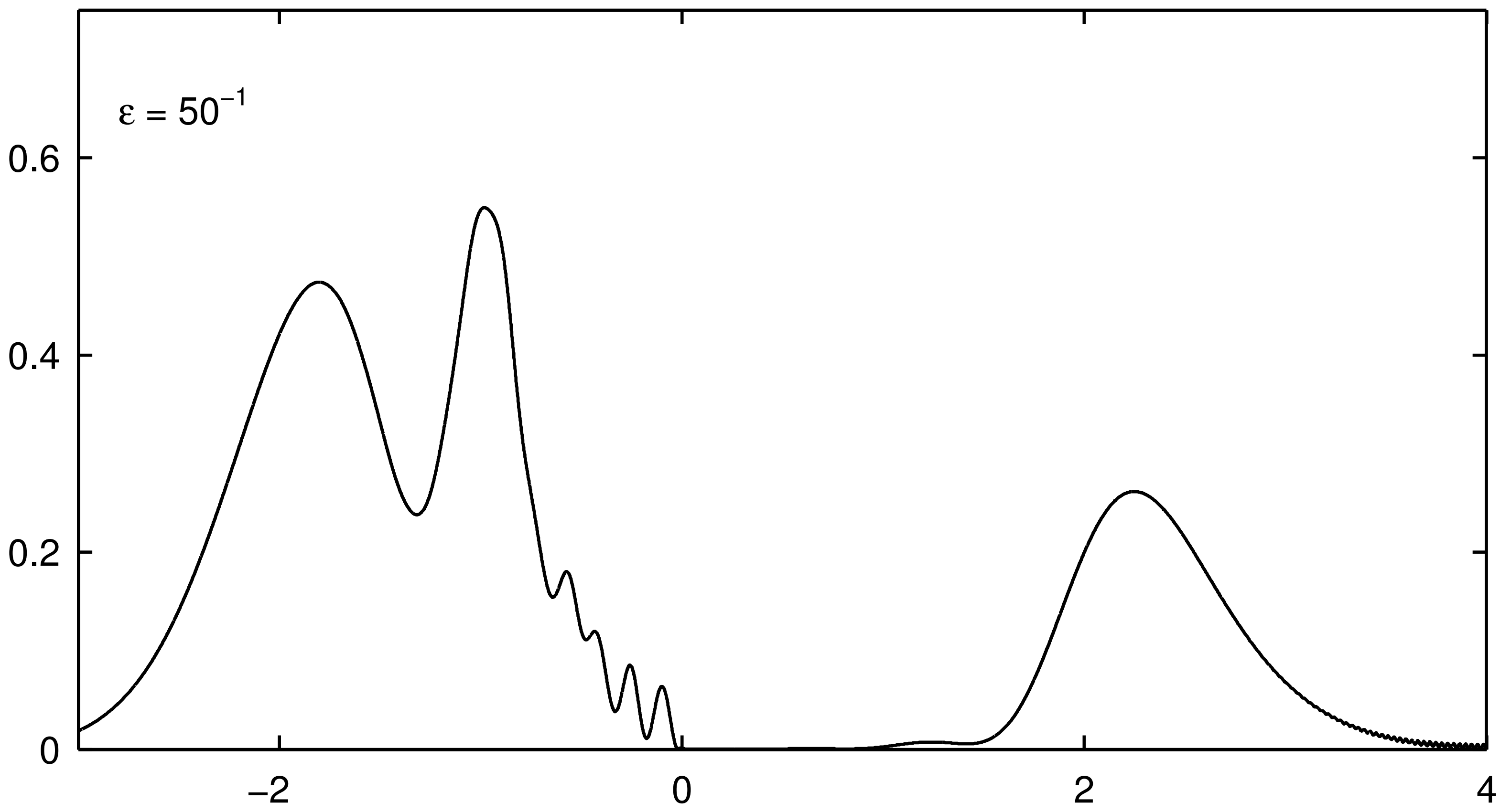


Resonant Tunneling Diode (RTD): Double-barrier quantum well



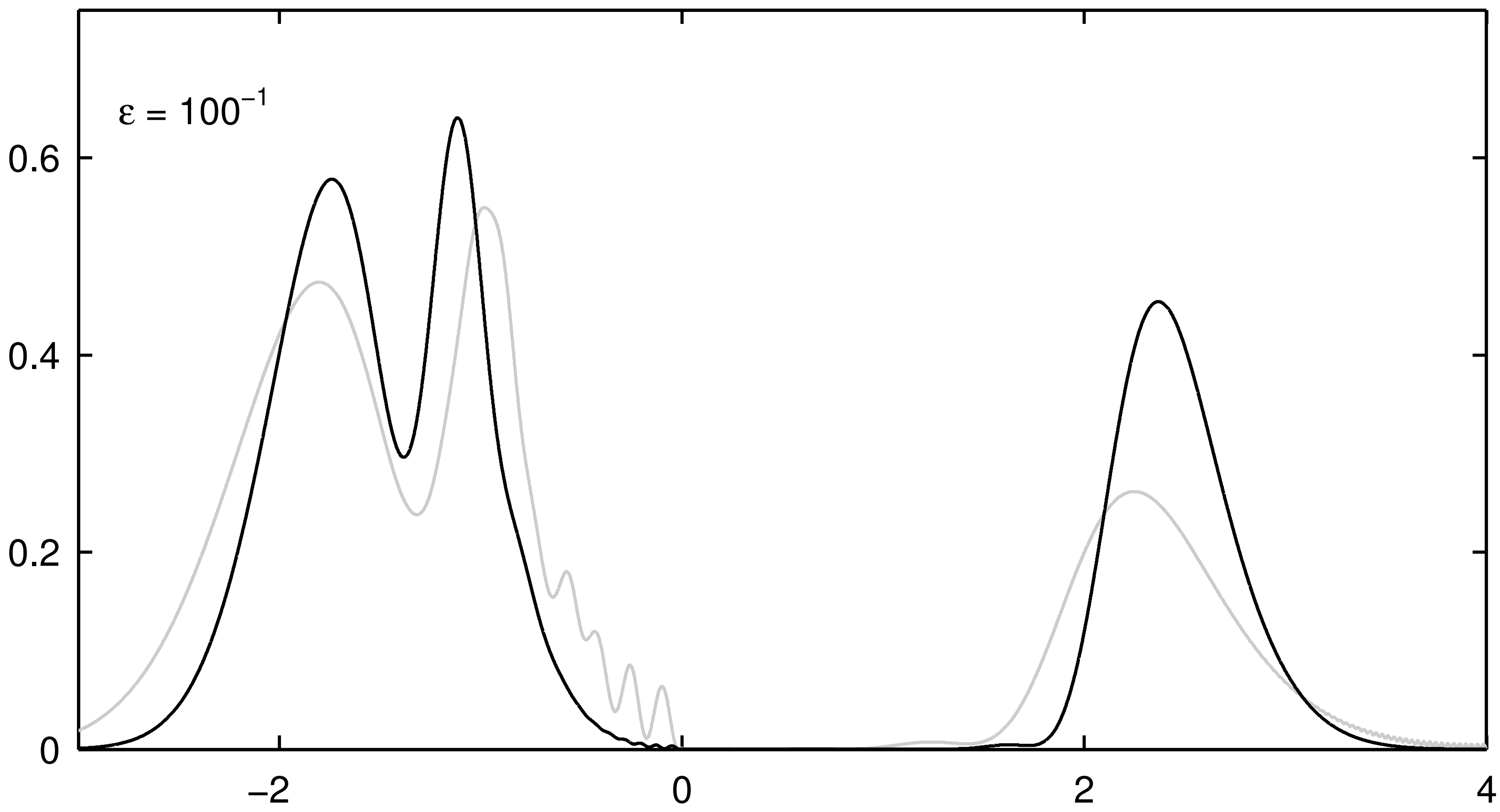
Example: Resonant tunneling mixed-state solution

