Quantum-mechanical Wave Packet Dynamics Using the Spectral Method

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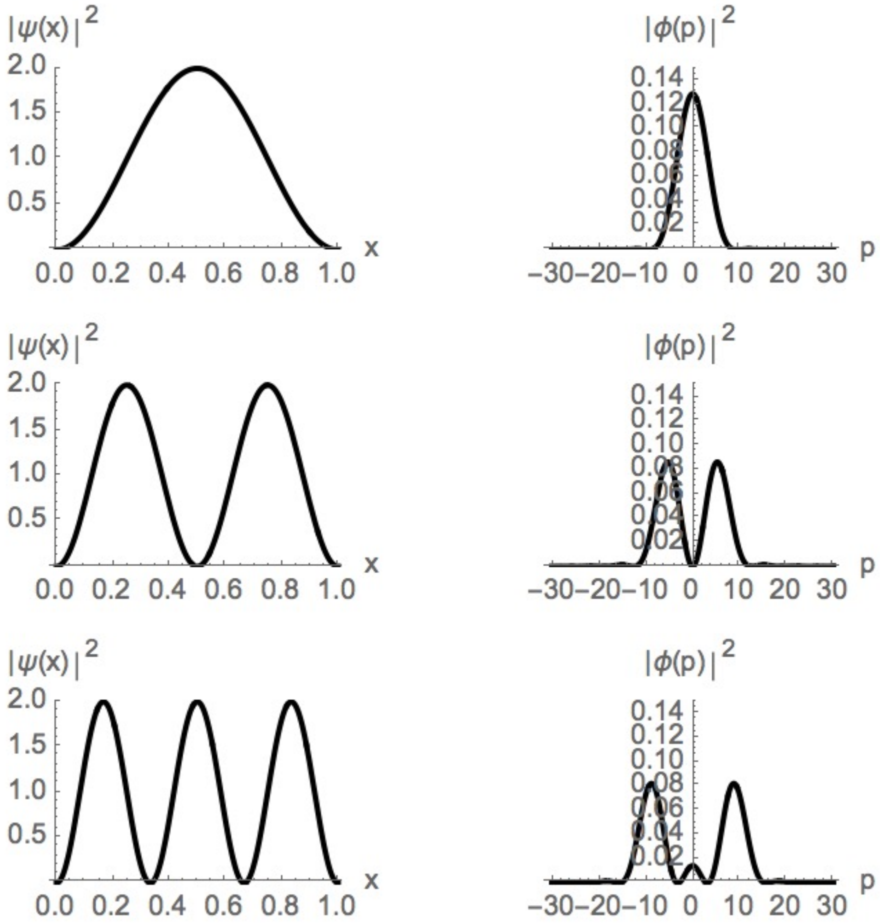
Quantum Mechanics: Intro

- Small Scale Physics
- Wave-Particle Duality
- Heisenberg Uncertainty Principle: $\Delta x \Delta p \geq \frac{\hbar}{2}$
- Schrödinger Equation: $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}, t) = i\hbar\frac{d}{dt}\psi(\boldsymbol{r}, t)$
- 1D, Time Independent SE: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$
- $\psi^*(x)\psi(x)$ gives the probability density for the object

