A Mixed Classical/Quantum Transport Model

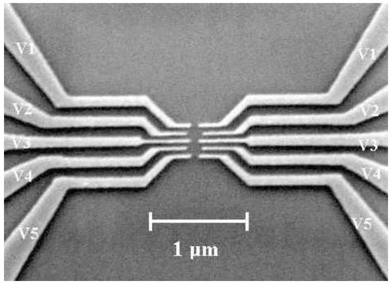
Kyle Novak

28 Sept 2005

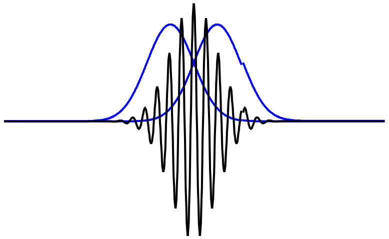
Overview

Motivation

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



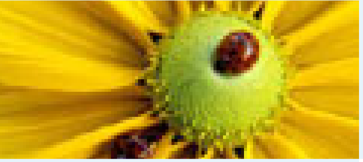
- Multi-scale problems
- High frequency limit, geometric optics, fluids
- Numerical PDEs

Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\Delta\Psi(x,t) + V(x)\Psi(x,t)$$

Physical interpretation

- $|\Psi|^2$: Position probability density $\rho(x,t)$
- $|\widehat{\Psi}|^2$: Momentum probability density
- Wavepacket $=$ particle



Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\Delta\Psi(x,t) + V(x)\Psi(x,t)$$

Physical interpretation

- $|\Psi|^2$: Position probability density $\rho(x,t)$
- $|\widehat{\Psi}|^2$: Momentum probability density
- Wavepacket = particle

Wave packet solution

$$\Psi(x,t;p_0) = \int_{-\infty}^{\infty} \phi(p-p_0)\psi_E(x,t)e^{iEt/\hbar}\,dp$$

where ψ_E solves $-\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi = E\psi$ with Hamiltonian $E = p^2/2m - V(x)$ along particle trajectory

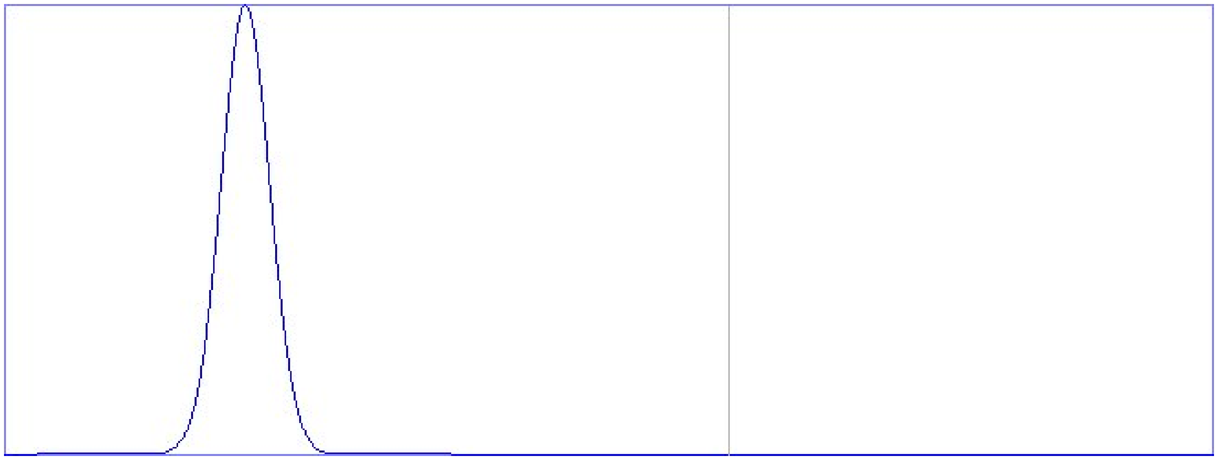
Gaussian Wave Packet

For symmetry in position and momentum ($\sigma_x \sim \sigma_p = \sqrt{eps/2}$), we take

$$\phi(p - p_0) = \exp(-(p - p_0)^2/2\varepsilon)/(\pi\varepsilon)^{1/4}$$

Simplified behavior of wave packet

- Away from quantum region acts like a particle
- Near a quantum region acts like a wave



Scale

Consider characteristic length and time:

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

Rescale x and t:

$$i\varepsilon \frac{\partial}{\partial t}\Psi_t = (-\frac{\varepsilon^2}{2m}\Delta + V(x))\Psi \quad \text{where} \quad \varepsilon = \hbar/L$$

What happens when $L \rightarrow \infty$ and $\varepsilon \rightarrow 0$?

Scale

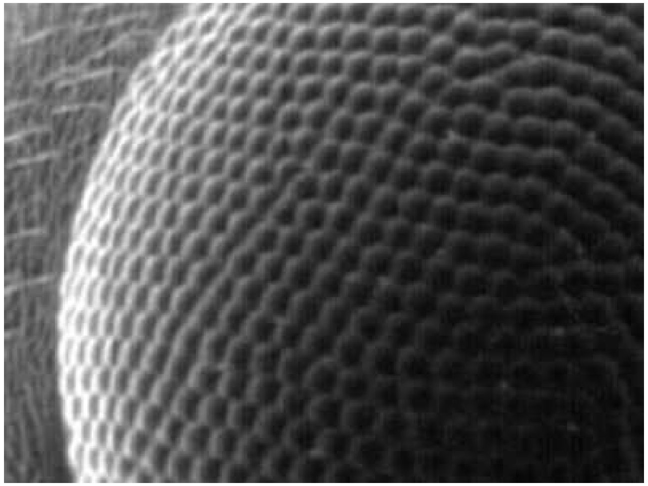
Consider characteristic length and time:

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

Rescale x and t:

$$i\varepsilon \frac{\partial}{\partial t}\Psi_t = (-\frac{\varepsilon^2}{2m}\Delta + V(x))\Psi \quad \text{where} \quad \varepsilon = \hbar/L$$

What happens when $L \to \infty$ and $\varepsilon \to 0$?



Scale

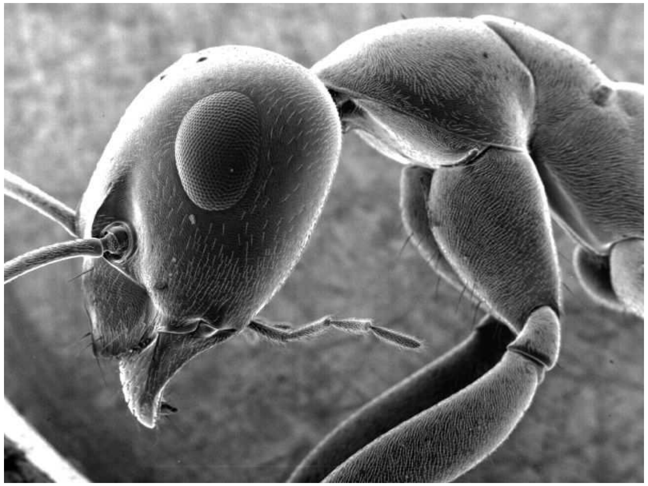
Consider characteristic length and time:

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

Rescale x and t:

$$i\varepsilon\frac{\partial}{\partial t}\Psi_t = \left(-\frac{\varepsilon^2}{2m}\Delta + V(x)\right)\Psi \quad \text{where} \quad \varepsilon = \hbar/L$$

What happens when $L \to \infty$ and $\varepsilon \to 0$?



Scale

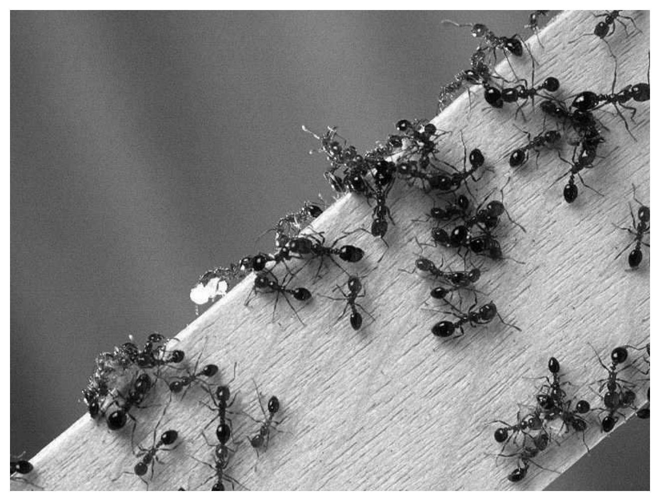
Consider characteristic length and time:

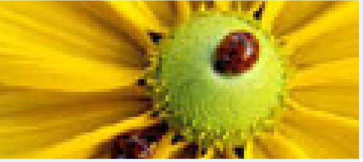
$$L\delta x \text{ and } L\delta t \text{ (where } \delta x = \lambda = \hbar/p)$$

Rescale x and t:

$$i\varepsilon \frac{\partial}{\partial t}\Psi_t = (-\frac{\varepsilon^2}{2m}\Delta + V(x))\Psi \quad \text{where} \quad \varepsilon = \hbar/L$$

What happens when $L \to \infty$ and $\varepsilon \to 0$?