Resonant Tunneling Diode (RTD): Double-barrier quantum well

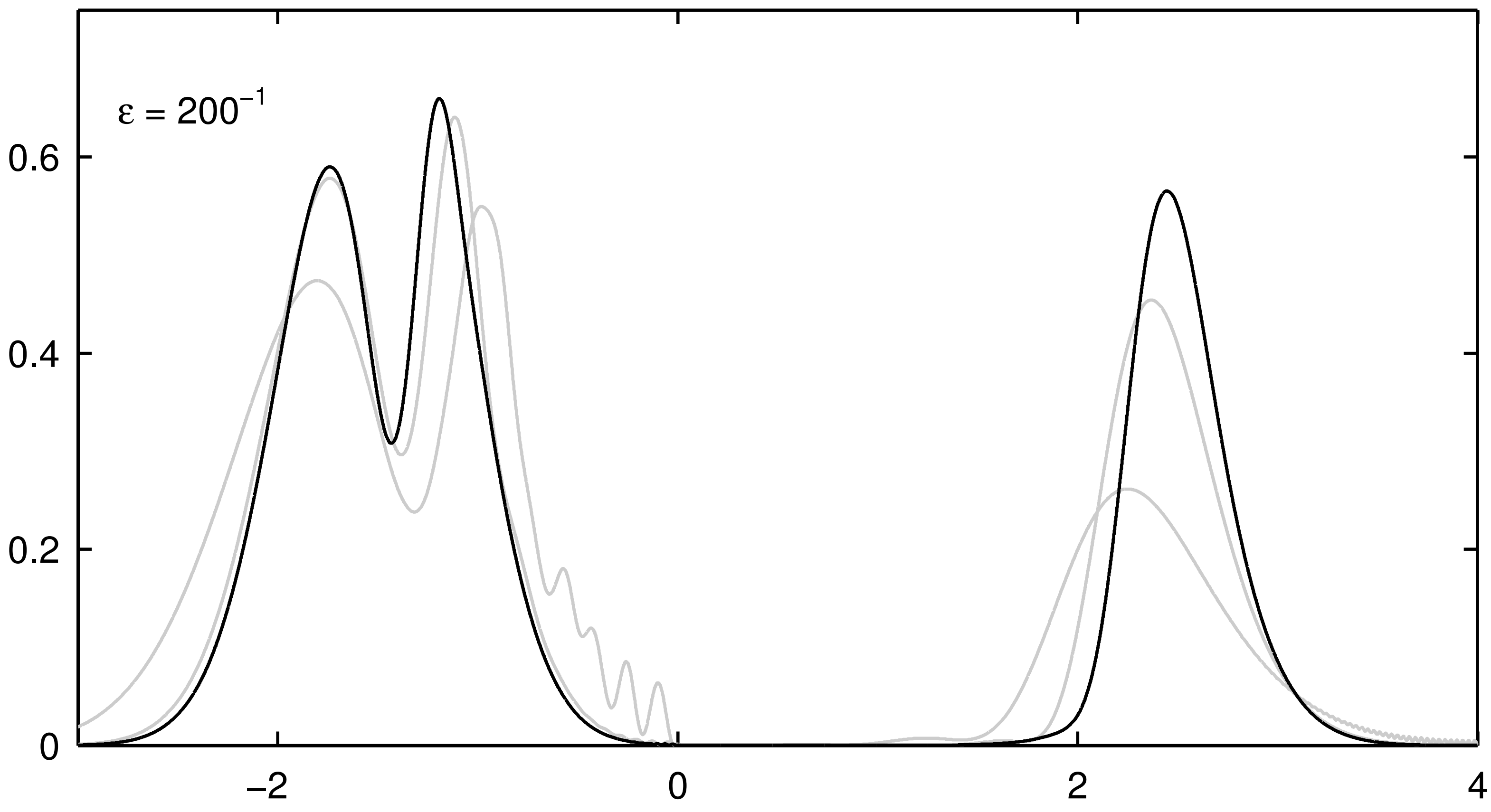


Example: Resonant tunneling mixed-state solution

Resonant Tunneling Diode (RTD): Double-barrier quantum well