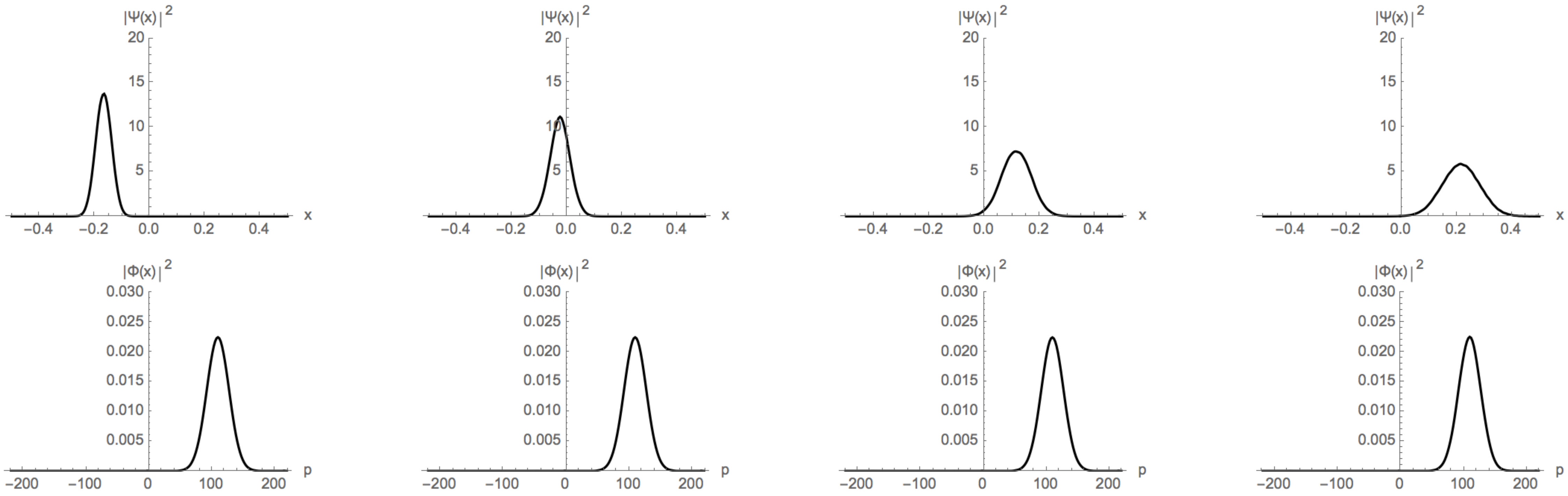
Infinite Square Well – Particle in a Box



- Infinitely hard walls at 0, L: object must be confined between them
- $\psi_n(x) = \sqrt{\frac{2}{L}}\, sin\left[\frac{n\pi x}{L}\right]$
- $\phi_n(p) = \frac{n\hbar\sqrt{\pi L\hbar}\left(1-e^{-\frac{ipL}{\hbar}}(-1)^n\right)}{n^2\pi^2\hbar^2-L^2p^2}$
- $E_n = \frac{n^2\pi^2\hbar^2}{2ML^2}$
- Symmetric ISW: walls at –L, L

Wave Packets in ISW

- $\Psi(x,t) = \sum_{n=1}^{\infty} c_n e^{-\frac{iE_n t}{\hbar}} \psi_n(x)$
- Coefficients chosen for a Gaussian shape