Wigner Equation

Schrödinger equation

$$\mathcal{S}\Psi(x,t) = \frac{\partial}{\partial t}\Psi(x,t) + \frac{\varepsilon}{2i}\Delta\Psi(x,t) - \frac{1}{\varepsilon i}V(x)\Psi(x,t) = 0$$

Wigner distribution function

$$f(x,p,t) = \mathcal{W}[\Psi,\Psi] = \int_{-\infty}^{\infty} \overline{\Psi}(x - \tfrac{1}{2}\varepsilon y, t)\Psi(x + \tfrac{1}{2}\varepsilon y, t)e^{ipy}\, dy$$

Wigner equation: $\mathcal{W}[\mathcal{S}\Psi,\Psi] + \mathcal{W}[\Psi,\mathcal{S}\Psi] = 0$

Wigner Equation

Schrödinger equation

$$\mathcal{S}\Psi(x,t) = \frac{\partial}{\partial t}\Psi(x,t) + \frac{\varepsilon}{2i}\Delta\Psi(x,t) - \frac{1}{\varepsilon i}V(x)\Psi(x,t) = 0$$

Wigner distribution function

$$f(x,p,t) = \mathcal{W}[\Psi,\Psi] = \int_{-\infty}^{\infty} \overline{\Psi}(x - \tfrac{1}{2}\varepsilon y, t)\Psi(x + \tfrac{1}{2}\varepsilon y, t)e^{ipy}\,dy$$

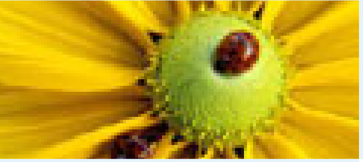
Wigner equation: $\mathcal{W}[\mathcal{S}\Psi,\Psi] + \mathcal{W}[\Psi,\mathcal{S}\Psi] = 0$

$$\frac{\partial}{\partial t}f + p\nabla f + \Theta = 0 \quad \text{where}$$

$$\Theta = -\frac{1}{\varepsilon i}\int \left[V(x + \tfrac{1}{2}\varepsilon y) - V(x - \tfrac{1}{2}\varepsilon y)\right]\hat{f}(x,y,t)e^{-ipy}\,dy$$

Semiclassical limit

$$\Theta = \nabla_x V \cdot \nabla_p f - \frac{1}{\varepsilon i} \sum_{n=1}^{\infty} \frac{(-1)^n \left(\frac{\varepsilon}{2}\right)^{2n}}{(2n+1)!} \nabla_x^{2n+1} V \nabla_p^{2n+1} f$$



Semiclassical limit

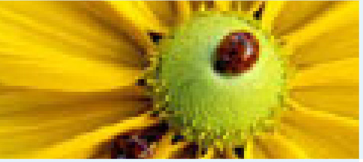
$$\Theta = \nabla_x V \cdot \nabla_p f - \frac{1}{\varepsilon i} \sum_{n=1}^{\infty} \frac{(-1)^n \left(\frac{\varepsilon}{2}\right)^{2n}}{(2n+1)!} \nabla_x^{2n+1} V \nabla_p^{2n+1} f$$

For $V(x)$ smooth, when $\varepsilon \to 0$

$$\Theta \to \nabla_x V \cdot \nabla_p f(x, p, t)$$

Liouville equation:

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



Semiclassical limit

$$\Theta = \nabla_x V \cdot \nabla_p f - \frac{1}{\varepsilon i} \sum_{n=1}^{\infty} \frac{(-1)^n \left(\frac{\varepsilon}{2}\right)^{2n}}{(2n+1)!} \nabla_x^{2n+1} V \nabla_p^{2n+1} f$$

For $V(x)$ smooth, when $\varepsilon \to 0$

$$\Theta \to \nabla_x V \cdot \nabla_p f(x,p,t)$$

Liouville equation:

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

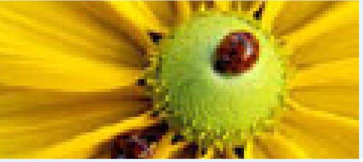
Characteristics $\equiv$ Hamiltonian system:

$$\dot{\mathbf{x}} = \frac{\mathbf{p}}{m}$$
$$\dot{\mathbf{p}} = -\nabla_x V(x) = \mathbf{F}$$

Why not use the Schrödinger Equation?

Liouville equation

- Arbitrary particle distribution, *but*
- No wave phenomena: tunneling, resonance, partial transmission/reflection, interference



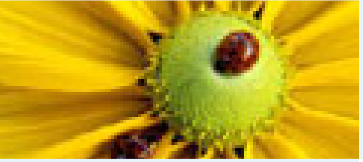
Why not use the Schrödinger Equation?

Liouville equation

- Arbitrary particle distribution, *but*
- No wave phenomena: tunneling, resonance, partial transmission/reflection, interference

Schrödinger equation

- Accurately models particle at any scale, *but*
- Single particle (x and p distribution are not independent)
- Numerically, we must resolve the de Broglie wavelength. Typically, $\Delta x = O(\varepsilon/p)$ or $\Delta x = o(\varepsilon/p)$
- Numerically, difficult to implement boundary conditions



Why not use the Schrödinger Equation?

Liouville equation

- Arbitrary particle distribution, *but*
- No wave phenomena: tunneling, resonance, partial transmission/reflection, interference

Schrödinger equation

- Accurately models particle at any scale, *but*
- Single particle (x and p distribution are not independent)
- Numerically, we must resolve the de Broglie wavelength. Typically, $\Delta x = O(\varepsilon/p)$ or $\Delta x = o(\varepsilon/p)$
- Numerically, difficult to implement boundary conditions

Idea!	Use Liouville equation globally. Use Schrödinger equation locally.

How do we do it?

Coupling a quantum barrier with a Liouville

- Solve the time-independent Schrödinger equation for the a local barrier/well
- Use the solution to determine scattering information
- Solve the Liouville equation everywhere else
- Use scattering information to connect across the barrier

Previous research

- N. Ben Abdallah, P. Degond and I.M. Gamba (2002)
- S. Jin and X. Wen (2005)

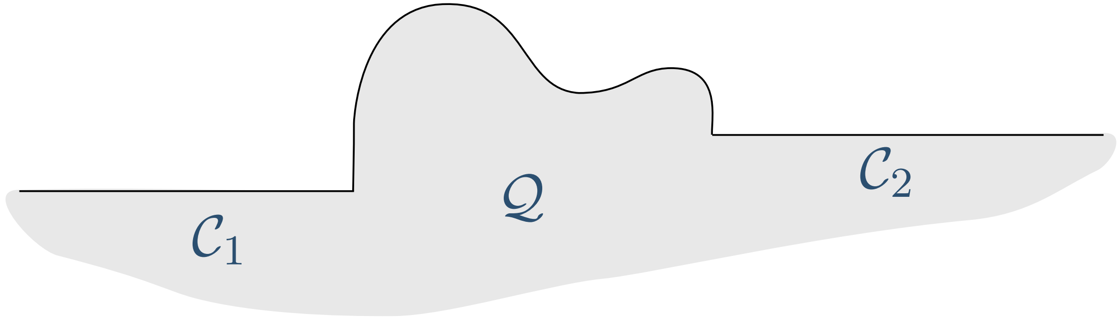
Simplifying assumptions

- We work in 1-d
- Particle moves instantaneously across the barrier
- Barrier is sufficiently local
- Particle has no phase information (no long range interaction)

Transfer Matrix

Solve $\frac{\varepsilon^2}{2m}\Delta\Psi - V(x)\Psi = E\Psi$ where

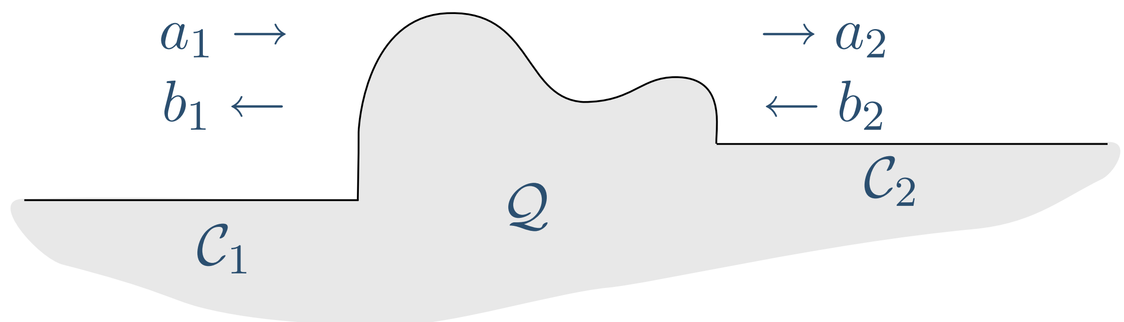
$$V(x) = \begin{cases} V_1, & x \in \mathcal{C}_1 \\ V_{\mathcal{Q}}(x), & x \in \mathcal{Q} \\ V_2, & x \in \mathcal{C}_2 \end{cases}$$



Transfer Matrix

$$\text{In } \mathcal{C} : \Psi(x) = \begin{cases} a_1 e^{i\kappa_1 x} + b_1 e^{-i\kappa_1 x}, & x \in \mathcal{C}_1 \\ b_2 e^{i\kappa_2 x} + b_2 e^{-i\kappa_2 x}, & x \in \mathcal{C}_2 \end{cases}$$

