A Semiclassical Transport Model for Thin Quantum Barriers

Kyle Novak

3 May 2006

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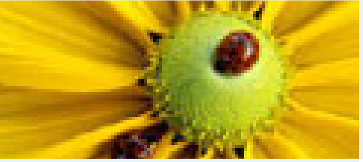
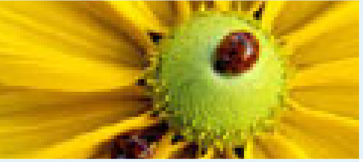


Motivation

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

Plasmas	Nanotechnology
Semiconductors	Quantum dots/films



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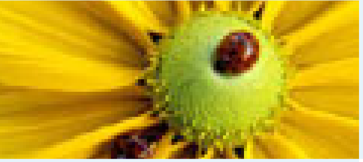

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! Consider a multiscale method for a thin quantum barrier

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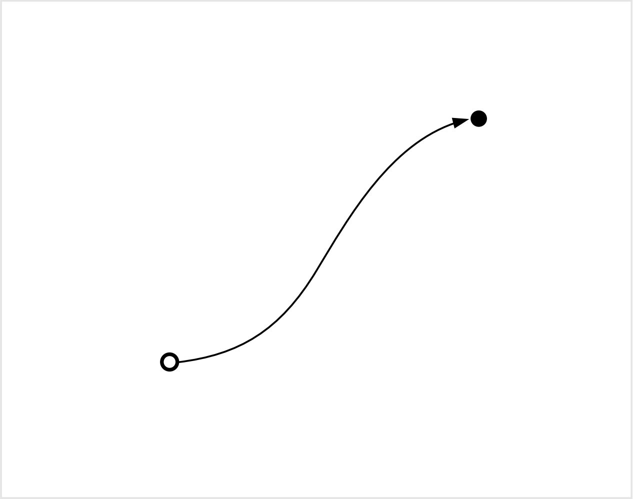
Hamilton's equations

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

Conservation of energy

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



Classical Mechanics

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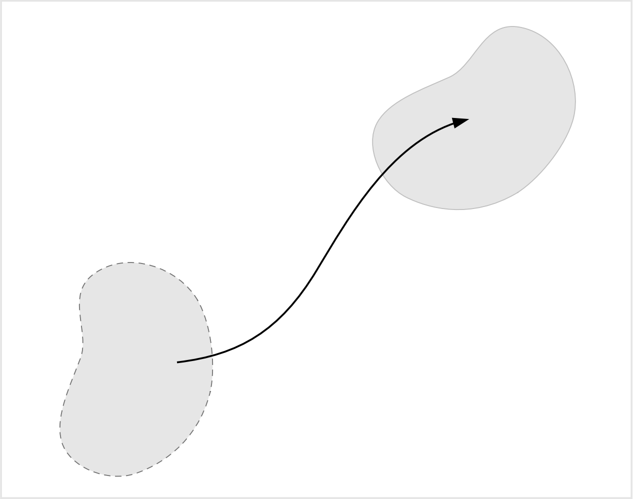
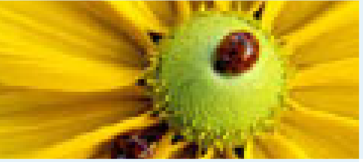
Probability distribution $f(x,p,t)$

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





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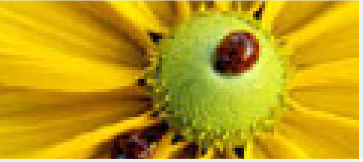

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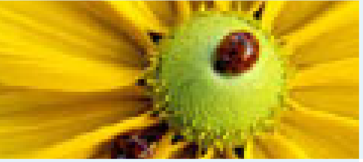
Liouville equation

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



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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

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

Conservation of energy

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

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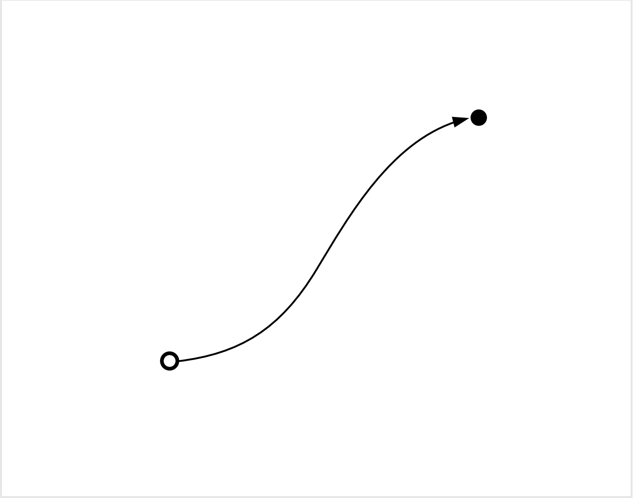
$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi = \Big(-\tfrac{1}{2}\hbar^2\Delta + V(x)\Big)\psi$$



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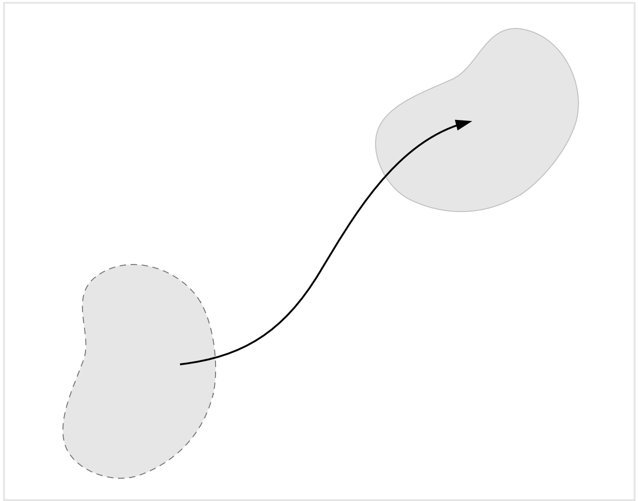
Macroscopic distribution $\tilde{f}(x,p)$



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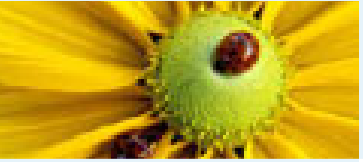
Density matrix

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



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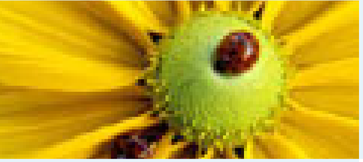
Von Neumann equation

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



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

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

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Characteristic length and time scale:

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

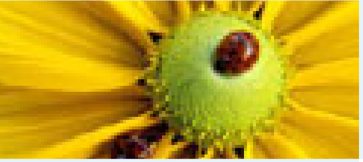
Rescale x, x', and t

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

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



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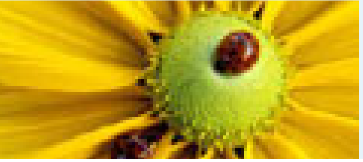
! What's the behavior of physical observables as $\varepsilon \to 0$?



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

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

von Neumann equation

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

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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

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

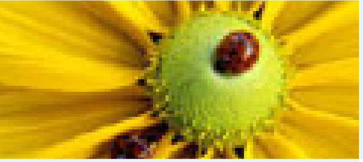
$$\Theta^{\varepsilon} W \longrightarrow \nabla_x V \cdot \nabla_p W \text{ as } \varepsilon \longrightarrow 0$$

Wigner equation ($\varepsilon \longrightarrow 0$)

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

Classical Liouville equation

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



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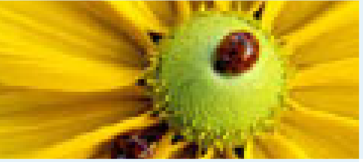
What if $V(x)$ is only *piecewise* continuous (as $\varepsilon \to 0$)?



Semiclassical Model

Approach

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

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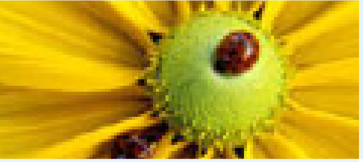
Idea

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.



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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.

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Bicharacteristics

A local bicharacteristic is an integral curve $\varphi(t) = (x(t), p(t))$ to

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

where $H(x,p)$ is differentiable.

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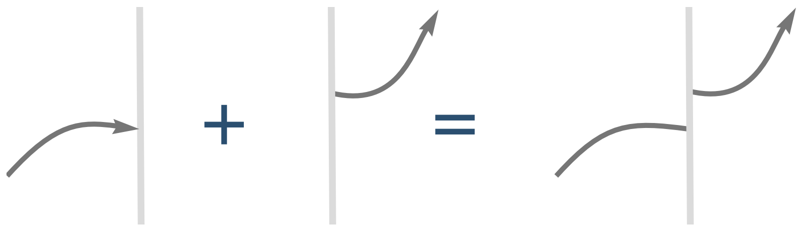
Equivalence class $[\varphi] = \{ \varphi^* \mid H(\varphi^*) = H(\varphi) \}$



Call this a global bicharacteristic.