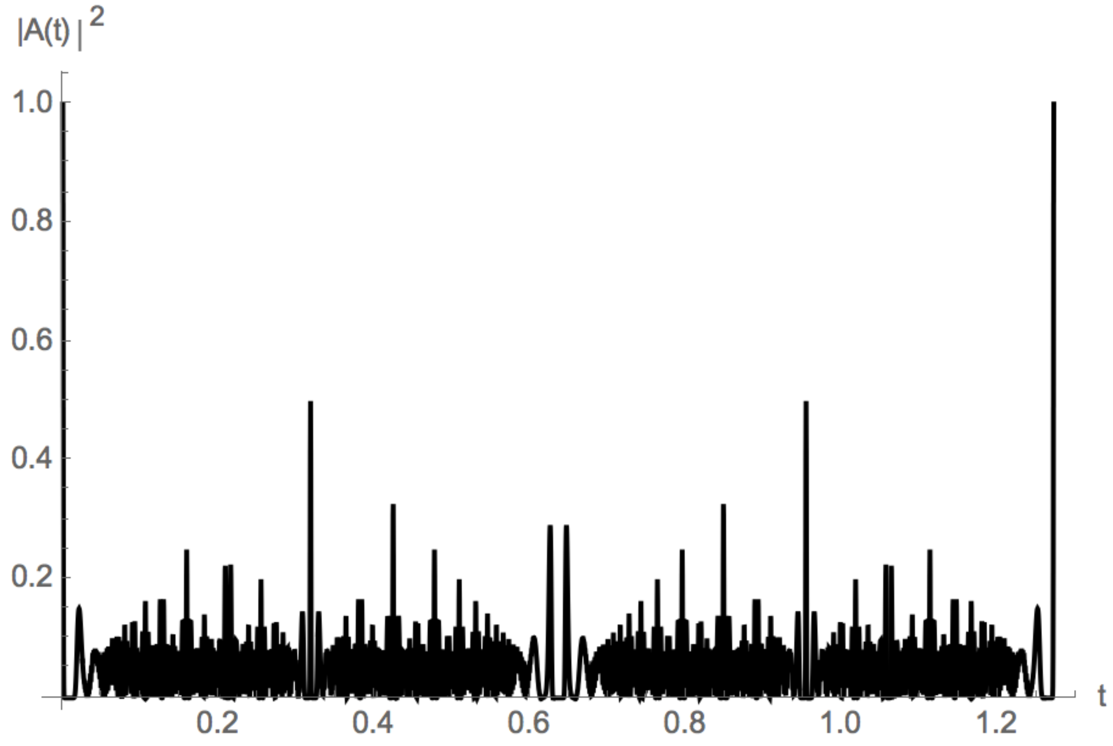
Wave Packets in ISW

- Autocorrelation Function:

  $A(t) = \int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(\mathrm{x},0)\mathrm{dx}$

- Exact revivals:

$$T_{Rev} = \frac{2\pi\hbar}{E_1} = \frac{16ML^2}{\pi\hbar}$$



Spectral Method

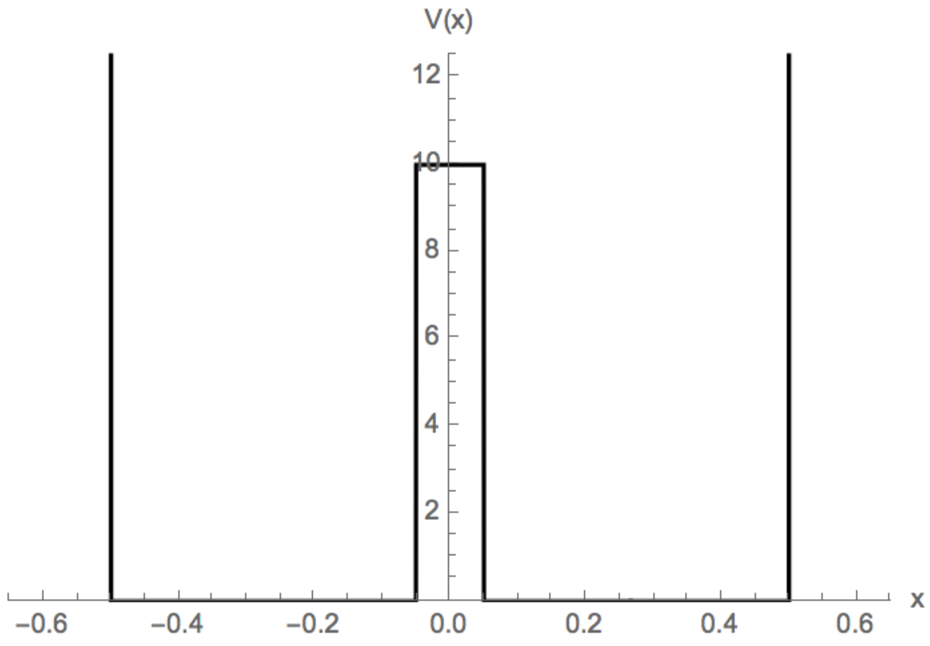
- Choose ISW as basis potential
- $\hat{H} = \hat{H}^{ISW} + V(x)$: $V(x)$ chosen to be a barrier or well to simulate scattering problems.
- Construct Hamiltonian matrix: $\mathcal{H}_{n,m} = \int_{-\infty}^{\infty} \psi_n^{*ISW} \hat{H} \psi_m^{ISW} \, dx$
- Eigenvalues give eigenenergies, eigenvectors give expansion coefficients for eigenstates
- $\psi_n(x) = \sum_{m=1}^{N} c_{n,m} \psi_m^{ISW}(x)$
- $\phi_n(p) = \sum_{m=1}^{N} c_{n,m} \phi_m^{ISW}(p)$
- Accuracy dependent on the size of the matrix, *N*.