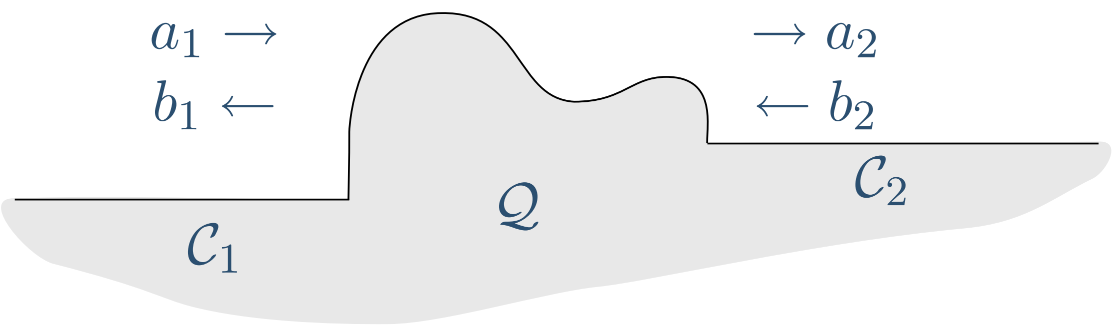
where $\kappa_j = \sqrt{p^2 - 2mV_j}/\varepsilon$



Transfer Matrix

In $\mathcal{C}$: $\Psi(x) = \begin{cases} a_1 e^{i\kappa_1 x} + b_1 e^{-i\kappa_1 x}, & x \in \mathcal{C}_1 \\ b_2 e^{i\kappa_2 x} + b_2 e^{-i\kappa_2 x}, & x \in \mathcal{C}_2 \end{cases}$

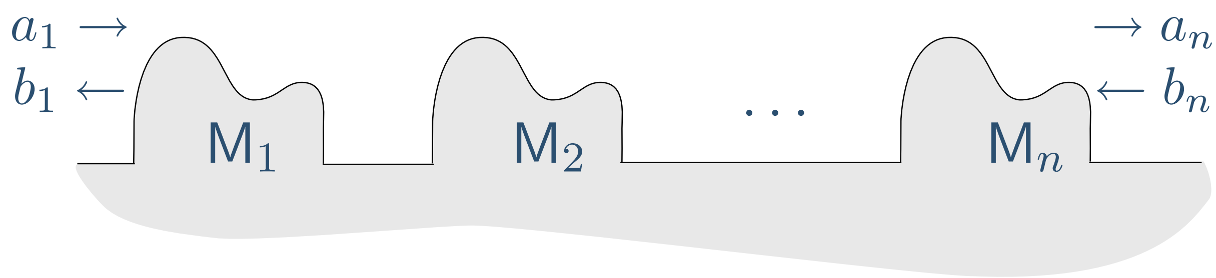
where $\kappa_j = \sqrt{p^2 - 2mV_j}/\varepsilon$



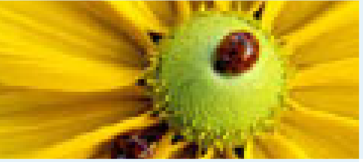
In $\mathcal{Q}$: linear, 2nd-order BVP, so $\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \mathsf{M} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$

Transfer Matrix

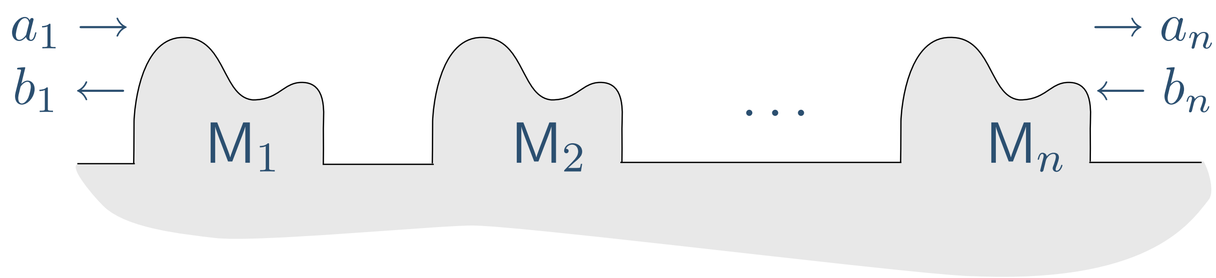
Multiple barriers



$$\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \underbrace{\mathsf{M}_{\mathsf{n}} \mathsf{M}_{n-1} \cdots \mathsf{M}_1}_{\mathsf{M}} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$$



Multiple barriers

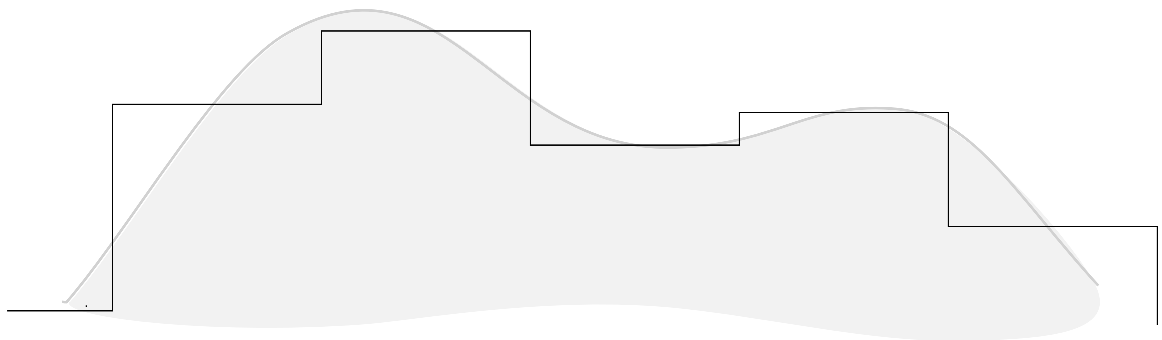


$$\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \underbrace{\mathsf{M}_\mathsf{n}\mathsf{M}_{n-1}\cdots\mathsf{M}_1}_{\mathsf{M}} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$$

Two simple barriers

- Step (D)
- Translation (P)

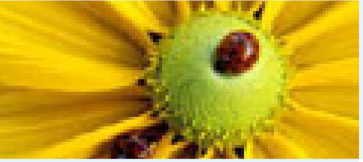
Arbitrary barrier



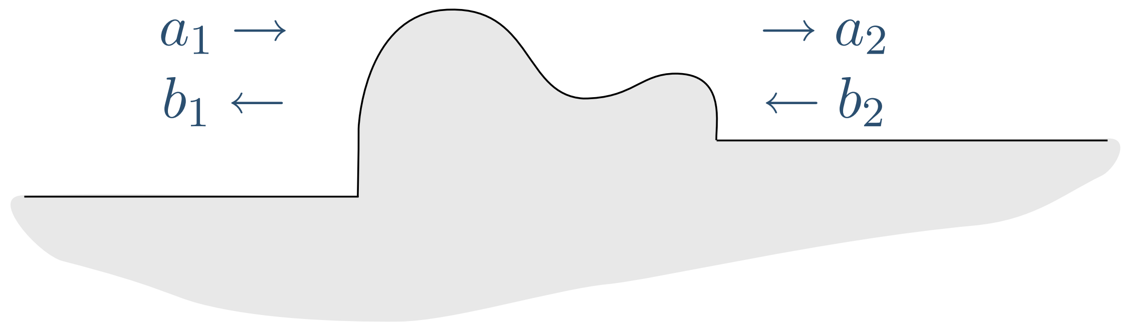
$$\mathsf{M}_j = \mathsf{P}_{j+1}^{1/2}\mathsf{D}_j\mathsf{P}_j^{1/2}$$

$$\mathsf{D}_j = \frac{1}{2}\begin{pmatrix} 1+\kappa_{j-1}/\kappa_j & 1-\kappa_{j-1}/\kappa_j \\ 1-\kappa_{j-1}/\kappa_j & 1+\kappa_{j-1}/\kappa_j \end{pmatrix}$$

$$\mathsf{P}_j = \begin{pmatrix} \exp(i\Delta x\kappa_j) & 0 \\ 0 & \exp(-i\Delta x\kappa_j) \end{pmatrix}$$



Scattering Matrix



Transfer matrix

$$\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \mathsf{M} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$$

Scattering matrix

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = \mathsf{S} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix}$$

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

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

Current Density

Schrödinger equation

$$\mathcal{S}\Psi(x,t) = \frac{\partial}{\partial t}\Psi(x,t) + \frac{\varepsilon}{2i}\varepsilon\Delta\Psi(x,t) - \frac{1}{\varepsilon i}V(x)\Psi(x,t) = 0$$

Consider:

$$2\mathrm{Re}\left[\overline{\Psi}\mathcal{S}\Psi\right] = \overline{\Psi}\mathcal{S}\Psi + \Psi\overline{\mathcal{S}\Psi} = 0$$

Current Density

Schrödinger equation

$$\mathcal{S}\Psi(x,t) = \frac{\partial}{\partial t}\Psi(x,t) + \frac{\varepsilon}{2i}\varepsilon\Delta\Psi(x,t) - \frac{1}{\varepsilon i}V(x)\Psi(x,t) = 0$$