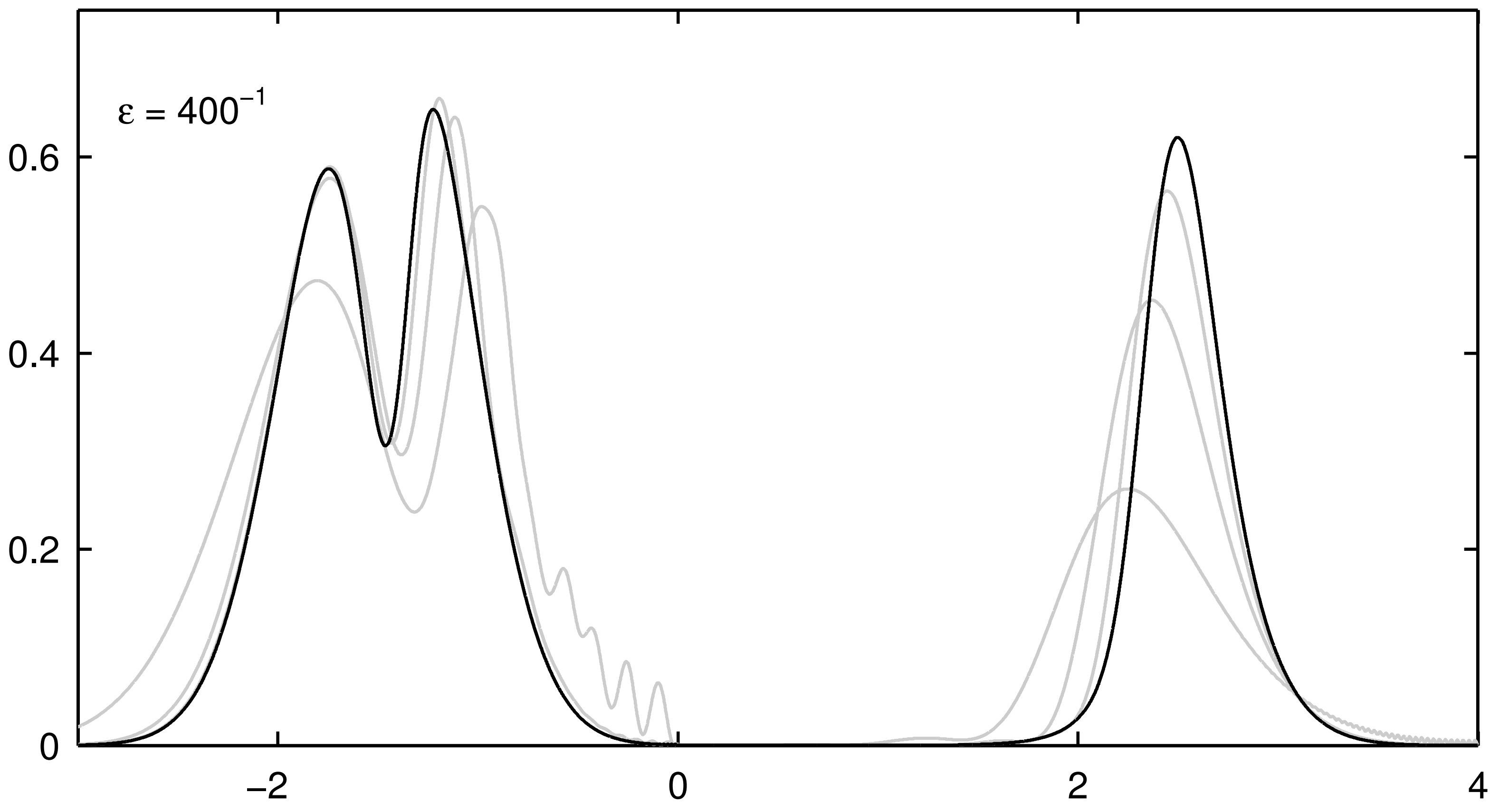


Resonant Tunneling Diode (RTD): Double-barrier quantum well



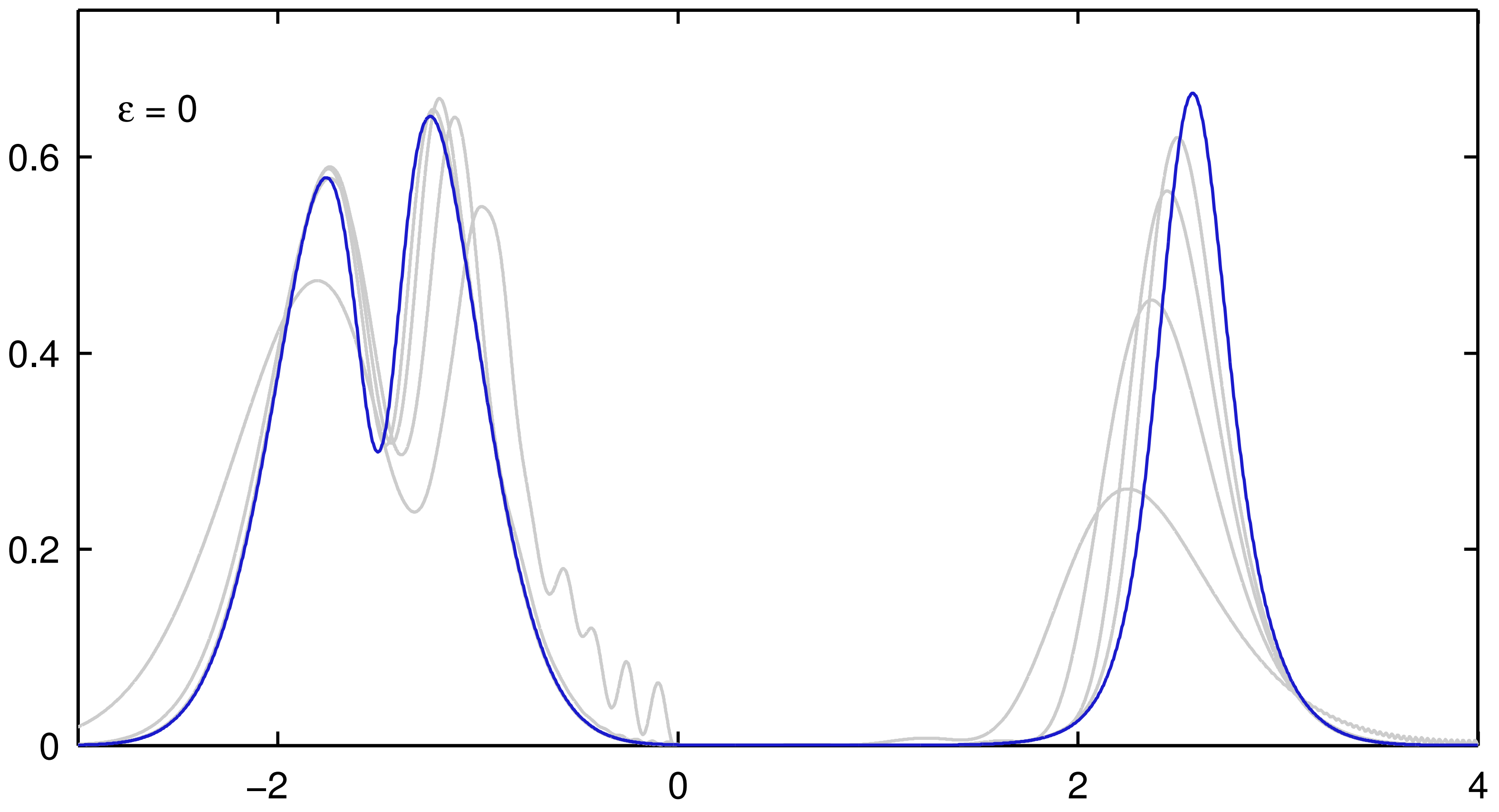
Example: Resonant tunneling mixed-state solution