Interface Condition (One Dimensional)

Push

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

Interface Condition (One Dimensional)

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- Lagrangian

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- Eulerian

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- Lagrangian
- One-to-many function

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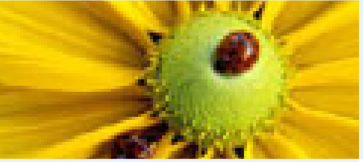
- Eulerian
- Many-to-one function



Entropy

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- Liouville and Schrödinger equations are time reversible
- Semiclassical model is time irreversible and entropy increasing

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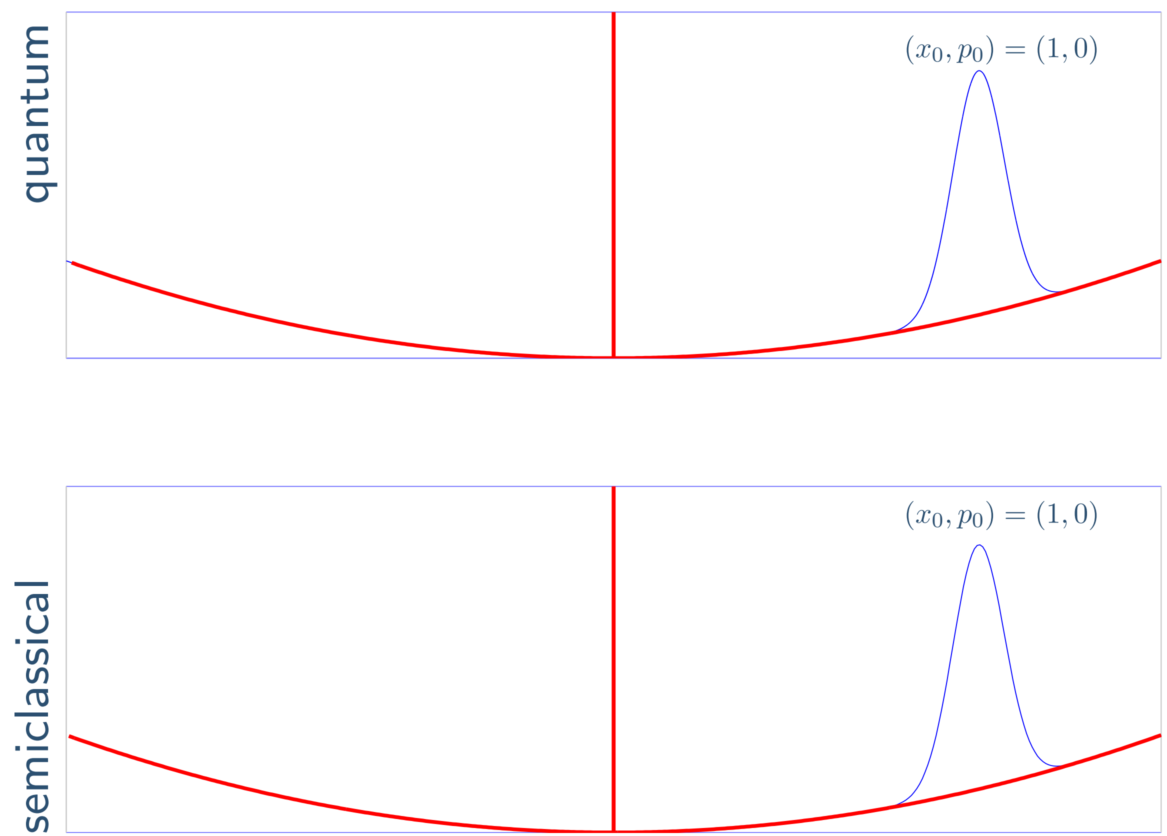
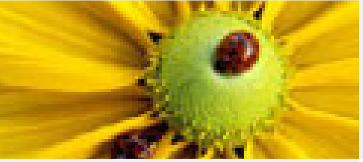
Example: $V(x) = \frac{1}{2}x^2 + \varepsilon\sqrt{3}\delta(x)$





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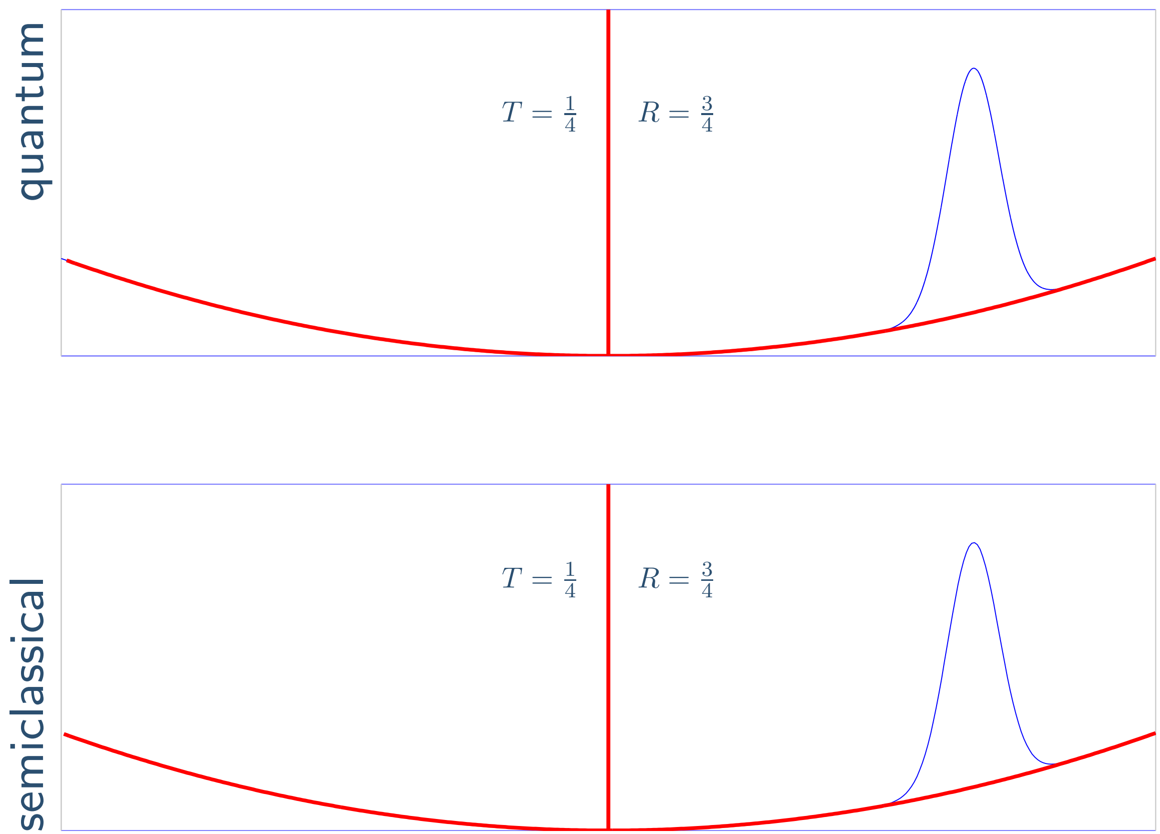