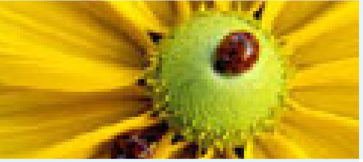
Consider:

$$2\text{Re}\left[\overline{\Psi}\mathcal{S}\Psi\right] = \overline{\Psi}\mathcal{S}\Psi + \Psi\overline{\mathcal{S}\Psi} = 0$$

Continuity equation

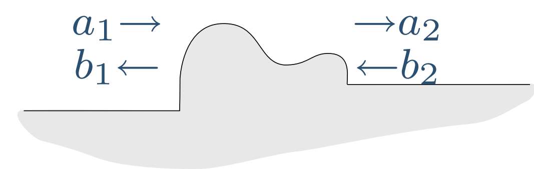
$$\frac{\partial}{\partial t}\rho(x,t) + \nabla\cdot J = 0$$

where probability current density $J = \varepsilon \text{Im}\left[\overline{\Psi}\nabla\Psi\right]$



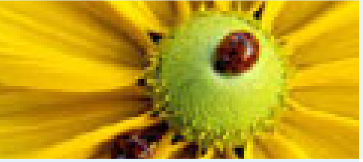
Scattering Coefficients

$$\Psi = \begin{cases} a_1 e^{i\kappa_1 x} + b_1 e^{-i\kappa_1 x}, & x \in \mathcal{C}_1 \\ a_2 e^{i\kappa_2 x} + b_2 e^{-i\kappa_2 x}, & x \in \mathcal{C}_1 \end{cases}$$



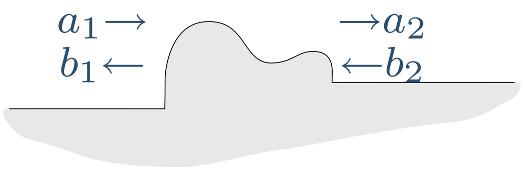
So,

$$J(x) = \varepsilon \mathsf{Im}\left[\overline{\Psi} \nabla \Psi\right] = \begin{cases} \kappa_1(|a_1|^2 - |b_1|^2), & x \in \mathcal{C}_1 \\ \kappa_2(|a_2|^2 - |b_2|^2), & x \in \mathcal{C}_2 \end{cases}$$



Scattering Coefficients

$$\Psi = \begin{cases} a_1 e^{i\kappa_1 x} + b_1 e^{-i\kappa_1 x}, & x \in \mathcal{C}_1 \\ a_2 e^{i\kappa_2 x} + b_2 e^{-i\kappa_2 x}, & x \in \mathcal{C}_1 \end{cases}$$



So,

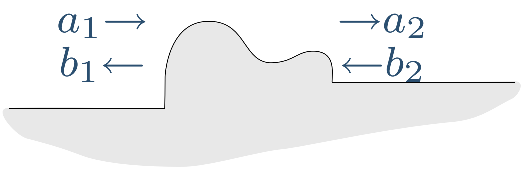
$$J(x) = \varepsilon \mathrm{Im}\,[\overline{\Psi} \nabla \Psi] = \begin{cases} \kappa_1(|a_1|^2 - |b_1|^2), & x \in \mathcal{C}_1 \\ \kappa_2(|a_2|^2 - |b_2|^2), & x \in \mathcal{C}_2 \end{cases}$$

Particle incident from left: $b_2 = 0$ then $a_2 = t_1 a_1$ and $b_1 = r_1 a_1$

$$J(x) = \begin{cases} \kappa_1 |a_1|^2 (1 - |r_1|^2), x \in \mathcal{C}_1 \\ \kappa_2 |a_2|^2 |t_1|^2, x \in \mathcal{C}_2 \end{cases}$$

Scattering Coefficients

$$\Psi = \begin{cases} a_1 e^{i\kappa_1 x} + b_1 e^{-i\kappa_1 x}, & x \in \mathcal{C}_1 \\ a_2 e^{i\kappa_2 x} + b_2 e^{-i\kappa_2 x}, & x \in \mathcal{C}_1 \end{cases}$$



So,

$$J(x) = \varepsilon \mathrm{Im}\left[\overline{\Psi}\nabla\Psi\right] = \begin{cases} \kappa_1(|a_1|^2 - |b_1|^2), & x \in \mathcal{C}_1 \\ \kappa_2(|a_2|^2 - |b_2|^2), & x \in \mathcal{C}_2 \end{cases}$$

Particle incident from left: $b_2 = 0$ then $a_2 = t_1 a_1$ and $b_1 = r_1 a_1$

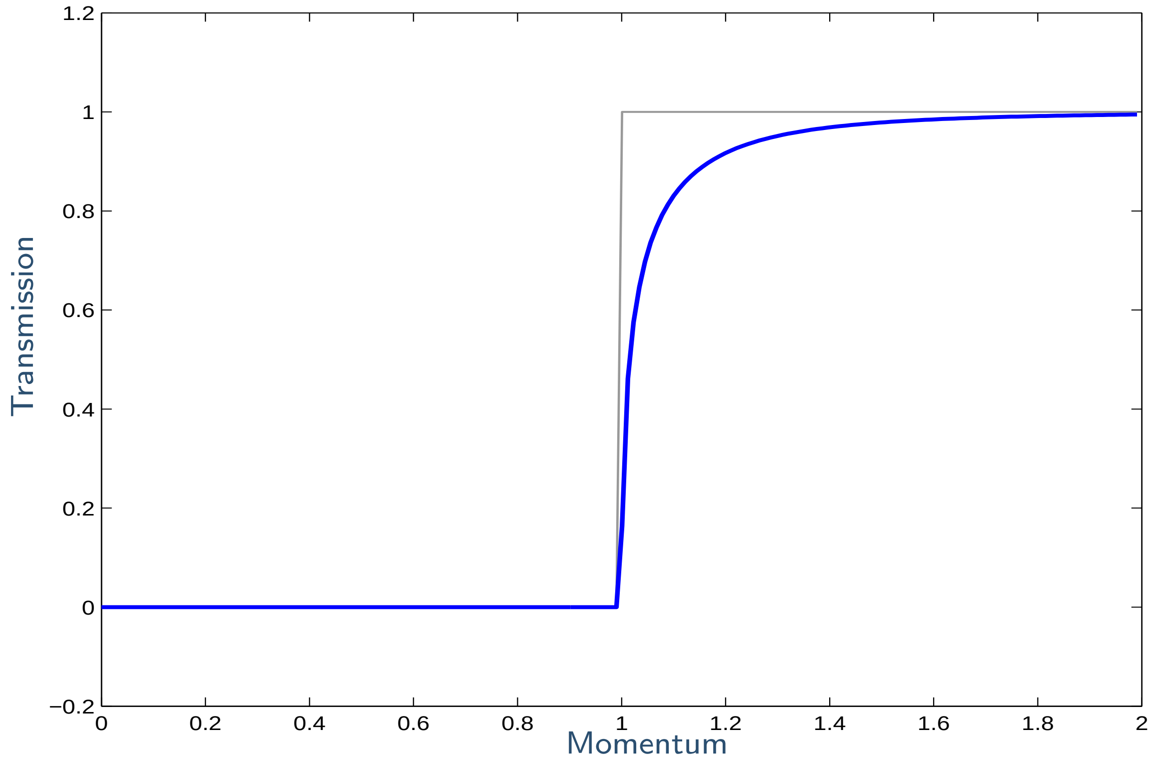
$$J(x) = \begin{cases} \kappa_1 |a_1|^2 (1 - |r_1|^2), x \in \mathcal{C}_1 \\ \kappa_2 |a_2|^2 |t_1|^2, x \in \mathcal{C}_2 \end{cases}$$

Reflection probability $R_1 = |r_1|^2$
Transmission probability $T_1 = (\kappa_2/\kappa_1)|t_1|^2$

Resonance and Tunneling

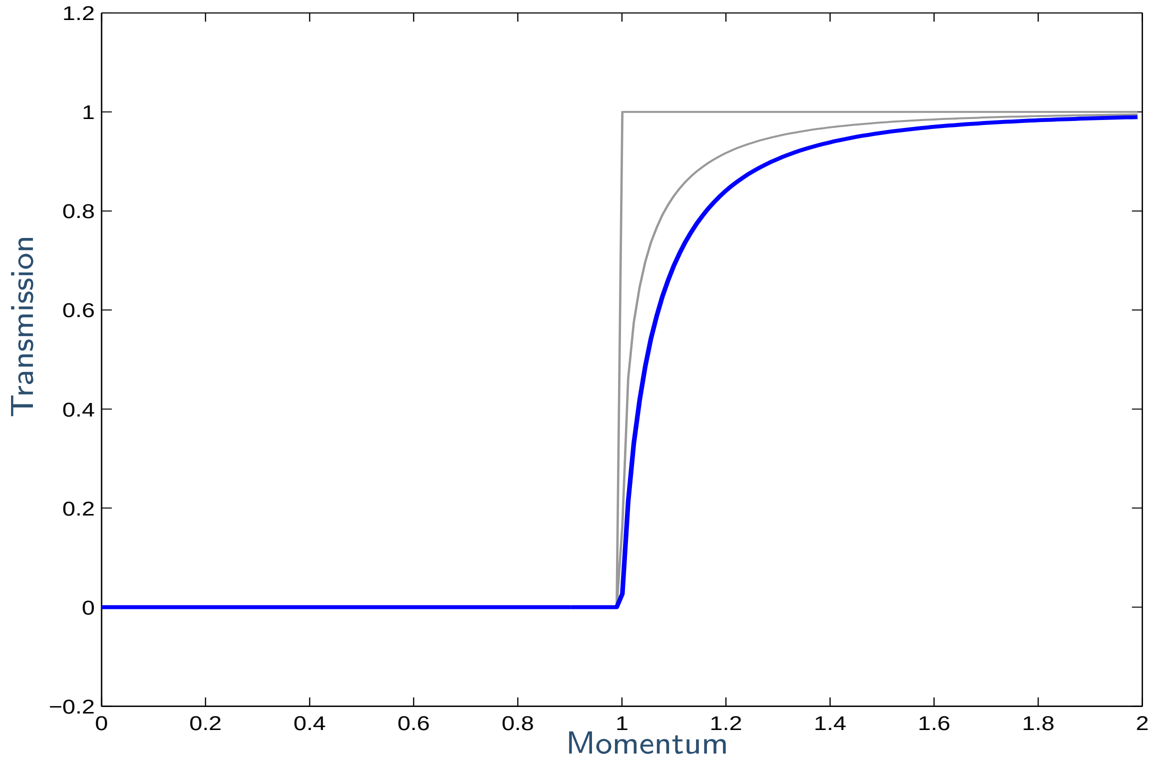
Rectangular potential with height $= 1/2$ and width 2ε