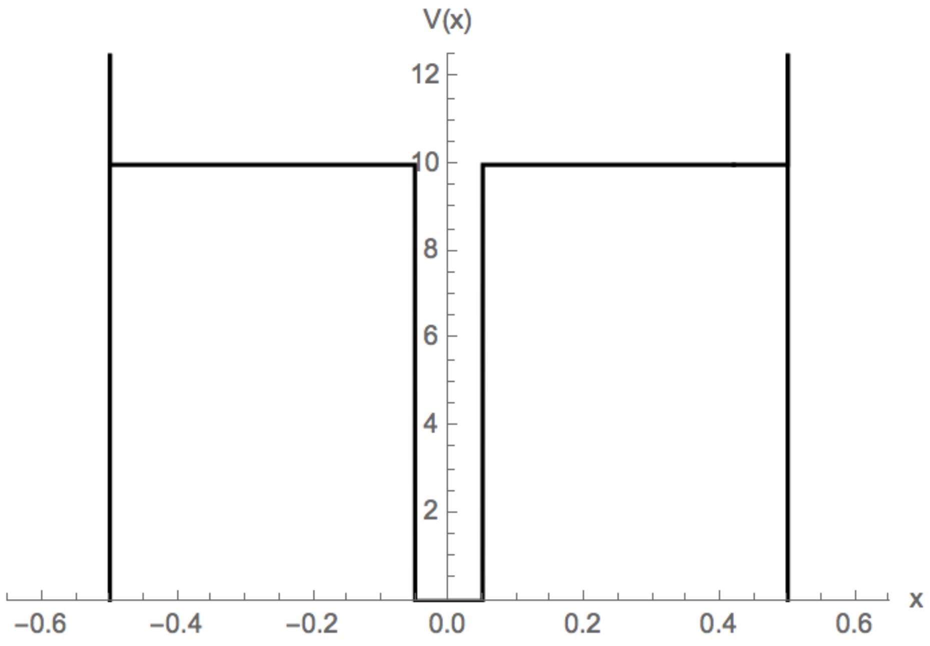
Process

- Define a scattering potential $V(x)$
- Use spectral method to determine eigenstates and energies
- Test and improve accuracy of results
- Construct wave packets from eigenstates
- Evolve wave packet in time
- Calculate regional probabilities, uncertainties, autocorrelation function, etc…
- Change parameters of potential for comparison