Resonant Tunneling Diode (RTD): Double-barrier quantum well



Example: Resonant tunneling mixed-state solution

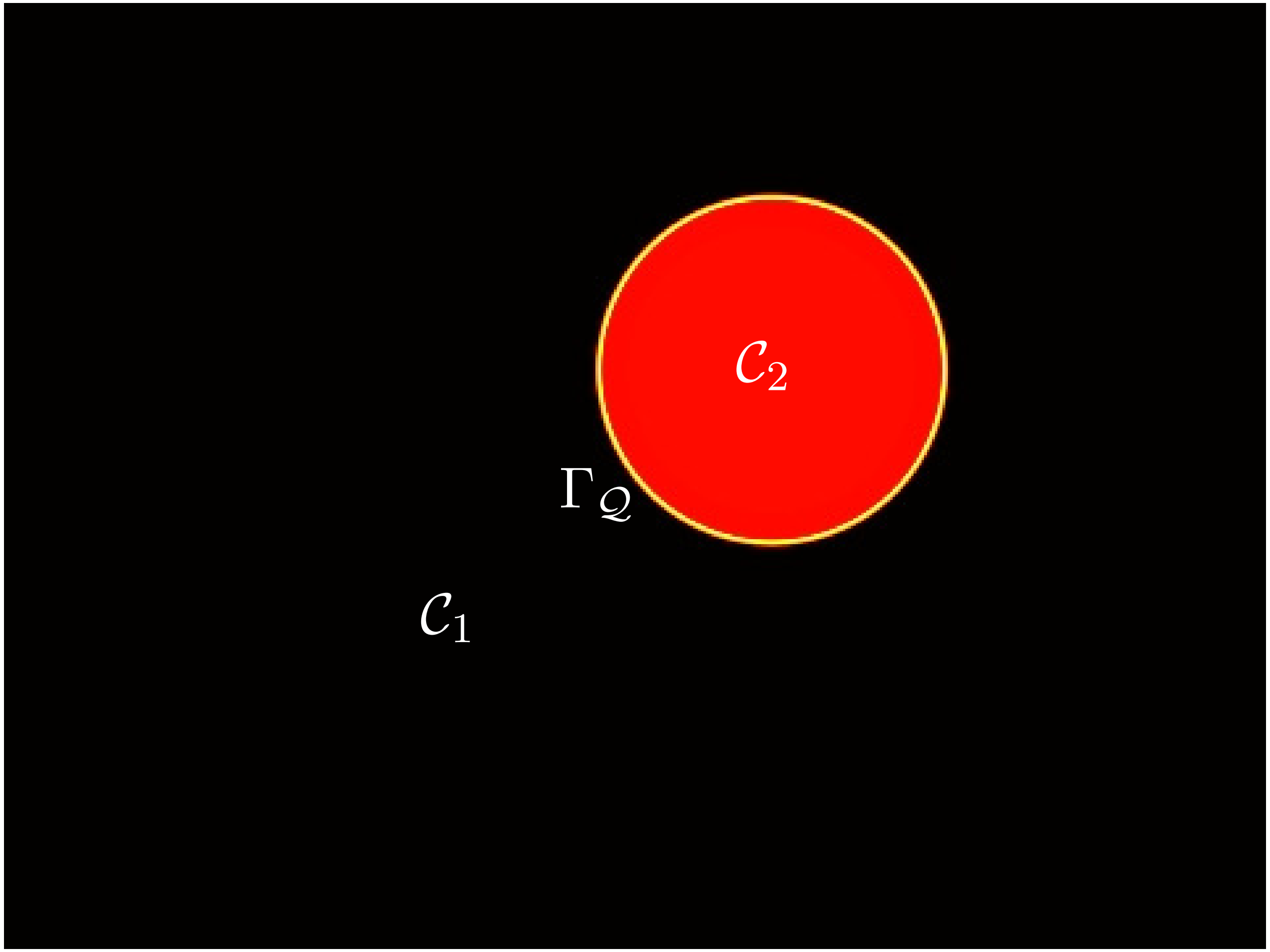
Resonant Tunneling Diode (RTD): Double-barrier quantum well



$O(\varepsilon)$ convergence to semiclassical solution

Two Dimensions

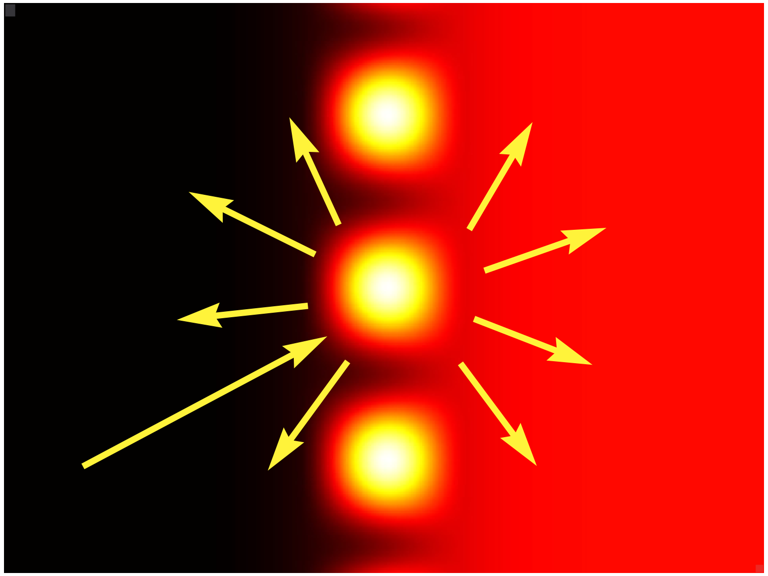
Overview



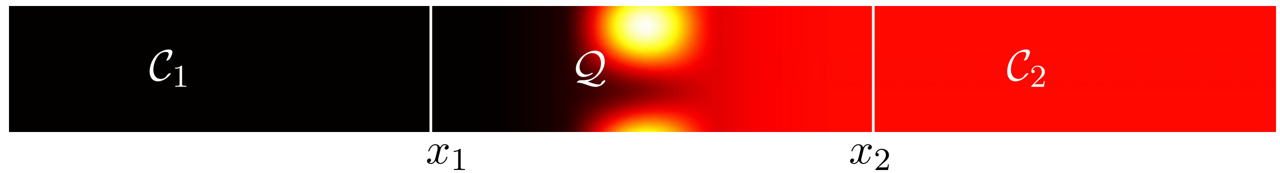
Overview

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

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



Scattering Probabilities



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

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

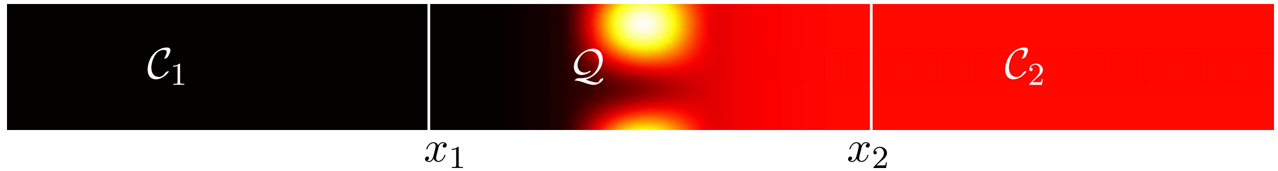
Solution in $\mathcal{C}_j$ for constant V_j