Step up



Rectangular potential with height $= 1/2$ and width 2ε

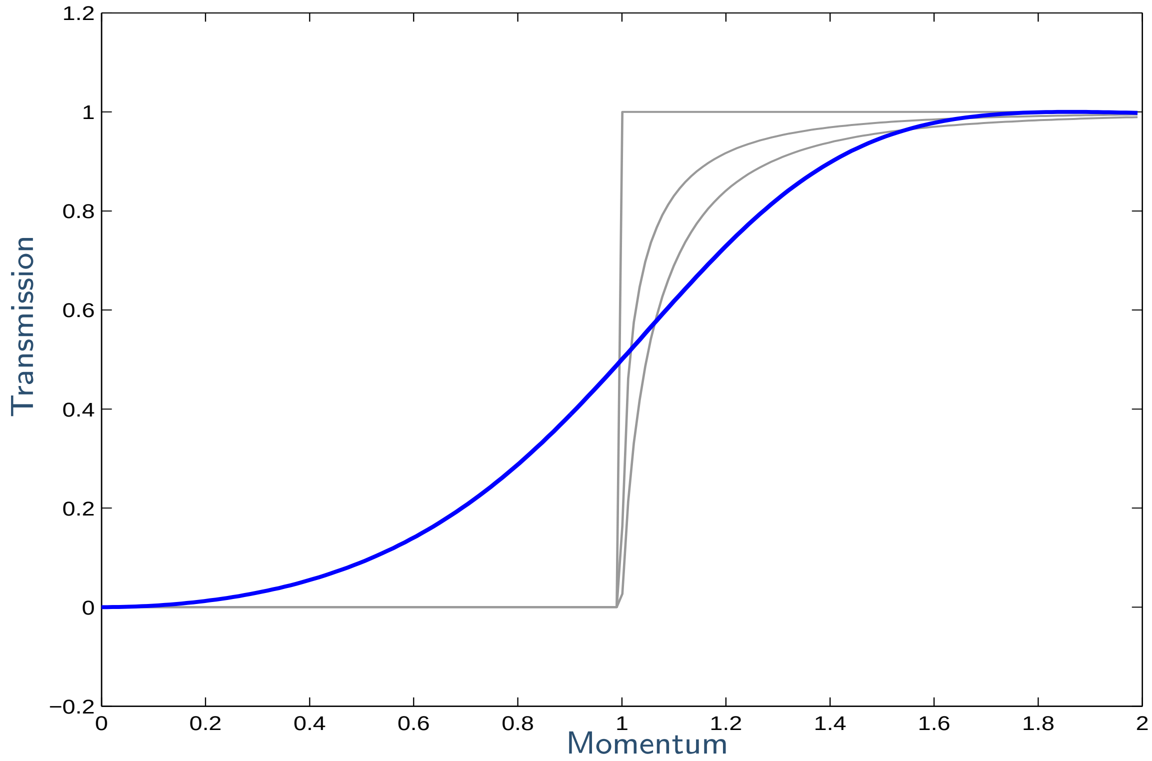
Step up + step down **independently**



Resonance and Tunneling

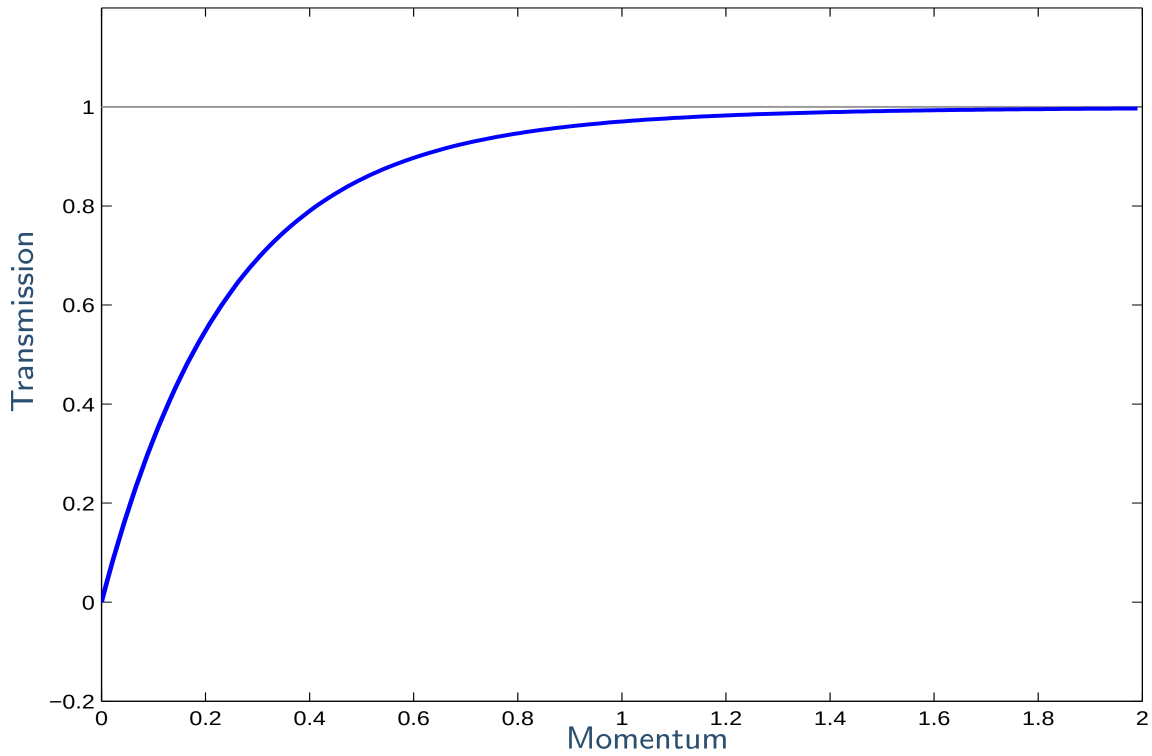
Rectangular potential with height $= 1/2$ and width 2ε