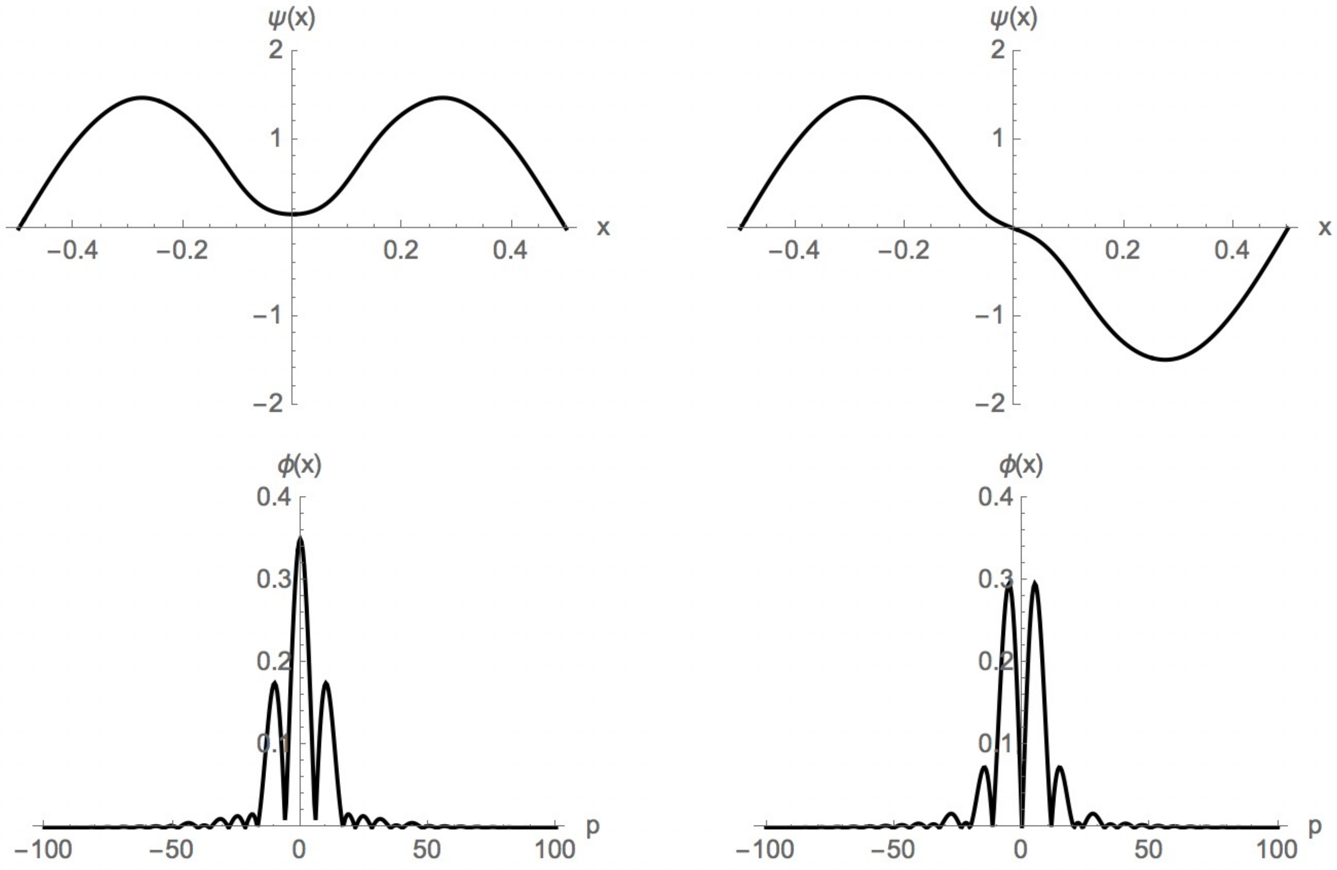
Barrier and Well Potentials

- Rectangular potential with height V_o and width a
- Other potentials written to have the same height (V_o) and same area ($V_o a$) as the rectangular potential





Eigenstates - Barriers



- Barrier causes dip in center of odd n states
- Can plot accurately with few states
- Degeneracies arise due to symmetry and can cause problems distinguishing states

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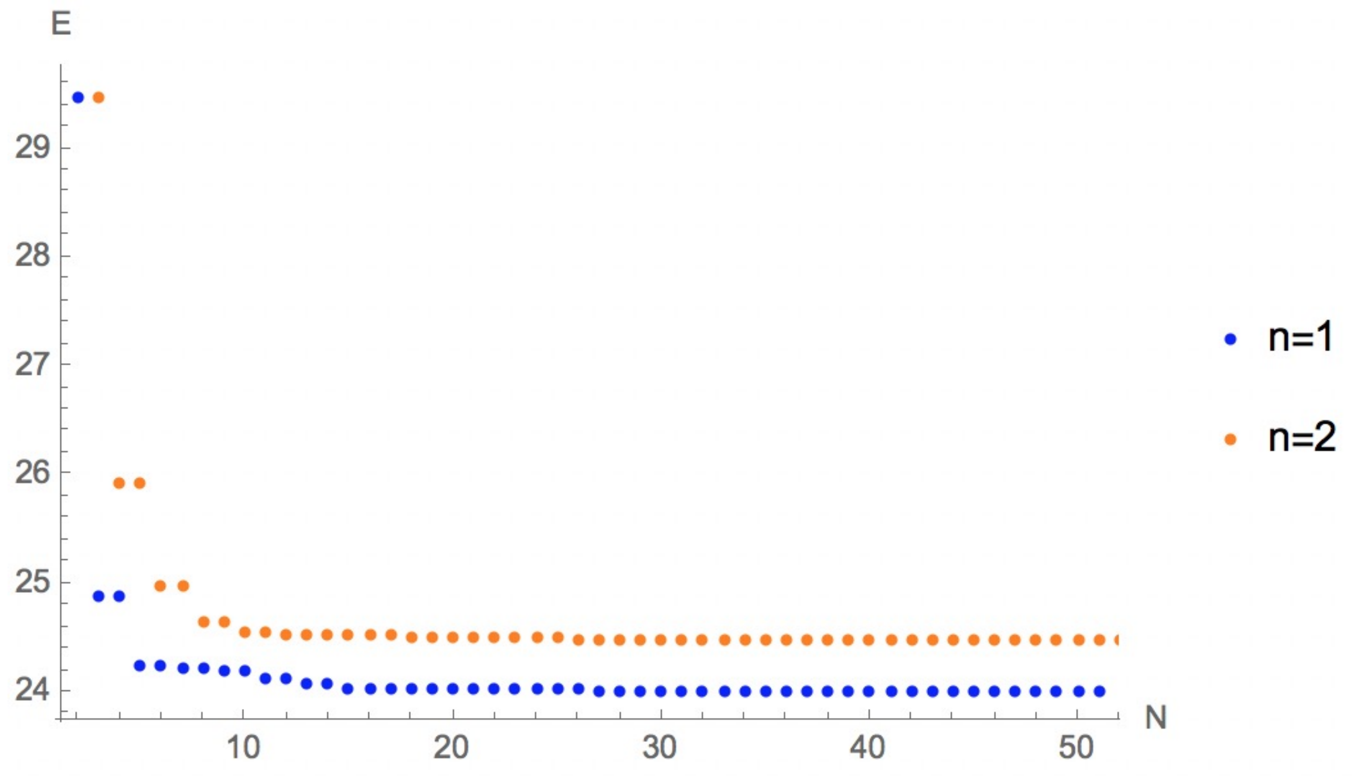