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

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}:

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

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

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

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

Solve the Schrödinger equation

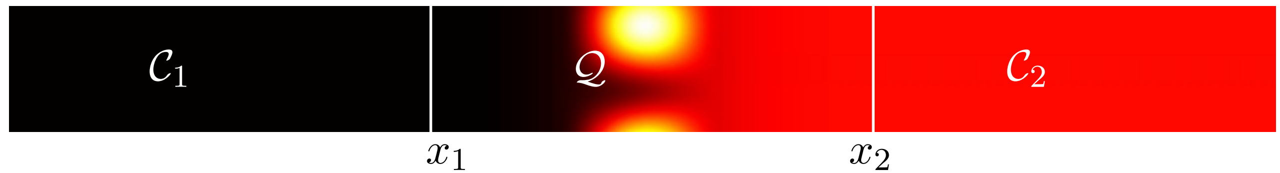
$$-\frac{\partial^2}{\partial x^2}\psi_{\mathcal{Q}}(x,y)-\frac{\partial^2}{\partial y^2}\psi_{\mathcal{Q}}(x,y)+2V_{\mathcal{Q}}(x,y)\psi_{\mathcal{Q}}(x,y)=p^2$$

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



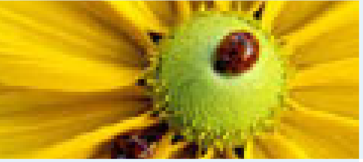
Fourier transform of ψ into momentum space $(y \mapsto \xi)$

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

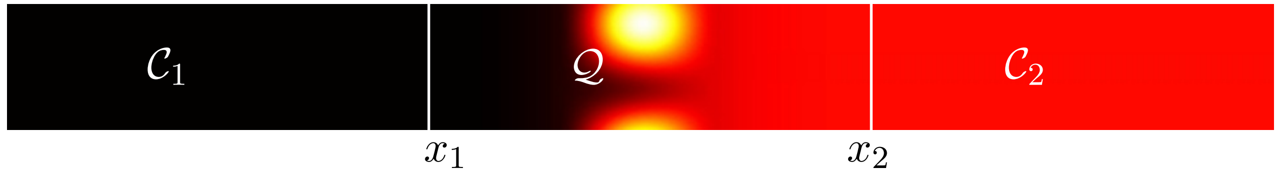
in $\mathcal{Q}$ with matching conditions

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

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

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

After solving the Schrödinger equation

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

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

Particle Method

- Initial conditions

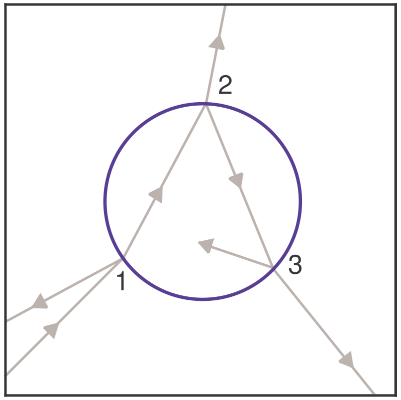
$$f_0(r) = \int_\Omega f_0(\tilde{r})\delta(r-\tilde{r})\,d\tilde{r} \quad \longrightarrow \quad f_0^h = \sum_{j=1}^{N} w_j \delta^h(r-r_j)$$