Step up + step down **combined**



Rectangular potential with height $= -1/2$ and width 8ε

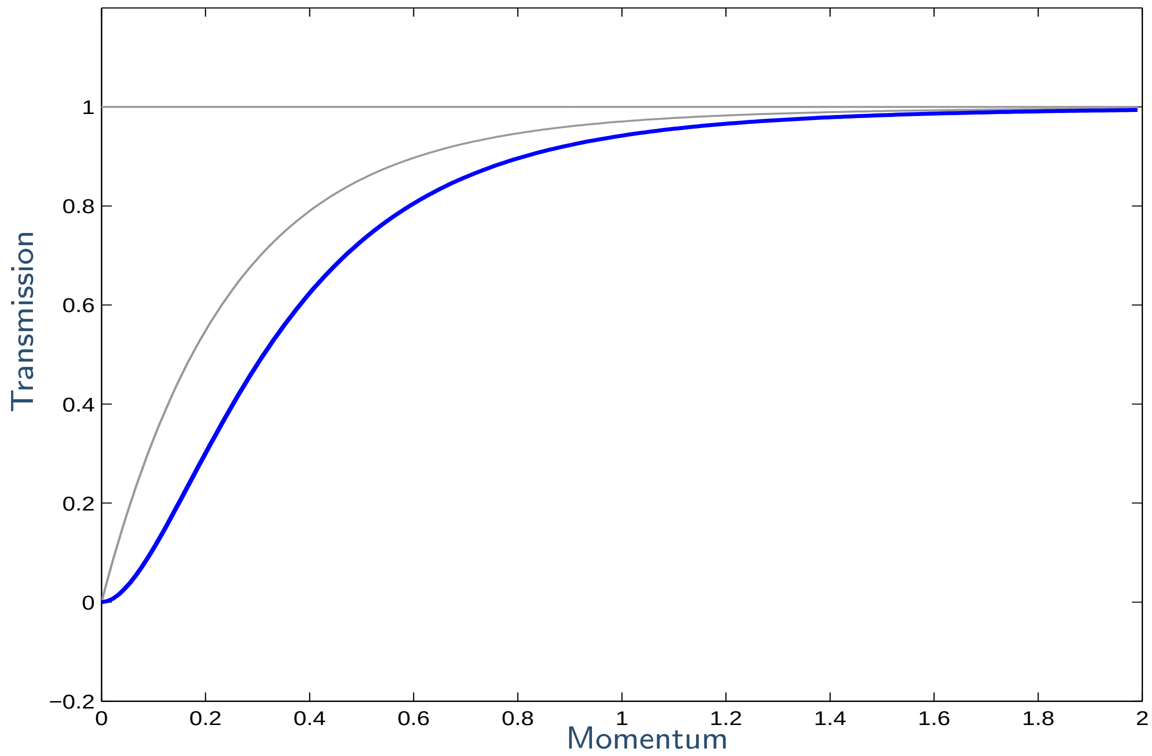
Step down



Resonance and Tunneling

Rectangular potential with height $= -1/2$ and width 8ε

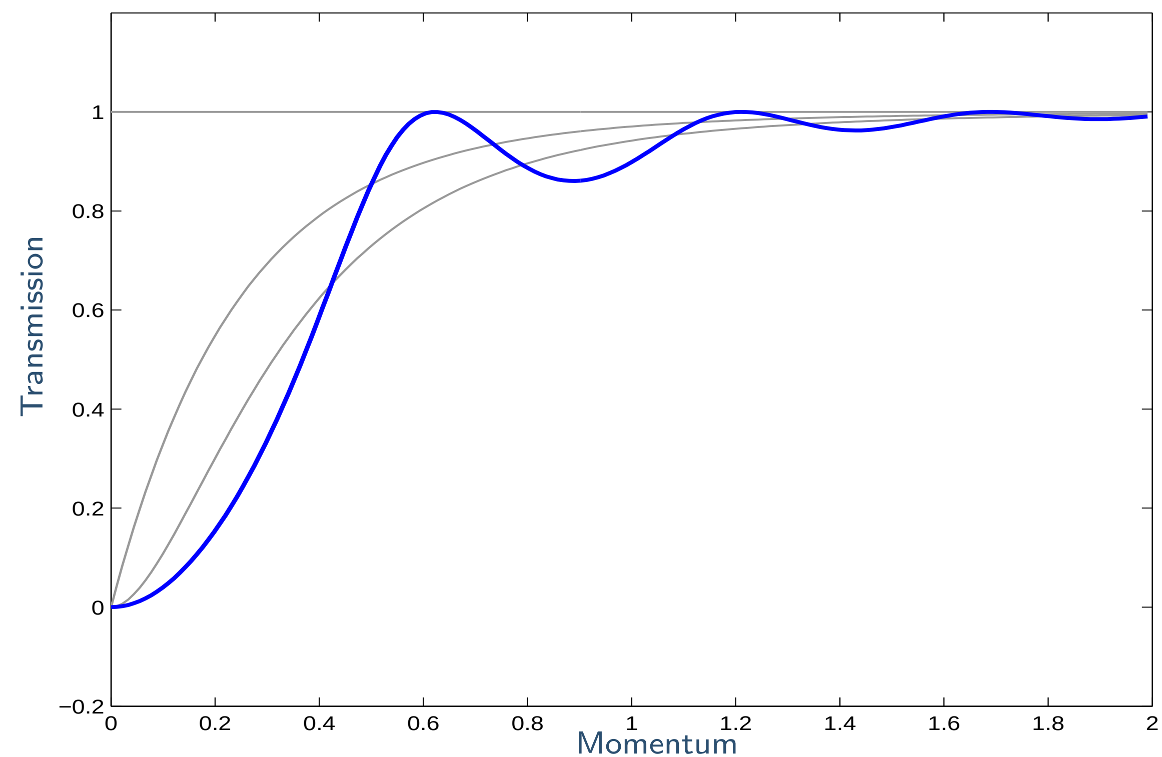
Step down + step up **independently**



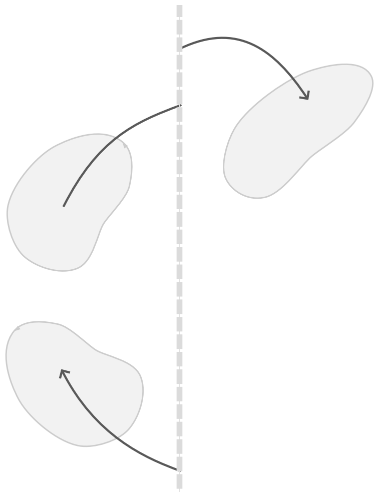
Resonance and Tunneling

Rectangular potential with height $= -1/2$ and width 8ε

Step down + step up **combined**



Semi-classical Liouville Equation



Bicharacteristics:

- Classical particle is either transmitted **or** reflected
- Quantum particle is generally both transmitted **and** reflected

- Hamiltonian $p^2/2m - V(x)$ constant along characteristics
- Particle density $f(x, p, t)$ carried along bicharacteristics

Finite Difference Scheme

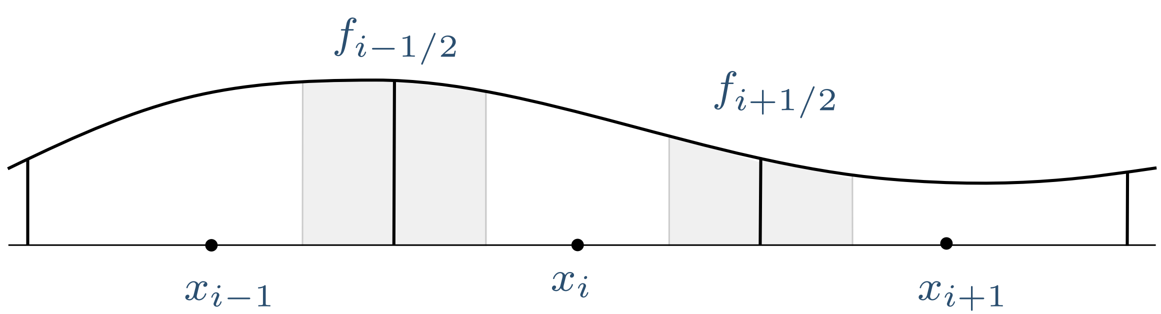
Background
Semi-classical Limit
Mixed Model
Schrödinger Solution
Liouville Solution
Semi-classical Liouville Equation
Finite Difference Scheme
Barrier Interface
2nd order method
Ghost fluid
Examples
Conclusions

$$\boxed{f_t + v f_x - V_x f_v = 0}$$

Grid points at (x_i, v_j). Barrier at $x_{Z+1/2}$.

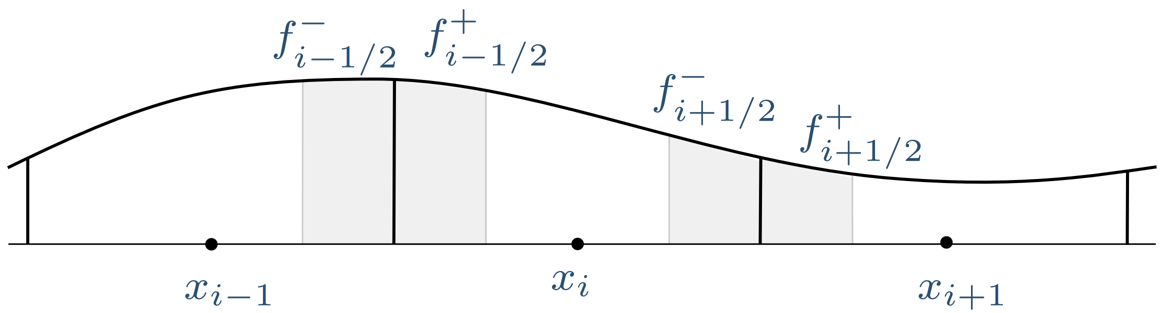
$$\partial_t f_{ij} + v_j \cdot \partial_x f_{ij} - \partial_x V_i \cdot \partial_v f_{ij} = 0$$

where $\partial_x f_{ij} = (f_{i+1/2,j} - f_{i-1/2,j})/\Delta x$



Stability requires upwinding to approximate $f_{i\pm1/2}$

Finite Difference Scheme



Where $f_{i\pm1/2}$ is continuous, $f^-_{i\pm1/2} = f^+_{i\pm1/2}$

$$\partial_x f_{ij} = \frac{f^-_{i+1/2,j} - f^-_{i-1/2,j}}{\Delta x} \quad \text{if} \quad v_j > 0$$

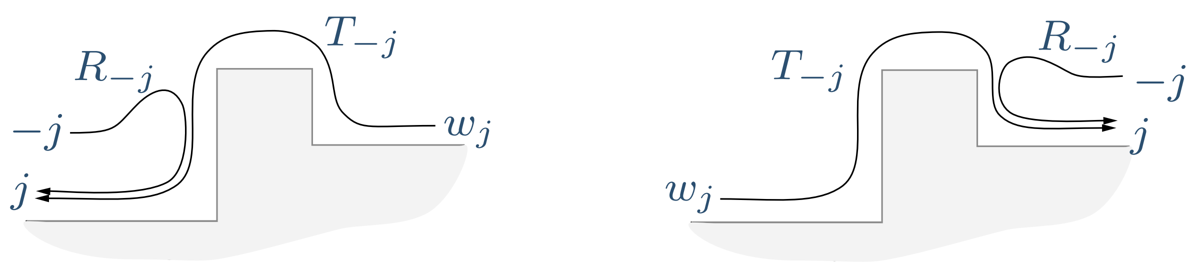
$$\partial_x f_{ij} = \frac{f^+_{i+1/2,j} - f^+_{i-1/2,j}}{\Delta x} \quad \text{if} \quad v_j < 0$$

Barrier Interface

At the quantum barrier $x_{Z+1/2}$, we need to incorporate information from two bicharacteristics.