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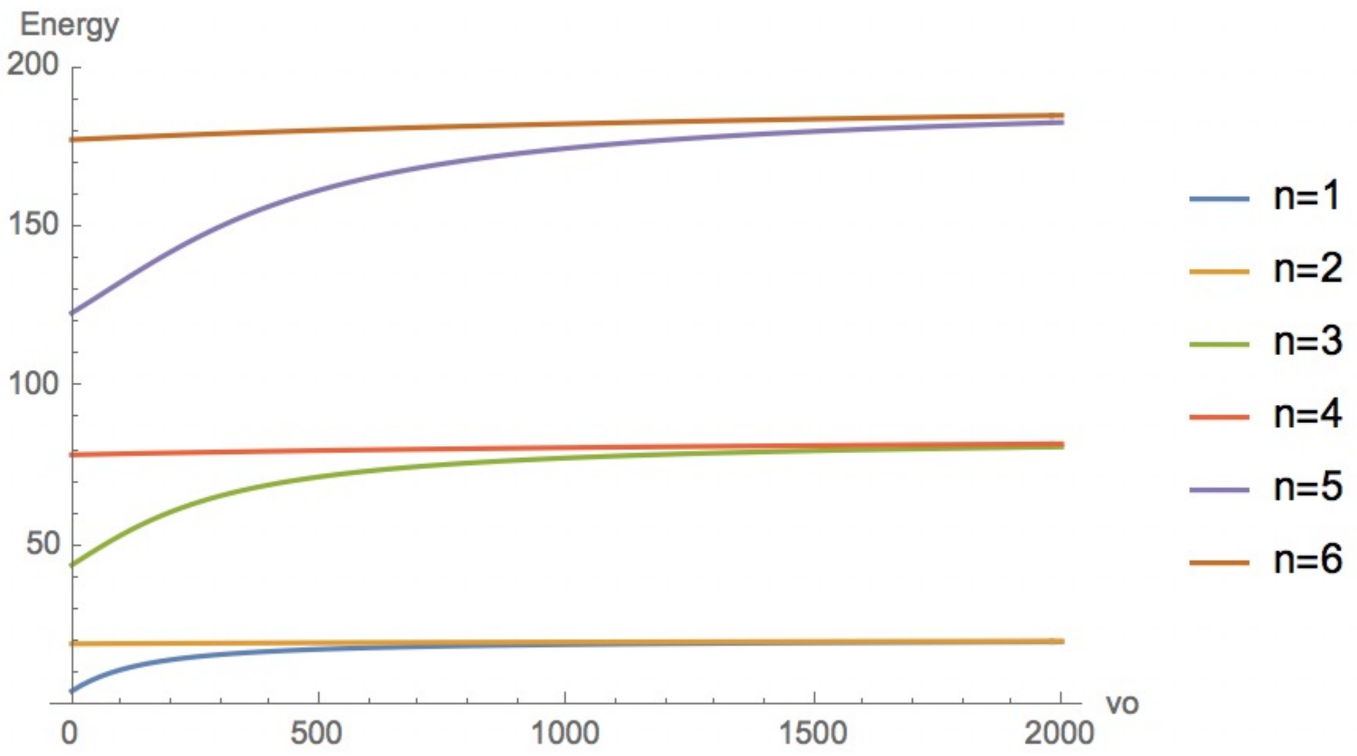