- Solve $\dfrac{dx}{dt} = p, \quad \dfrac{dp}{dt} = -\nabla_x V$

- Interface condition

Monte Carlo sample $S(\theta_{\text{out}}; p, \theta_{\text{in}})$

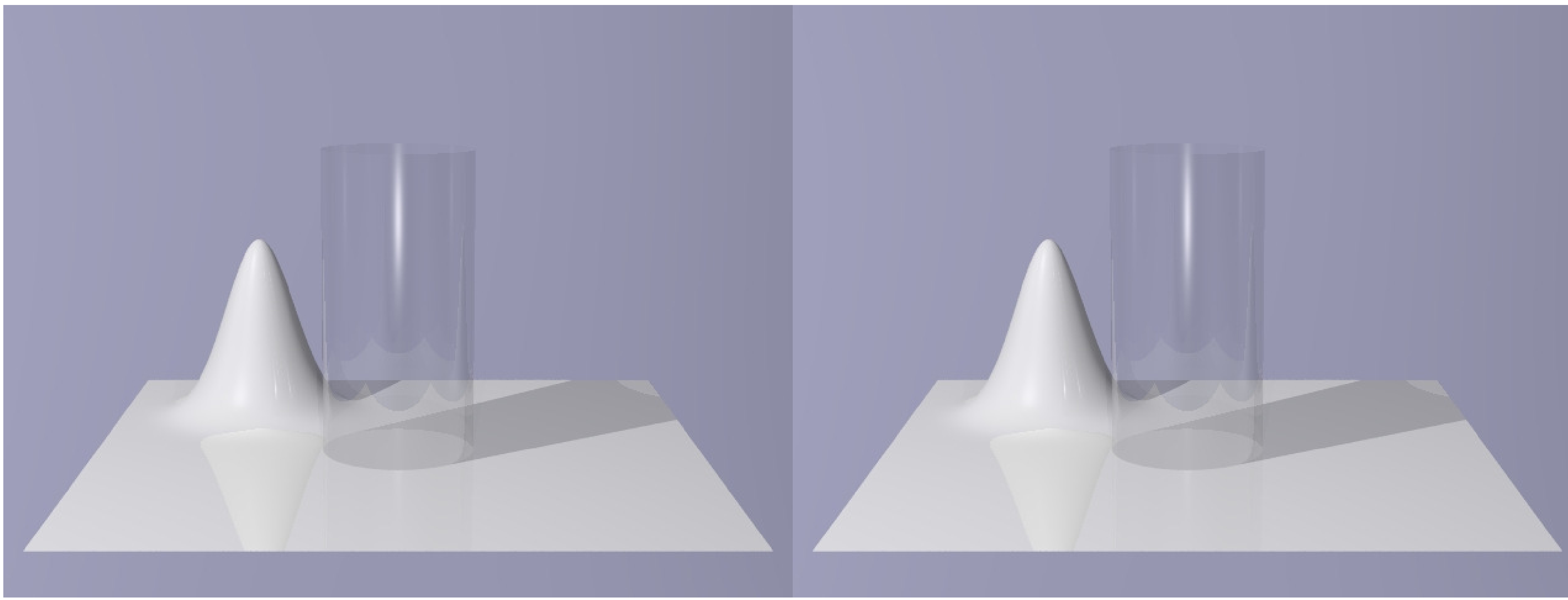
Deterministic take all paths



- Reconstruct density distribution with bicubic cutoff function

Example: Circular Barrier

Schrödinger ($\varepsilon = 1/400$) Semiclassical

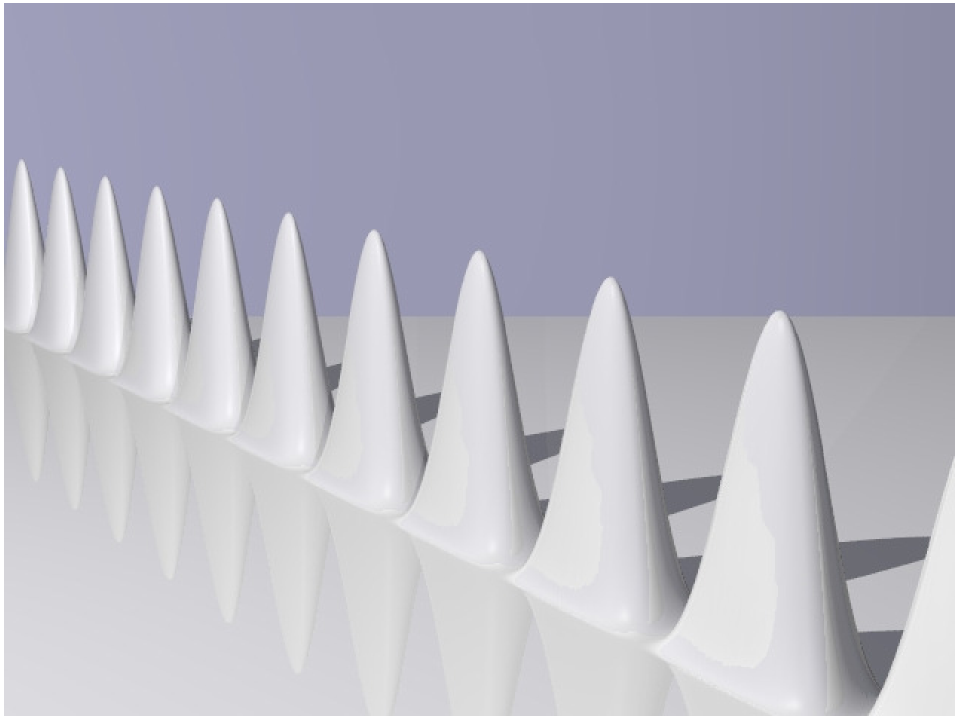


Example: Circular Barrier

Schrödinger ($\varepsilon = 1/400$) Semiclassical

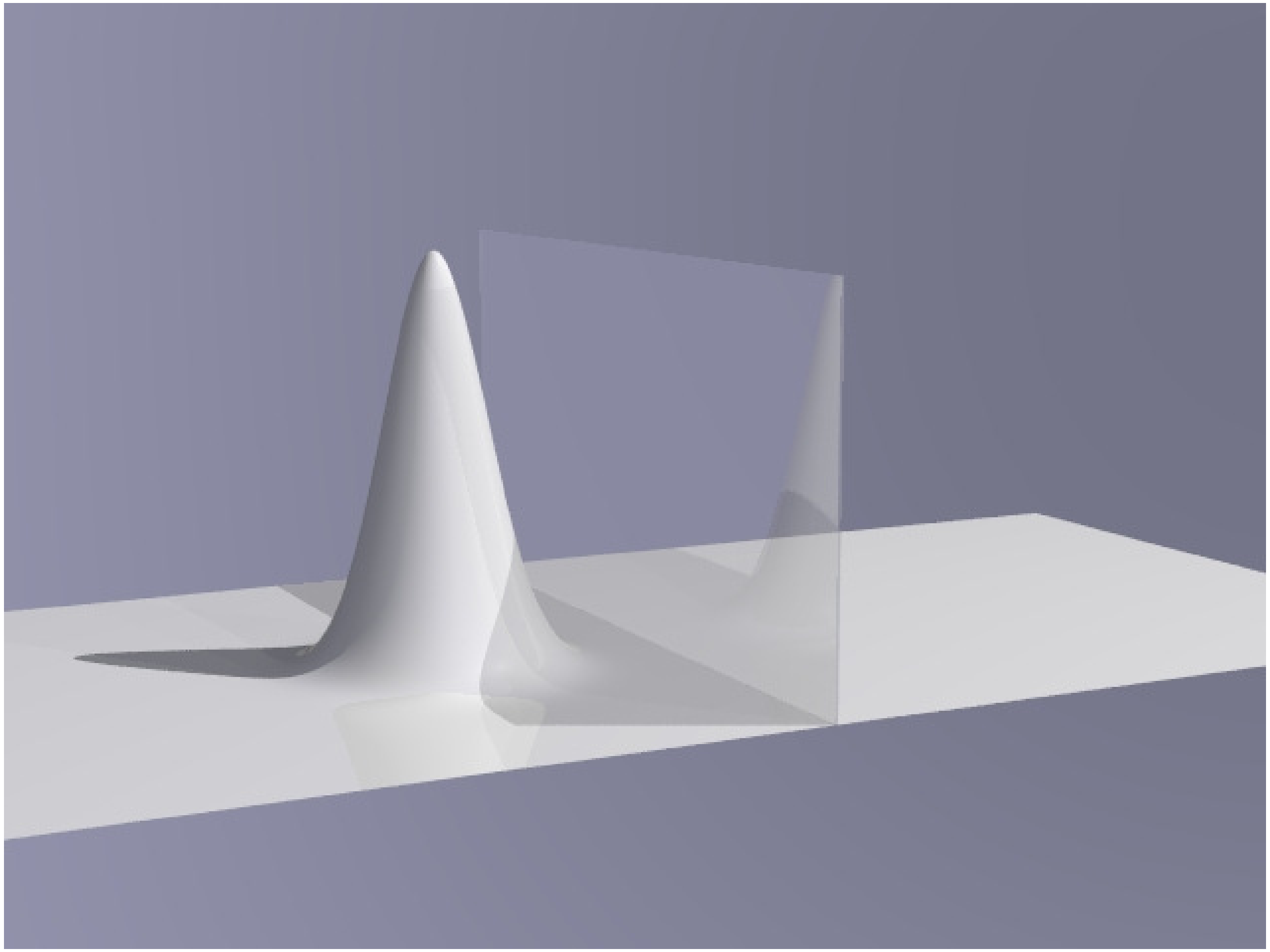
Example: Diffraction Grating

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



Example: Diffraction Grating

Semiclassical ($p = 1$ and $\theta_{\text{in}} = 10°$)