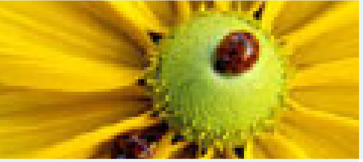

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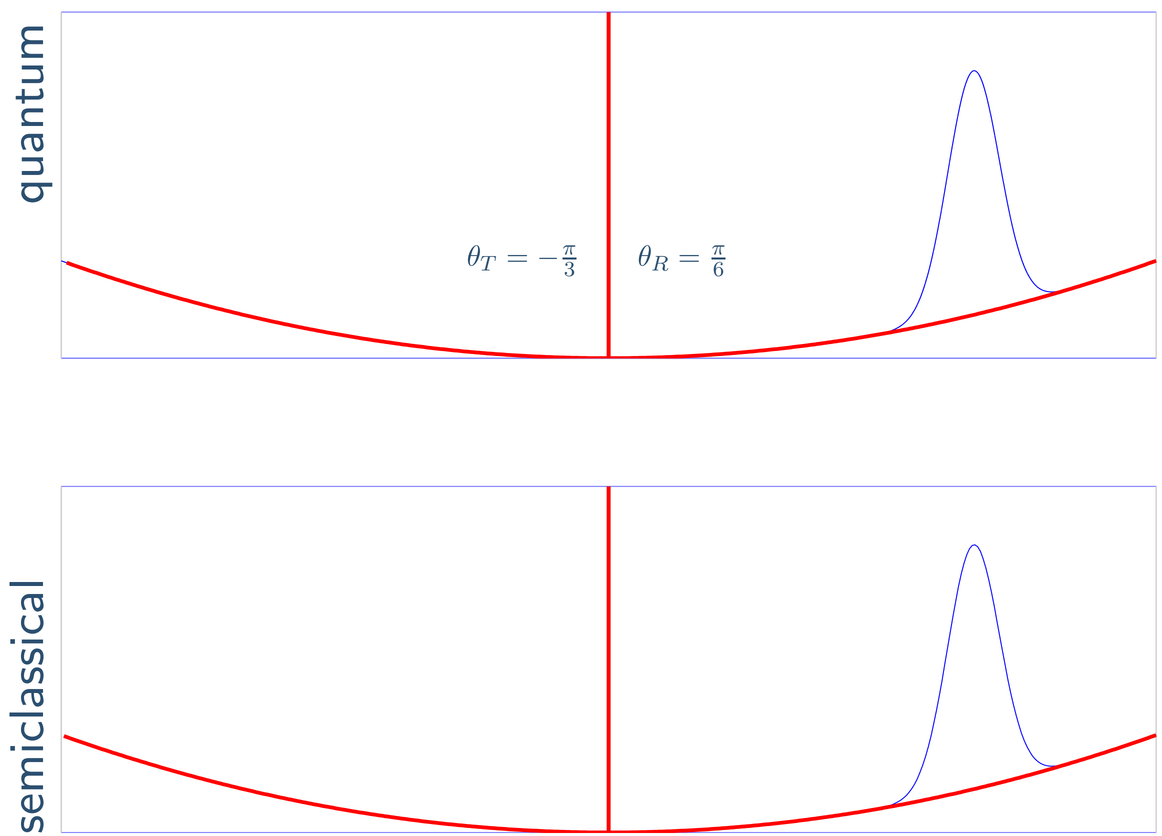
Example: $V(x) = \frac{1}{2}x^2 + \varepsilon\sqrt{3}\delta(x)$



Entropy

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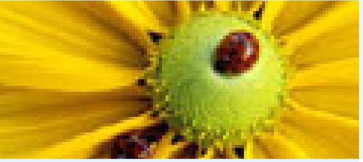
- Liouville and Schrödinger equations are time reversible
- Semiclassical model is time irreversible and entropy increasing

Example: $V(x) = \frac{1}{2}x^2 + \varepsilon\sqrt{3}\delta(x)$

quantum

semiclassical

One Dimension



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Implementation

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Scattering

Liouville Solver

Interface Condition

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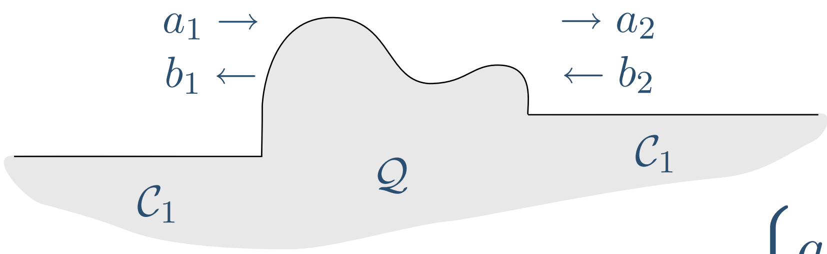
Example 2

Two Dimensions

Future Directions

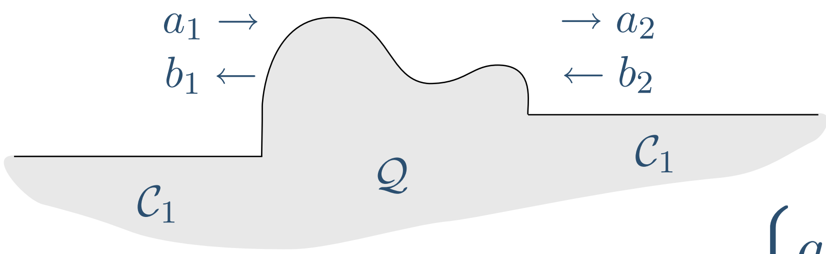
- Initialization
  - Solve time-independent Schrödinger equation for $E = \frac{1}{2}p^2$ (using transfer matrix method)
  - Calculate $T(p)$ and $R(p)$ to get interface condition
- Liouville Solver
  - Use finite volume method globally
  - Incorporate interface condition at quantum barrier

Transfer Matrix



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

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



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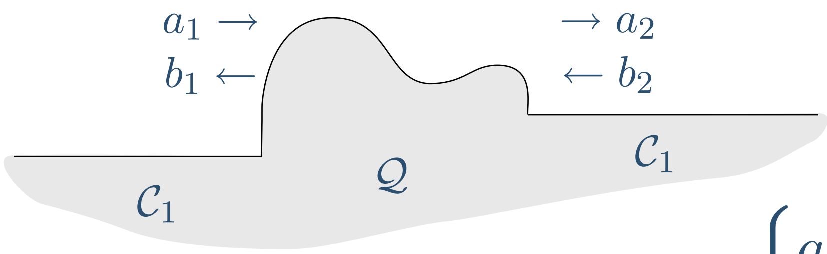
Transfer matrix M

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

Transfer Matrix



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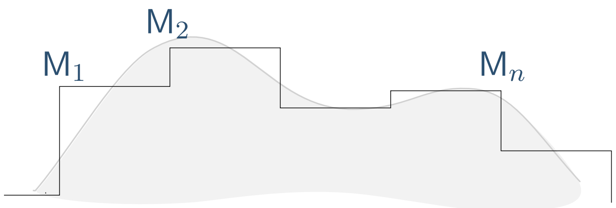
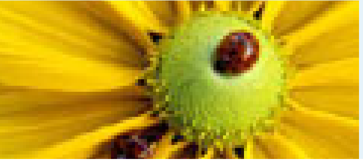
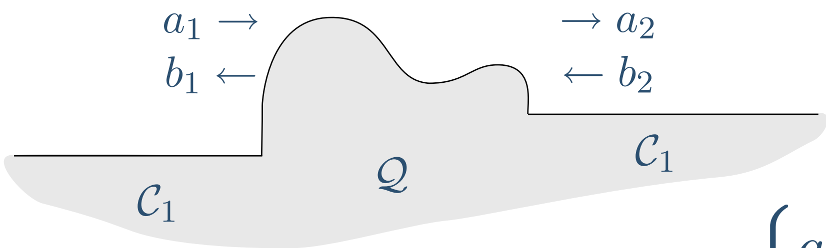


$$\mathsf{M} = \mathsf{M}_n \cdots \mathsf{M}_2 \mathsf{M}_1$$



Transfer Matrix



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

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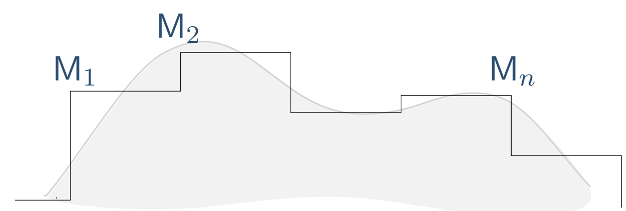

$$\mathsf{M} = \mathsf{M}_n \cdots \mathsf{M}_2 \mathsf{M}_1$$

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 coefficients

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

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

Transmission and reflection coefficients

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

Continuity equation

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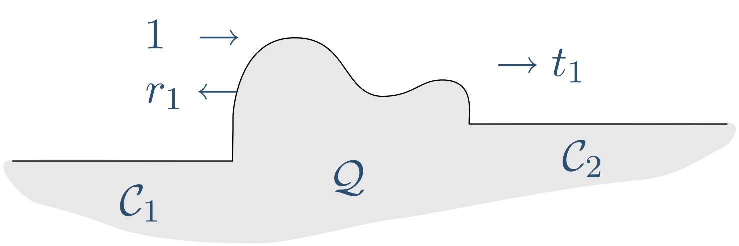
Wave incident from the left ($a_1 = 1$, $b_1 = r_1$, $a_2 = t_1$ and $b_2 = 0$)



Scattering coefficients

Transmission and reflection coefficients

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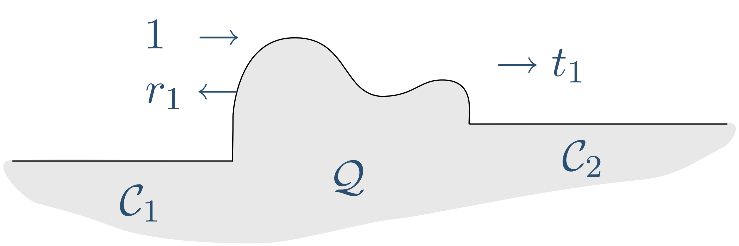


$$J(x) = \begin{cases} \kappa_1 \left(1 - |r_1|^2\right), & x \in \mathcal{C}_1 \\ \kappa_2 \left(|t_2|^2\right), & x \in \mathcal{C}_2 \end{cases}$$