Barrier interface condition

$$
\begin{aligned}
f^+_{Z+1/2,j} &= R_{-j} f^+_{Z+1/2,-j} + T_{-j} f^-_{Z+1/2,w(j)} \\
f^-_{Z+1/2,j} &= R_{-j} f^-_{Z+1/2,-j} + T_{-j} f^+_{Z+1/2,w(j)}.
\end{aligned}
$$



Barrier Interface

At the quantum barrier $x_{Z+1/2}$, we need to incorporate information from two bicharacteristics.

Barrier interface condition

$$f^+_{Z+1/2,j} = R_{-j} f^+_{Z+1/2,-j} + T_{-j} f^-_{Z+1/2,w(j)}$$
$$f^-_{Z+1/2,j} = R_{-j} f^-_{Z+1/2,-j} + T_{-j} f^+_{Z+1/2,w(j)}.$$

We use the approximation

$$T_{-j} f^+_{Z+1/2,w(j)} = \frac{1}{v_j \Delta v} \int_{w(v_{j-1/2})}^{w(v_{j+1/2})} T(v) v f^- \, dv$$

where we use Hamiltonian to determine w

$$w(v_{\pm|j|}) = \pm\sqrt{v_j^2 \pm 2(V^+_{Z+1/2} - V^-_{Z+1/2})}$$

2nd order method

Piecewise linear:

$$f^{+}_{i-1/2,j} = f_{i,j} - \tfrac{1}{2}\left(1 - \lambda_j\right)\Delta x \sigma^x_{ij}$$
$$f^{-}_{i+1/2,j} = f_{i,j} + \tfrac{1}{2}\left(1 - \lambda_j\right)\Delta x \sigma^x_{ij}$$

with the slope σ^x_{ij} calculated using the Van Leer slope limiter

$$\sigma^x_{ij} = \left(\frac{f_{ij} - f_{i-1,j}}{\Delta x}\right)\phi\left(\frac{f_{i+1,j} - f_{ij}}{f_{ij} - f_{i-1,j}}\right) \quad \text{where} \quad \phi(\theta) = \frac{\theta + |\theta|}{1 + |\theta|}$$

and the Courant number $\lambda_j = |v_j|\Delta t/\Delta x$

We can't do this directly across at the barrier!

Ghost fluid

Across the barrier, we need to reconstruct “unmixed” flux.

For $j > 0$,

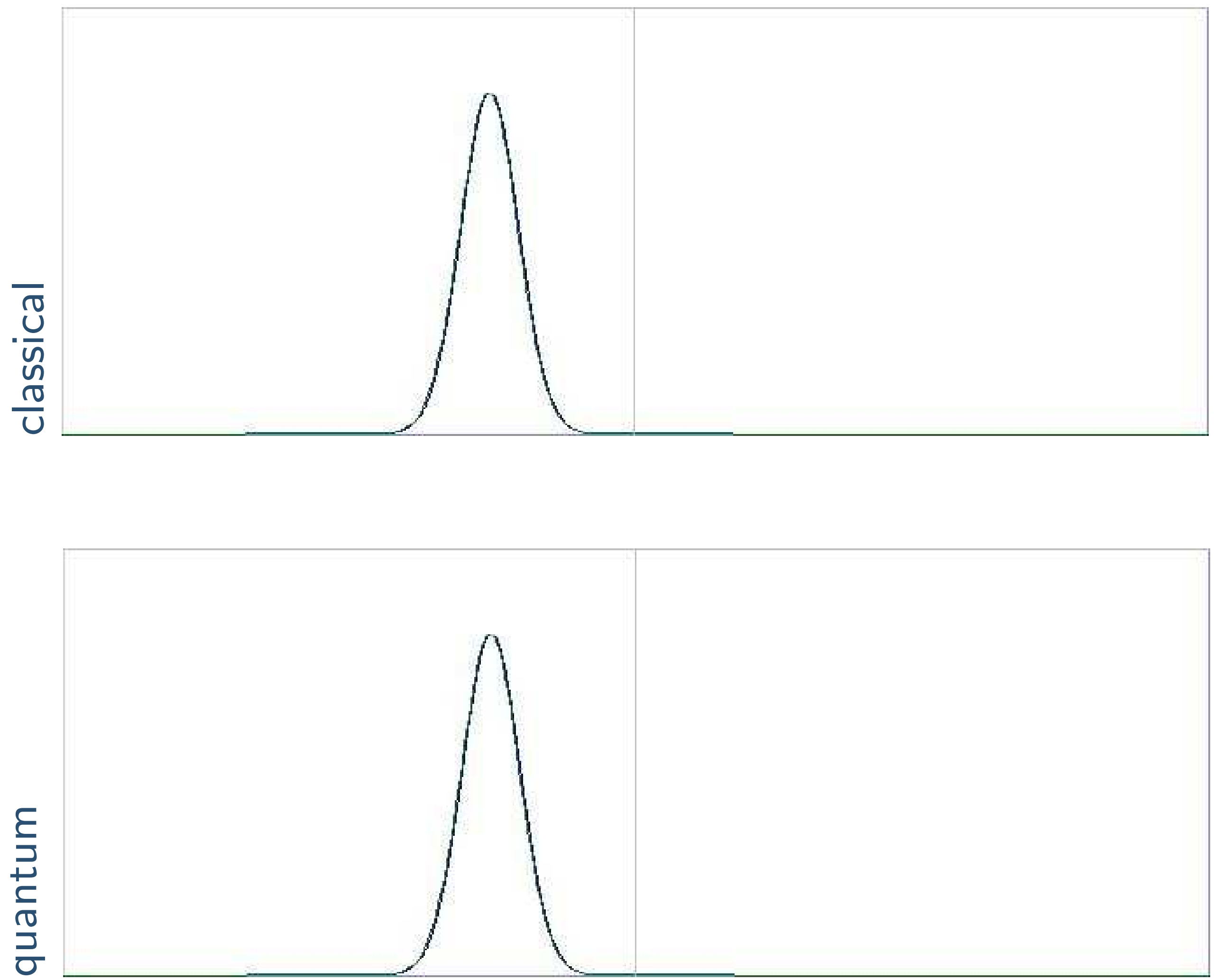
$$
\begin{aligned}
f_{Z+1,-w(-j)} &= T_j \tilde{f}_{Z+1,j} + R_j \tilde{f}_{Z,w(-j)} \\
f_{Z,-j} &= R_j \tilde{f}_{Z+1,j} + T_j \tilde{f}_{Z,w(-j)}
\end{aligned}
$$

with a similar system for $j < 0$. By inverting this system of equations, we have the unmixed state downwind of the barrier

$$
\begin{aligned}
\tilde{f}_{Z+1,j} &= \frac{T_j f_{Z+1,-w(-j)} - R_j f_{Z,-j}}{T_j - R_j} \qquad \text{when } j > 0 \\
\tilde{f}_{Z,j} &= \frac{T_j f_{Z,-w(-j)} - R_j f_{Z+1,-j}}{T_j - R_j} \qquad \text{when } j < 0
\end{aligned}
$$