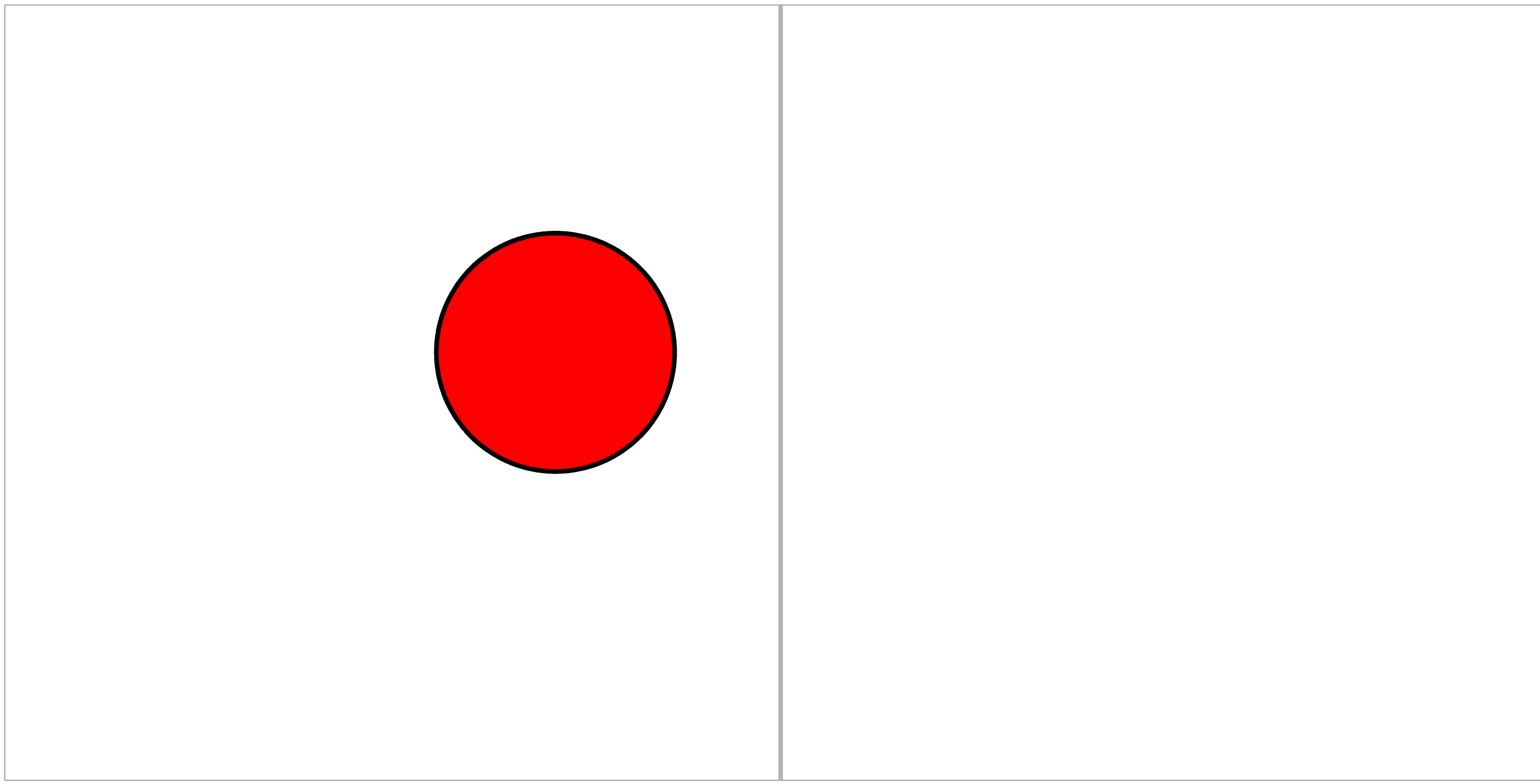


Example: Diffraction Grating

Semiclassical ($p = 1$ and $\theta_{\text{in}} = 10°$)

Fraunhofer diffraction

Example: Diffraction Grating



Schrödinger ($\varepsilon = 1/800$)— red
Semiclassical — black contour

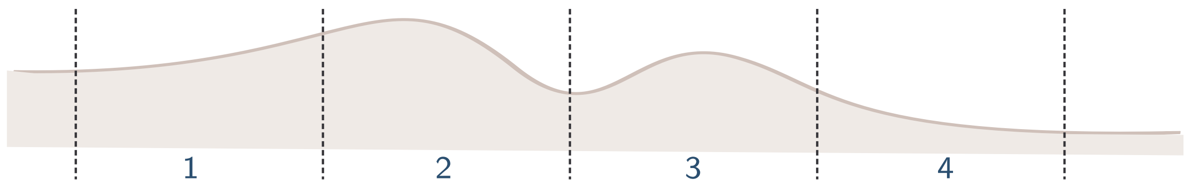
Example: Diffraction Grating

Schrödinger ($\varepsilon = 1/800$)— red
Semiclassical — black contour

Coherent Model

Extending the Thin Barrier Model

Idea Combine several thin barriers.



Problem Wigner transform discards phase information,
so barrier interactions are mutually independent.

ψ Quantum	$\longrightarrow$	Wigner Transform	$\longrightarrow$	f Semiclassical

Approach Track both $f(x, p, t)$ and phase offset $\theta(x, p, t)$.

Example: Harmonic Oscillator with Delta Barrier

$$V(x) = \frac{1}{2}x^2 + \varepsilon\alpha\delta(x)$$

$\alpha = \sqrt{3}$: $\frac{1}{4}$ transmission probability

quantum

semiclassical

Example: Harmonic Oscillator with Delta Barrier

$$V(x) = \frac{1}{2}x^2 + \varepsilon\alpha\delta(x)$$

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quantum

semiclassical

$$V(x) = \frac{1}{2}x^2 + \varepsilon\alpha\delta(x)$$

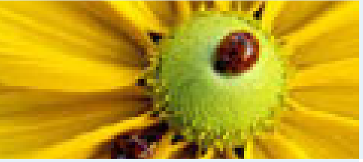
$\alpha = \sqrt{3}$: $\frac{1}{4}$ transmission probability

quantum

semiclassical

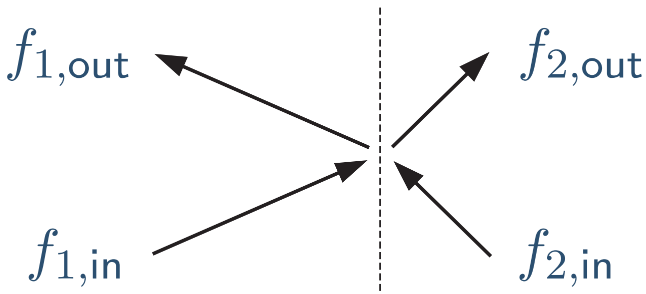
Numerical Implementation

- Initialization
  - Solve time-independent Schrödinger equation to get the complex scattering coefficients
- Eulerian Solver/Lagrangian Solver
  - Use finite volume/particle method method locally
  - Incorporate interface condition at quantum barrier



Eulerian Implementation

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - \frac{dV}{dx}\frac{\partial f}{\partial p} = 0$$