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

Liouville Equation

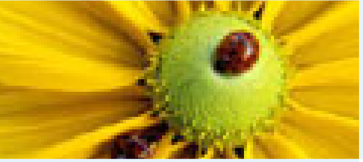
$$\frac{\partial f}{\partial t} = -p\frac{\partial f}{\partial x} + \frac{dV}{dx}\frac{\partial f}{\partial x}$$

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

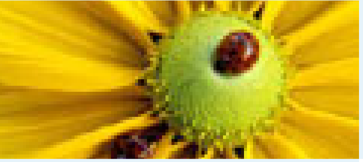
The discrete operators $\partial_x f_{ij}$, $\partial_p f_{ij}$ and $\partial_x V_i$ are

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

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

Pull interface condition

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

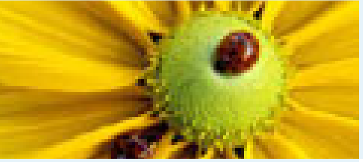
$$f^{-}_{Z+1/2,j} = R(q_j) f^{-}_{Z+1/2,-j} + T(q_j) f(x^{+}_{Z+1/2}, q_j) \qquad \text{for } j < 0$$

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

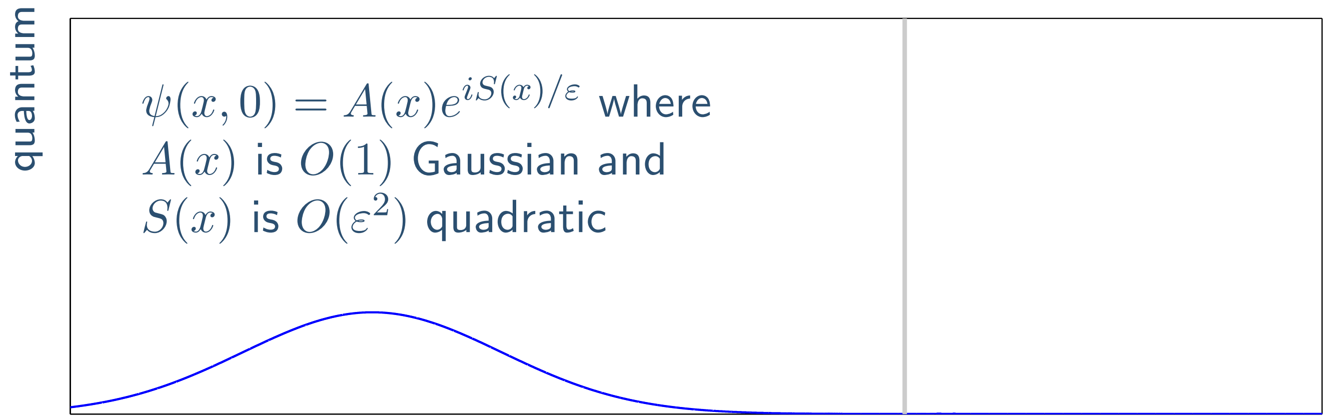
$$f(x^{-}_{Z+1/2}, q_j) = \frac{1}{p_j \Delta p} \int_{q_{j-1/2}}^{q_{j+1/2}} p f(x^{-}_{Z+1/2}, p)\, dp$$

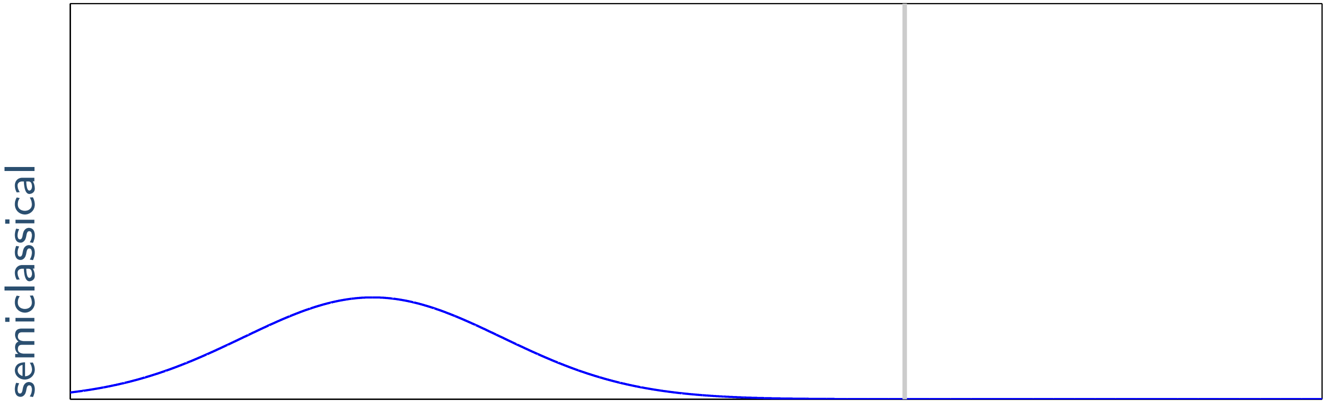
where $q_{j\pm1/2} = \sqrt{p^2_{j\pm1/2} + 2(V^{+}_{Z+1/2} - V^{-}_{Z+1/2})}$. The integral is approximated by a composite mid-point rule.



Example: Schrödinger solution for step potential

$\psi(x,0) = A(x)e^{iS(x)/\varepsilon}$ where
$A(x)$ is $O(1)$ Gaussian and
$S(x)$ is $O(\varepsilon^2)$ quadratic





Example: Schrödinger solution for step potential

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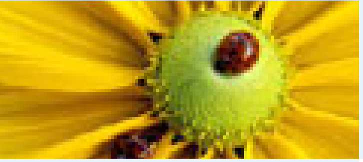
semiclassical



Example: Schrödinger solution for step potential

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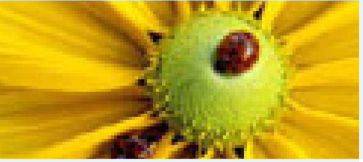
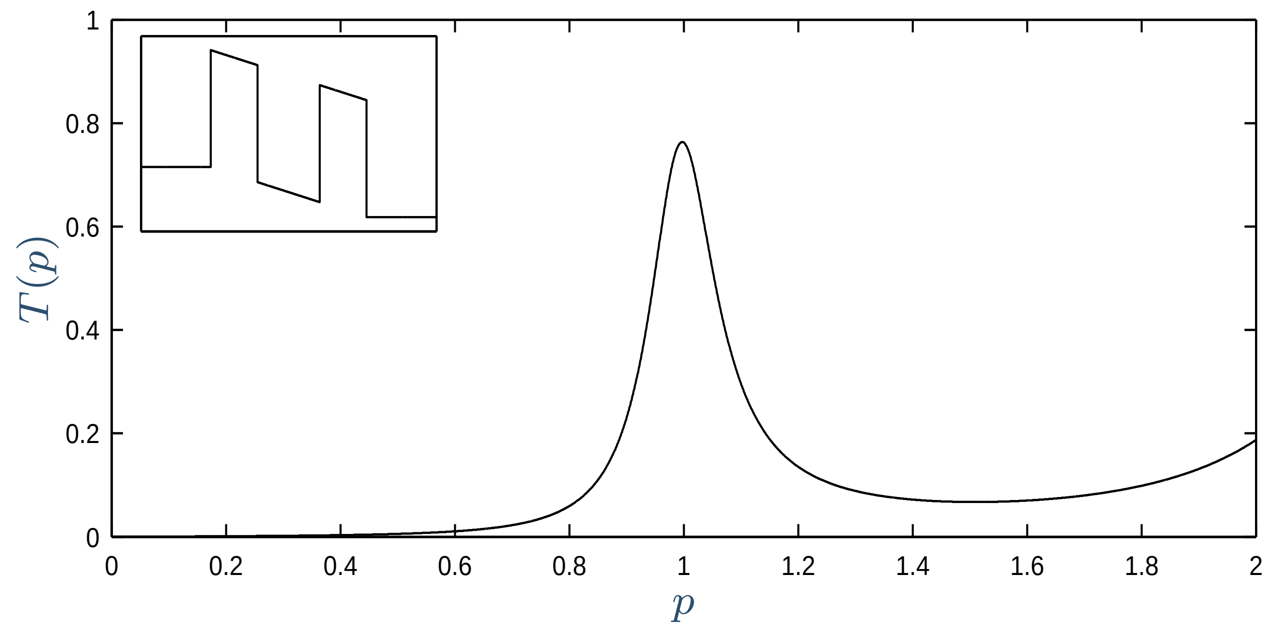
$O(\varepsilon)$ convergence of Schrödinger solution