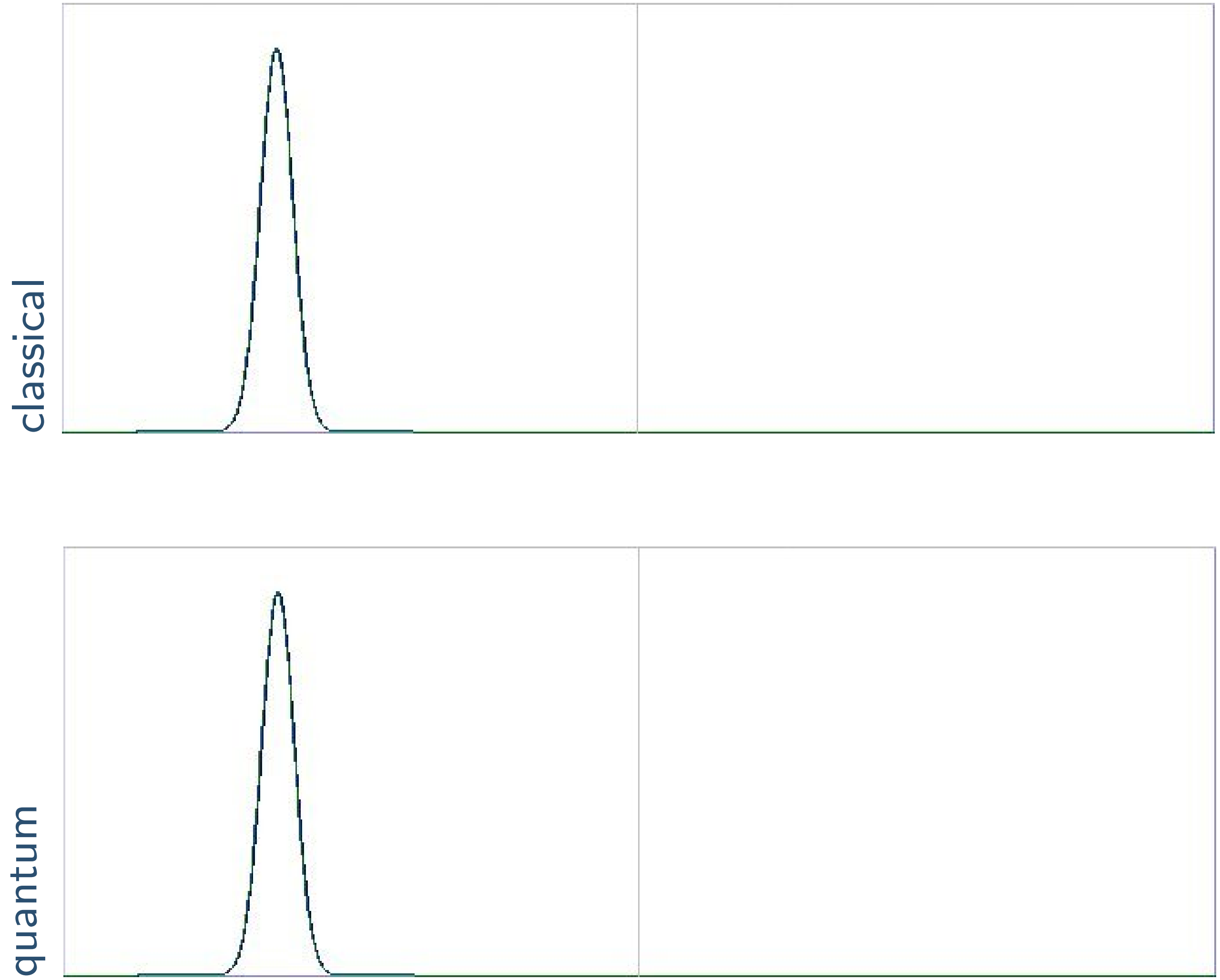
Step Potential

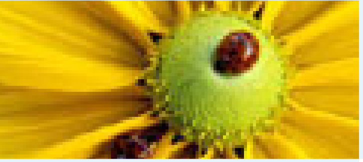
$V(x) = 0$ if $x < 0$ and $V(x) = -\frac{1}{2}$ if $x > 0$, $v_0 = \frac{1}{4}$, $\varepsilon = .005$



Eckart Potential

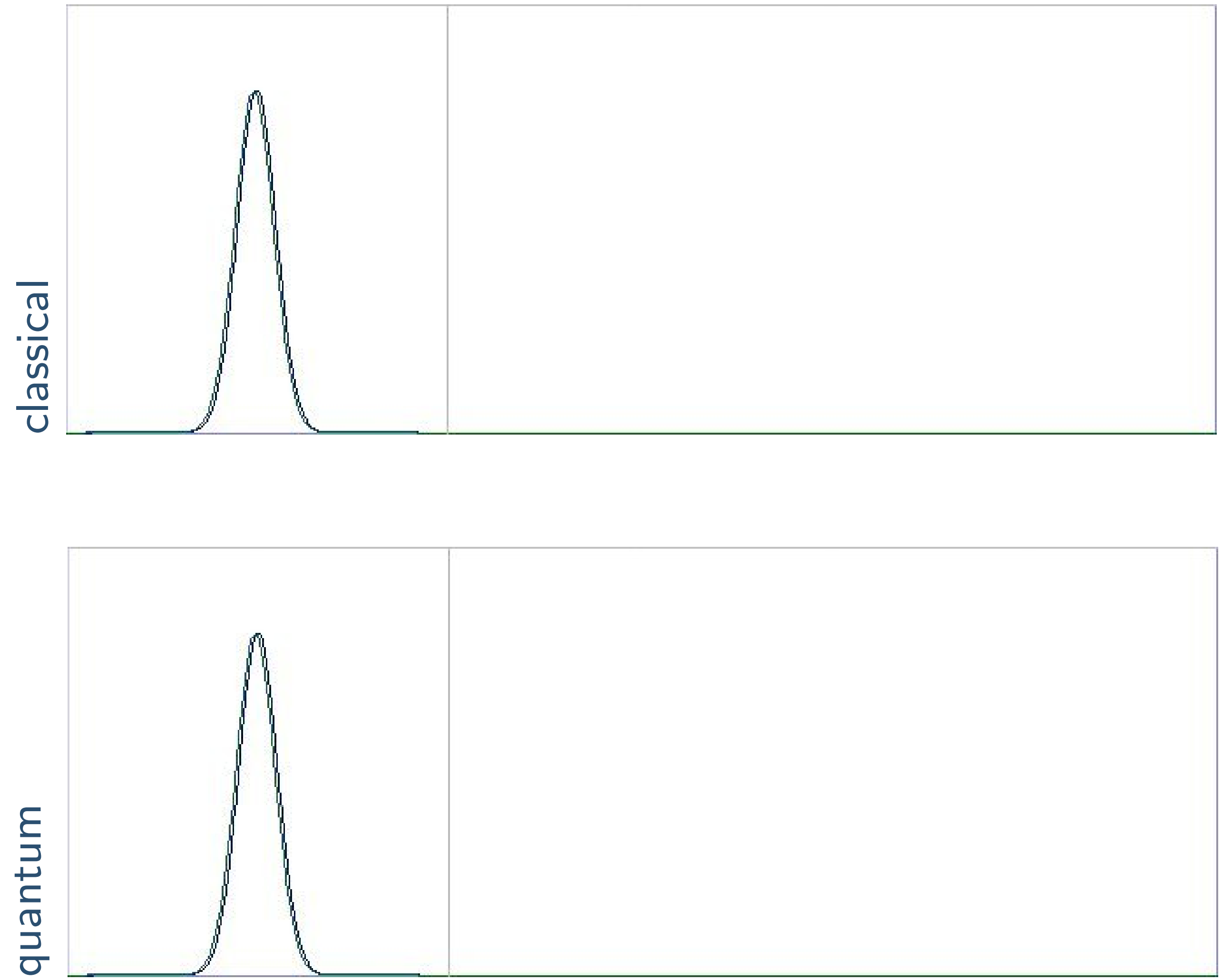
$V(x) = -2\,\mathrm{sech}^2(4x/\varepsilon)$ with $\varepsilon = .005$





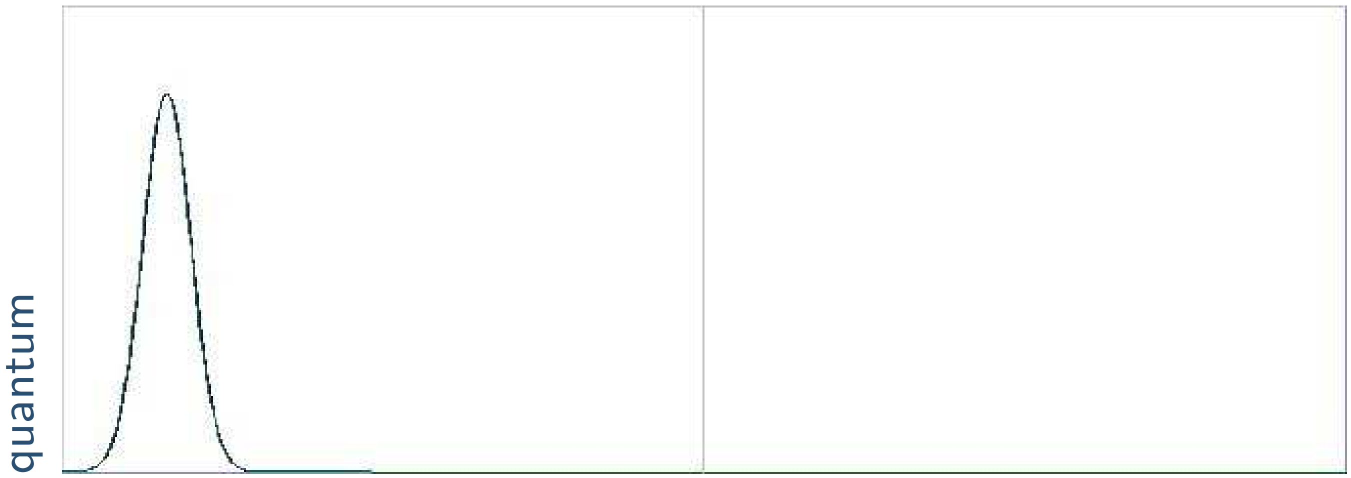
Tunneling Diode

$V(x) = -x + \text{Rect}[-\varepsilon/2, \varepsilon/2](x)$ with $\varepsilon = .005$



Rectangular Potential

$V = \frac{1}{2}$, width $= 25\varepsilon$, $v_0 = 0$, $\varepsilon = 0.005$



Research Directions

Simplifying assumptions

- Particle moves instantaneously across the barrier
- Barrier is sufficiently local
- Particle has no phase information (no long range interaction)

Incorrect/inaccurate for

- Larger quantum structures
- Smaller domains (nonvanishing ε)
- Periodic crystalline structures
- Highly resonant barriers

Extension of model

- Introduce time delay
- Introduce phase information
- Reconstruct solution inside the quantum barrier

Thank you

Questions?