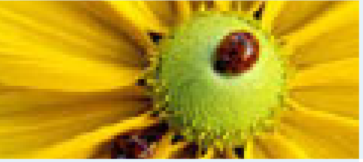
$$f_{1,\text{out}} + f_{2,\text{out}} = f_{1,\text{in}} + f_{2,\text{in}}$$

Build wave interference into the interface conditions

$$\rho_{1+2} = |\psi_1 + \psi_2|^2 = \rho_1 + \rho_2 + 2\sqrt{\rho_1\rho_2}\cos\theta$$

So,

$$f_{1,\text{out}} = Rf_{1,\text{in}} + Tf_{2,\text{in}} + 2\sqrt{RTf_{1,\text{in}}f_{2,\text{in}}}\cos\theta$$
$$f_{2,\text{out}} = Tf_{1,\text{in}} + Rf_{2,\text{in}} - 2\sqrt{RTf_{1,\text{in}}f_{2,\text{in}}}\cos\theta$$



Eulerian: Tracking the phase θ

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

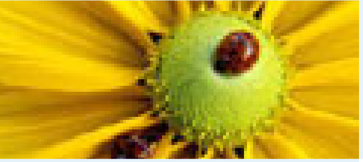
$$\frac{d\Phi}{dt} = \frac{\partial\Phi}{\partial t} + p\frac{\partial\Phi}{\partial x} - \frac{dV}{dx}\frac{\partial\Phi}{\partial p} = 0$$

with the interface condition

$$\Phi_{1,\text{out}} = r_1\Phi_{1,\text{in}} + \sqrt{\frac{p_1}{p_2}}t_2\Phi_{2,\text{in}}$$

$$\Phi_{2,\text{out}} = \sqrt{\frac{p_2}{p_1}}t_1\Phi_{1,\text{in}} + r_2\Phi_{2,\text{in}}$$

Then $e^{i\theta} = \Phi/|\Phi|$.



Implementation Issues

- $\Phi(x,p,t) = \sqrt{f(x,p,t)}e^{i\theta(x,p)}$ is a hybrid of f and ψ.
- We could have simply solved

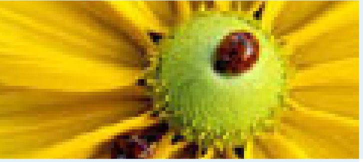
$$\frac{\partial \Phi}{\partial t} + p\frac{\partial \Phi}{\partial x} - \frac{dV}{dx}\frac{\partial \Phi}{\partial p} = 0$$

but scheme does not conserve $\rho(x,t) = \int |\Phi(x,p,t)|^2 \, dp$.

- Solve in (x,E)-domain rather than (x,p)-domain.

$$\frac{d}{dt}F(x,E) = \frac{\partial F}{\partial t} + p\frac{\partial F}{\partial x} = 0$$

  - Prevent numerical mixing of the characteristics.
  - Simplifies the scheme for discontinuous potentials.



Lagrangian Solver

$$\frac{dx}{dt} = p, \ \frac{dp}{dt} = -\frac{dV}{dx} \text{ with } \Phi_k(x,p,0) = \sqrt{f_k(x,p,0)}.$$

Solution $f(x,p,t) = \left| \sum_k s_k(H(x,p))\Phi_k(x,p,t) \right|^2$

Linear Interface Condition: $\quad r\Phi_{1,\text{out}} + t\Phi_{2,\text{out}} = \Phi_{1,\text{in}}.$

Lagrangian Solver

$$\frac{dx}{dt} = p,\ \frac{dp}{dt} = -\frac{dV}{dx} \text{ with } \Phi_k(x,p,0) = \sqrt{f_k(x,p,0)}.$$

Solution $f(x,p,t) = \left|\sum_k s_k(H(x,p))\Phi_k(x,p,t)\right|^2$

Linear Interface Condition: $\quad r\Phi_{1,\text{out}} + t\Phi_{2,\text{out}} = \Phi_{1,\text{in}}.$

Monte Carlo ($\xi \in [0,1]$) $\begin{cases} \text{transmission,} & \text{if } \xi < \frac{|t|}{|t|+|r|} \\ \text{reflection,} & \text{otherwise.} \end{cases}$

$$s_k \leftarrow (|t| + |r|)e^{i\theta}s_k \quad \text{with} \quad e^{i\theta} = \begin{cases} t/|t|, & \text{for transmission} \\ r/|r|, & \text{for reflection} \end{cases}$$

Example: Double-delta Barrier

$$V(x) = \alpha\varepsilon \left[\delta(x - \ell/2) + \delta(x + \ell/2)\right], \quad \ell = 10\varepsilon$$

Example: Double-delta Barrier

$$V(x) = \alpha\varepsilon \left[\delta(x - \ell/2) + \delta(x + \ell/2)\right], \quad \ell = 10\varepsilon$$

Thin Barrier

Example: Double-delta Barrier

$$V(x) = \alpha\varepsilon \left[\delta(x - \ell/2) + \delta(x + \ell/2)\right], \quad \ell = 10\varepsilon$$

Two Thin Barriers

Example: Double-delta Barrier

$$V(x) = \alpha\varepsilon \left[\delta(x - \ell/2) + \delta(x + \ell/2) \right], \quad \ell = 10\varepsilon$$

Coherent Model

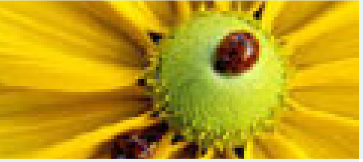
Example: Double-delta Barrier

$$V(x) = \alpha\varepsilon\left[\delta(x-\ell/2)+\delta(x+\ell/2)\right], \quad \ell = 10\varepsilon$$

Coherent Model (Averaged Solution)

Example: Crystalline Barrier

$$V(x) = \alpha\varepsilon \sum_{k=-5}^{5} \delta(x - k\ell), \quad \ell = 20\varepsilon$$



Example: Crystalline Barrier

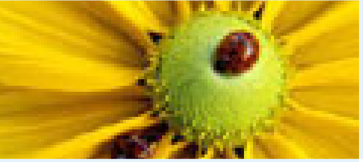
$$V(x) = \alpha\varepsilon \sum_{k=-5}^{5} \delta(x - k\ell), \quad \ell = 20\varepsilon$$

Several Decoherent Thin Barriers

Example: Crystalline Barrier

$$V(x) = \alpha\varepsilon \sum_{k=-5}^{5} \delta(x - k\ell), \quad \ell = 20\varepsilon$$

Coherent Model



Example: Crystalline Barrier

$$V(x) = \alpha\varepsilon \sum_{k=-5}^{5} \delta(x - k\ell), \quad \ell = 20\varepsilon$$

Coherent Model (Averaged Solution)

Conclusion

$O(\varepsilon)$ semiclassical model captures a variety of quantum effects

- partial reflection
- partial transmission
- tunneling
- resonance
- caustics
- internal scattering
- refraction
- diffraction
- time delay
- trapping