Example: Resonant tunneling von Neumann solution

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



- Convergence of von Neumann solution
- Convergence of numerical semiclassical solution

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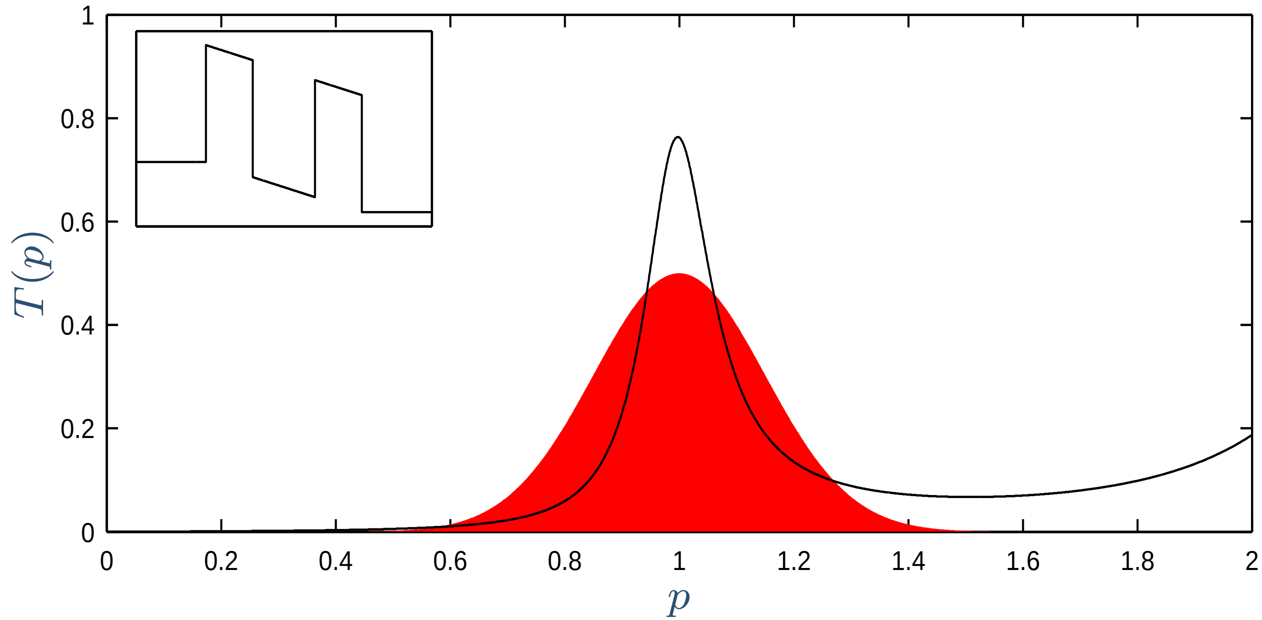
Resonant Tunneling Diode (RTD): Double-barrier quantum well



- Convergence of von Neumann solution
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Example: Resonant tunneling von Neumann solution

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$O(\varepsilon)$ convergence of von Neumann solution

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$O(\Delta x)$ convergence of numerical solution

Two Dimensions

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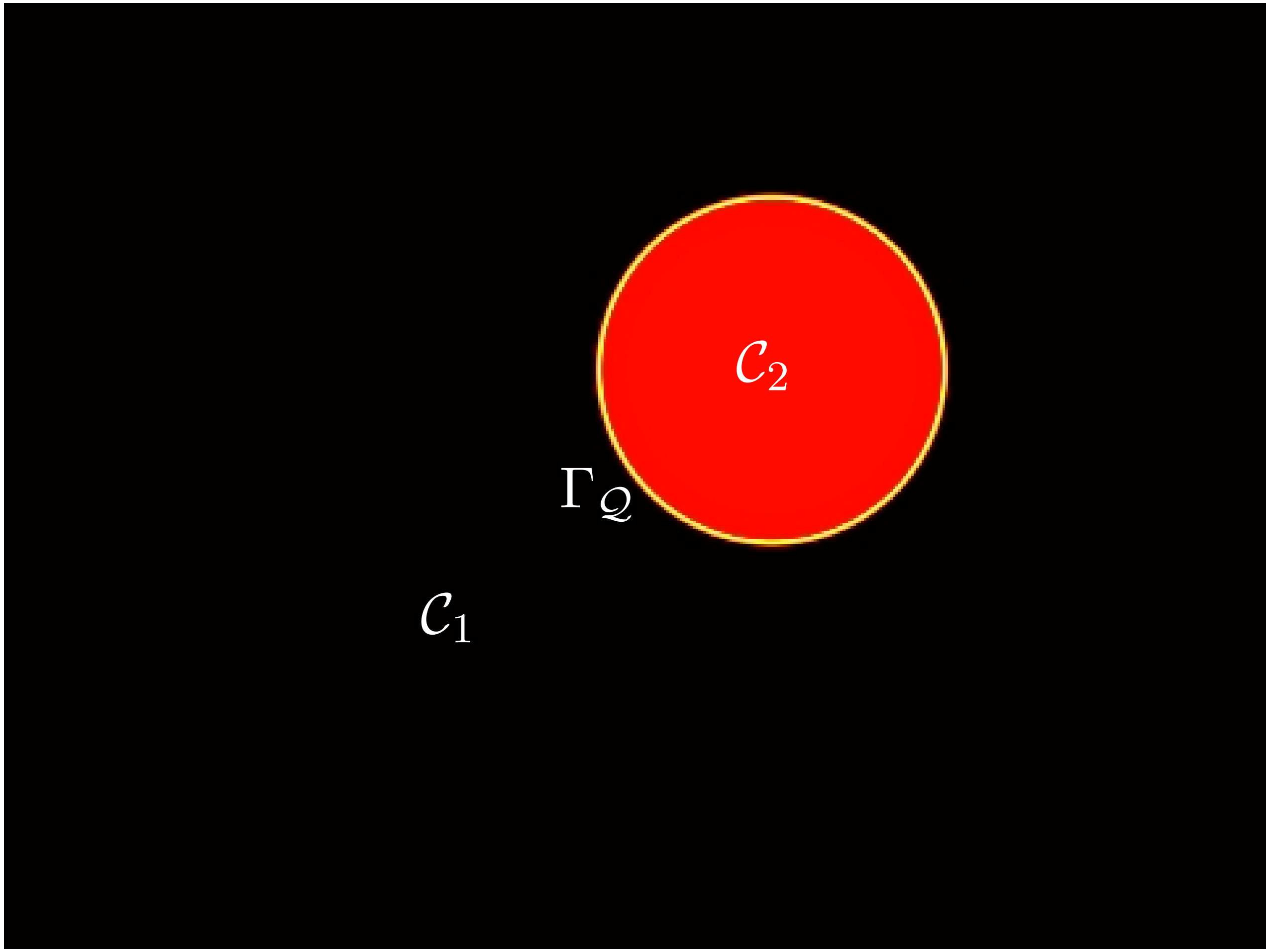

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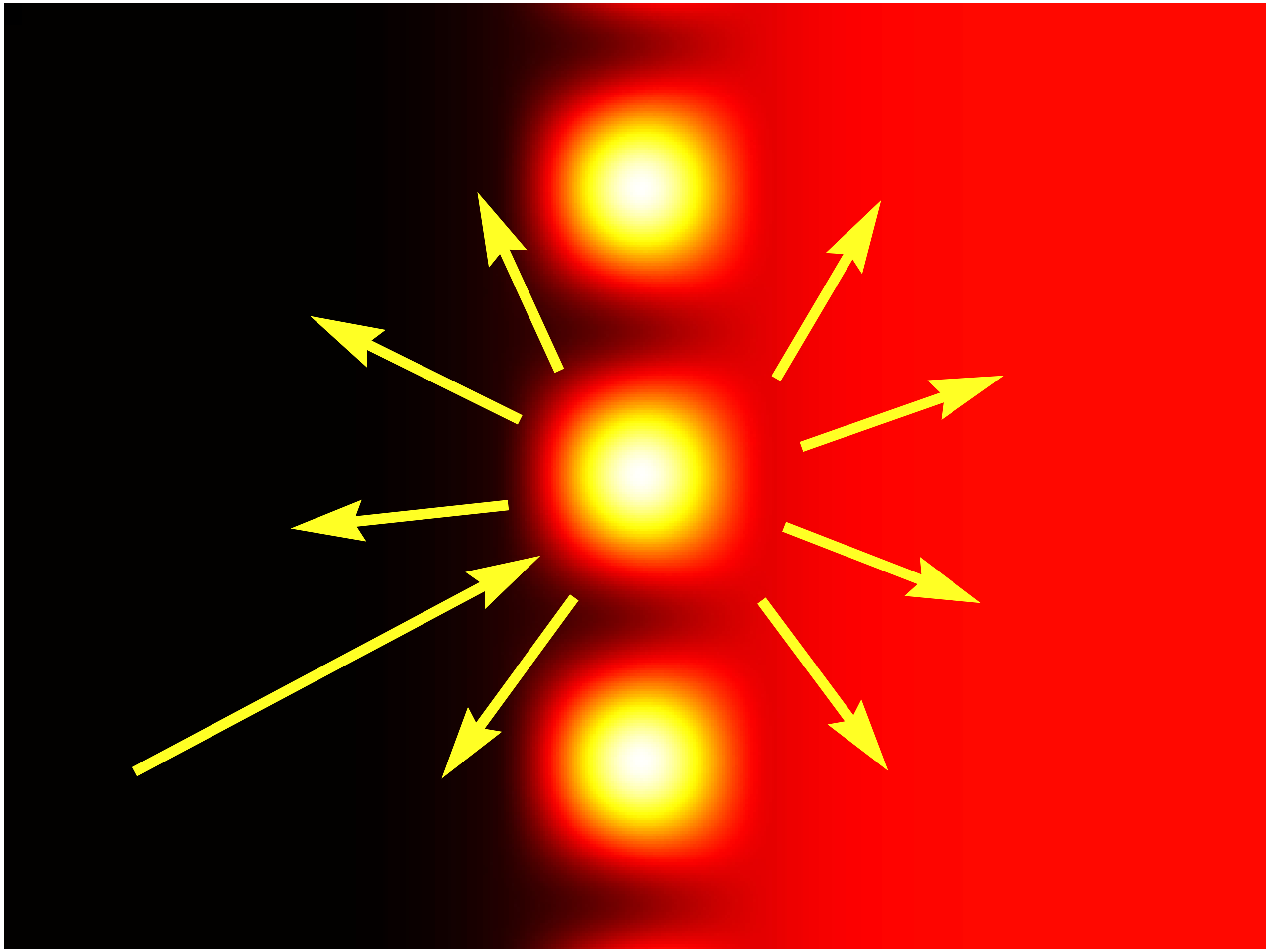


2D interface condition

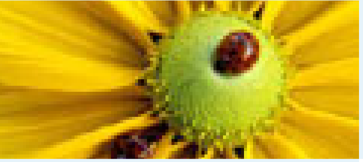
Pull interface condition

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

Push interface condition

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

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



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! Computer memory: We need at least 100 mesh points to resolve each direction. 100^4 floating-point numbers $=$ 380MB with an equal amount for a "swap" array

- 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

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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

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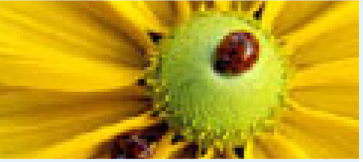
For particle incident from left at angle θ_{in}:

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

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

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

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



Quantum Transmitting Boundary Method

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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

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

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

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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

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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

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

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

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- Difficult to solve. Iterative solver:

$$Au^{(n+1)} = Bu^{(n)}$$

where u_{ij} discretization of $\hat{\psi}_{\mathcal{Q}}(x_i, \xi_j)$

$$A = -\tfrac{1}{2\Delta x^2}\delta_{i+1,j} + \left(\tfrac{1}{\Delta x^2} + \eta_1^2(\xi_j)\right)\delta_{ij} - \tfrac{1}{2\Delta x^2}\delta_{i-1,j}$$
$$B = -2\mathcal{F}V_{\mathcal{Q}}\mathcal{F}^{-1}$$

- If $V_{\mathcal{Q}}(x, y)$ is independent in y, Schrödinger equation is separable and problem reduces to one-dimensional case.
- Otherwise, exploit geometry of the barrier.

Particle Method

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

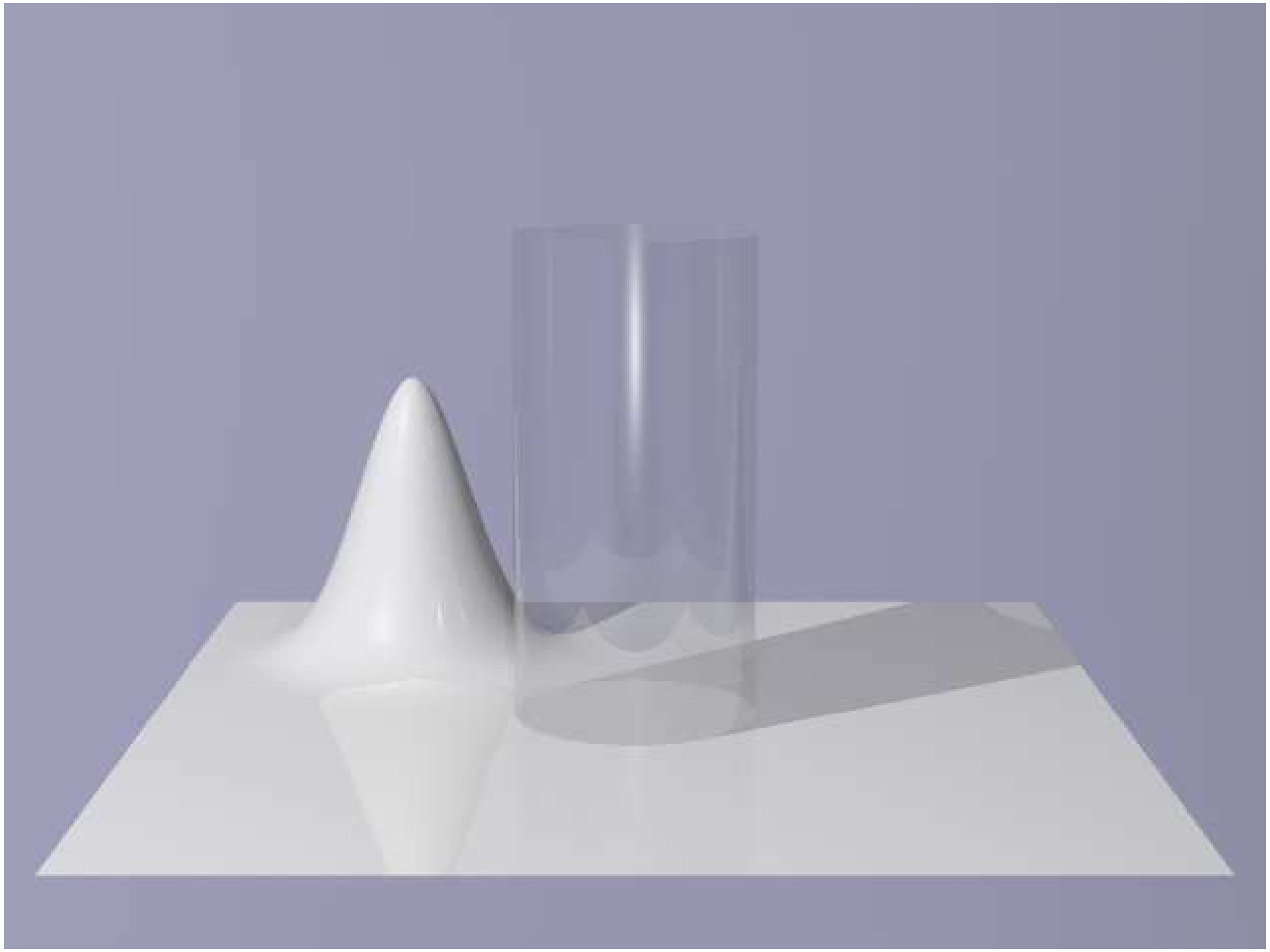
  Monte Carlo take a path randomly from $S(\theta_{\text{out}}; p, \theta_{\text{in}})$

  Deterministic take all paths (binary tree)

- Reconstruct density distribution with bicubic cutoff function

Example: Circular Barrier

$\varepsilon = 50^{-1}, 100^{-1}, 200^{-1}$ and 400^{-1}



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Schrödinger with $\varepsilon = 50^{-1}$

Example: Circular Barrier

Schrödinger with $\varepsilon = 100^{-1}$

Example: Circular Barrier

Schrödinger with $\varepsilon = 200^{-1}$

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Schrödinger with $\varepsilon = 400^{-1}$

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Semiclassical Liouville

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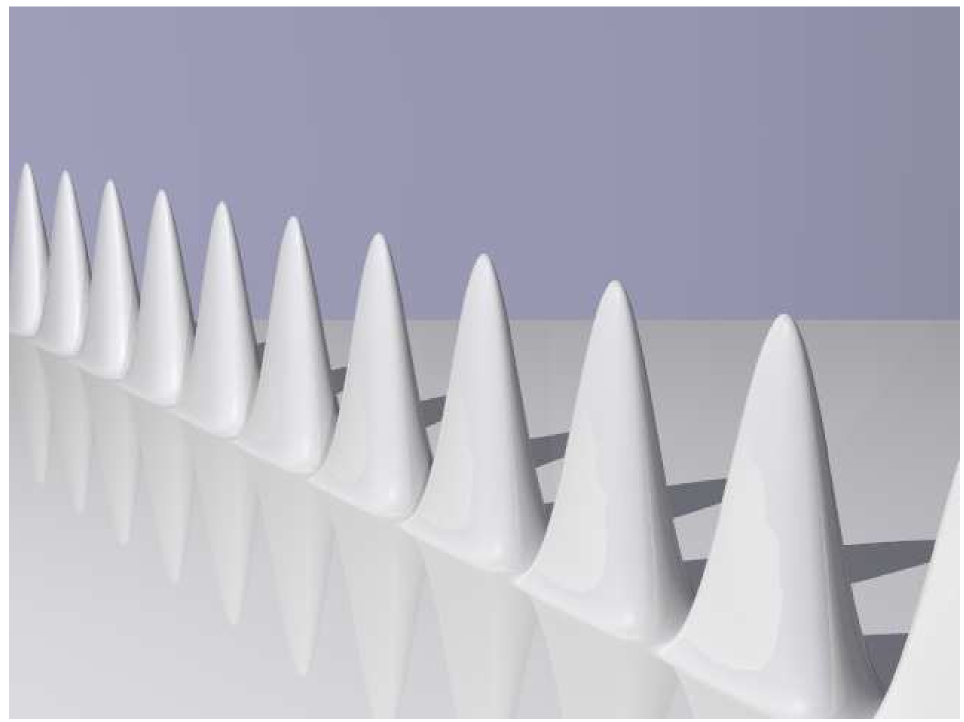
Classical

Example 2: 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 2: Diffraction Grating

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

with boundary conditions

$$\begin{aligned} i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} &= 2i\eta(\xi)\delta(\xi - \xi_{\text{in}}) && x = -1 \\ i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} &= 0 && x = +1 \end{aligned}$$

Example 2: Diffraction Grating

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

with boundary conditions

$$i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 2i\eta(\xi)\delta(\xi - \xi_{\mathsf{in}}) \qquad x = -1$$

$$i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 0 \qquad x = +1$$

$$\frac{\partial^2}{\partial x^2}\hat{\psi}_{\mathcal{Q}}(x,\xi) + \eta^2(\xi)\hat{\psi}_{\mathcal{Q}}(x,\xi) - \underbrace{2\int_{-\infty}^{\infty} \overbrace{V_{\mathcal{Q}}(x,y)}^{f(x)\cos^2(\alpha y/2)} \psi(x,y) e^{-i\xi y}\, dy}_{f(x)\left(\hat{\psi}_{\mathcal{Q}}(x,\xi+\alpha) + 2\hat{\psi}_{\mathcal{Q}}(x,\xi) + \hat{\psi}_{\mathcal{Q}}(x,\xi-\alpha)\right)} = 0$$

with boundary conditions

$$i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 2i\eta(\xi)\delta(\xi - \xi_{\text{in}}) \qquad x = -1$$

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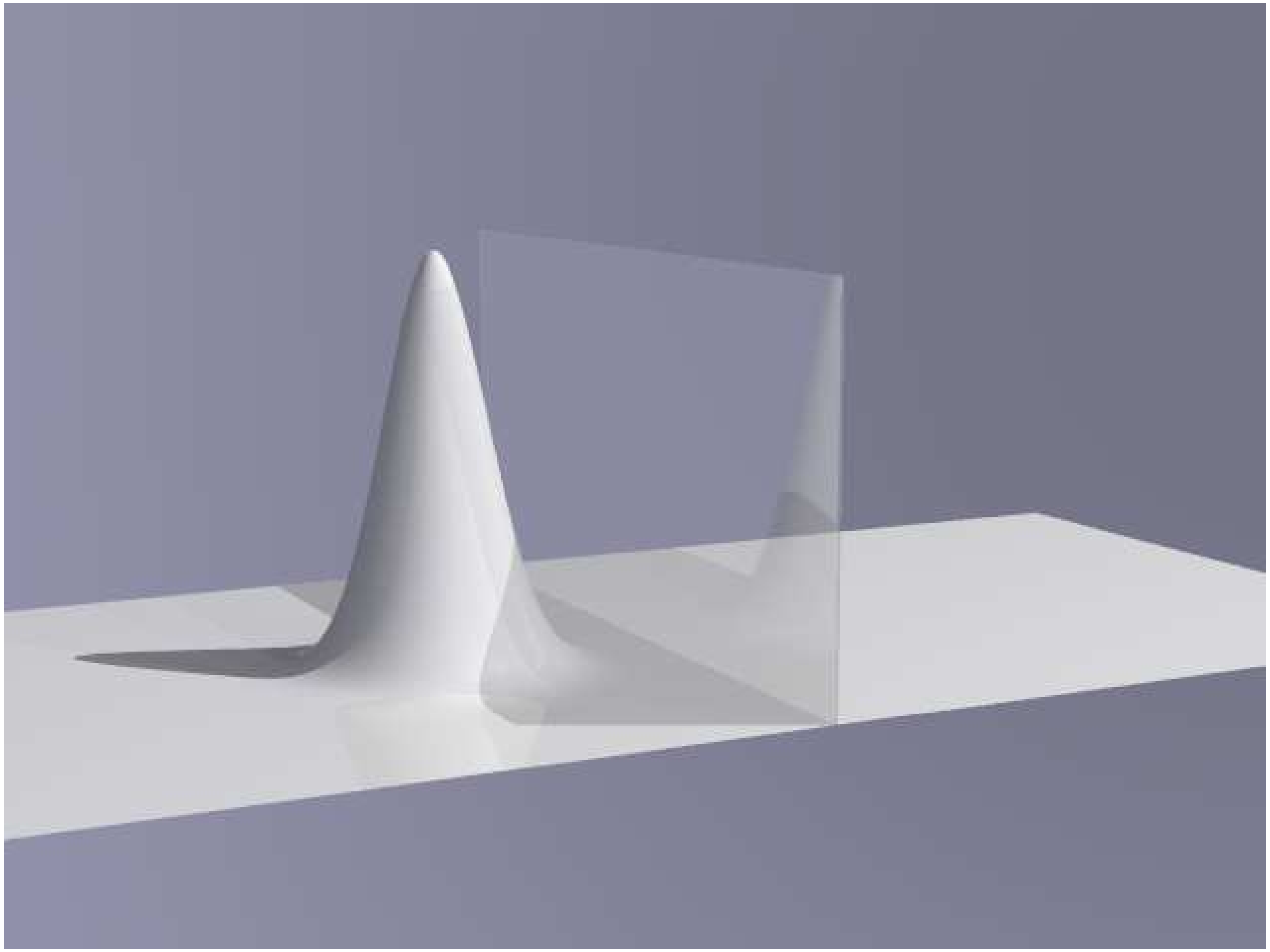
$$i\eta(\xi)\hat{\psi}_{\mathcal{Q}} + \frac{\partial}{\partial x}\hat{\psi}_{\mathcal{Q}} = 0 \qquad x = +1$$

- Linear system. Block tridiagonal matrix.
- Discrete scattering angles correspond to the Fraunhofer diffraction grating $m\lambda = (\sin\theta_{\text{in}} + \sin\theta_m)$

Example 2: Diffraction Grating

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



Example 2: Diffraction Grating

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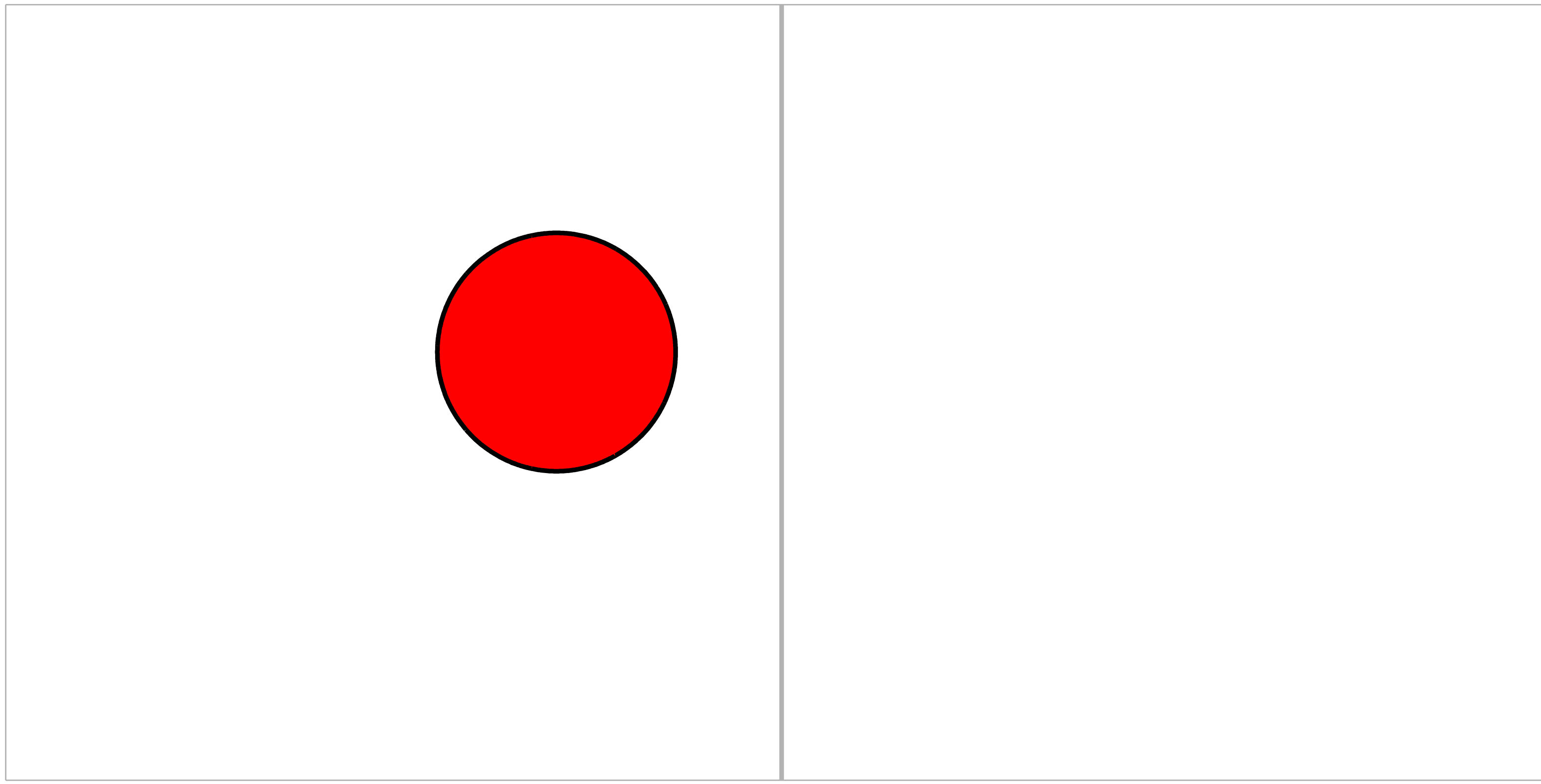
Semiclassical ($p = 1$ and $\theta_{\text{in}} = 10°$)

Example 2: Diffraction Grating

$\varepsilon = 100^{-1}, 200^{-1}, 400^{-1}$ and 800^{-1}



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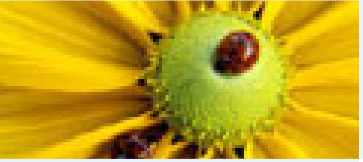
$$\varepsilon = 100^{-1}$$



Example 2: Diffraction Grating

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$$\varepsilon = 200^{-1}$$

Example 2: Diffraction Grating

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$$\varepsilon = 400^{-1}$$

Example 2: Diffraction Grating

$$\varepsilon = 800^{-1}$$

Future Directions

Coherent Semiclassical Model

Where do we go from here?

- Mesoscopic barriers
- Periodic crystalline structures

Coherent Semiclassical Model

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Assumptions require that each barrier be independent.
We need to construct a coherent semiclassical model.

Coherent Semiclassical Model

Where do we go from here?

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Assumptions require that each barrier be independent.
We need to construct a coherent semiclassical model.

Naive approach

$$\Phi(x,p,t) = \sqrt{f(x,p,t)}e^{i\theta(p)} \qquad (f = |\Phi|^2)$$

$$\frac{\partial \Phi}{\partial t} + p\frac{\partial \Phi}{\partial x} - V(x)\frac{\partial \Phi}{\partial p} = 0$$

with the interface condition $\Phi^+ = r\Phi_1^- + t\Phi_2^-$

Example (Revisited)

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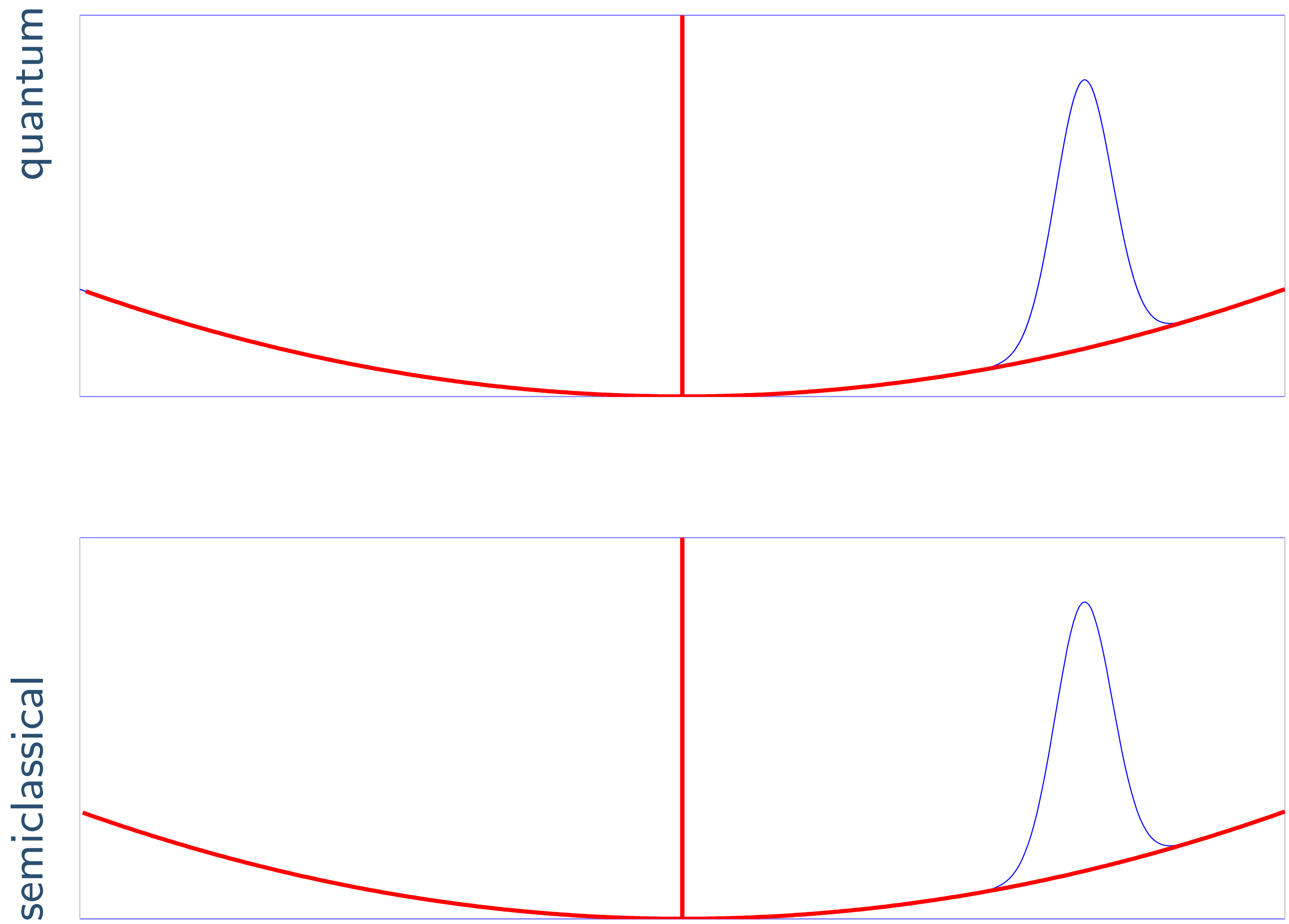

Example (Revisited)

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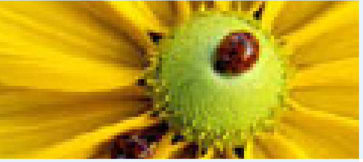
quantum

semiclassical

Conclusion

- $O(\varepsilon)$ semiclassical model captures a variety of quantum effects in both one dimension and two dimensions
  - partial reflection
  - partial transmission
  - tunneling
  - resonance
  - caustics
  - internal scattering
  - refraction
  - diffraction
  - time delay
- Open problem: extend the model to wider class of barriers



Conclusion

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Questions?