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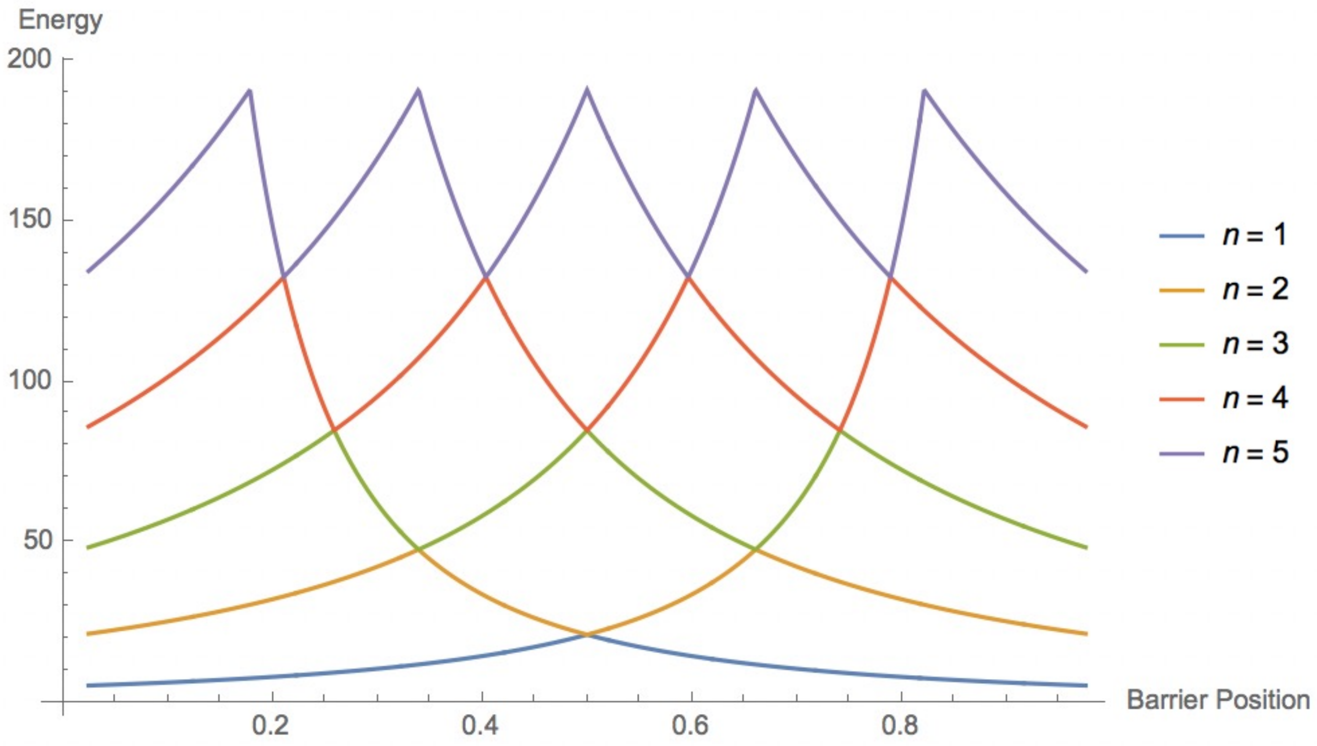

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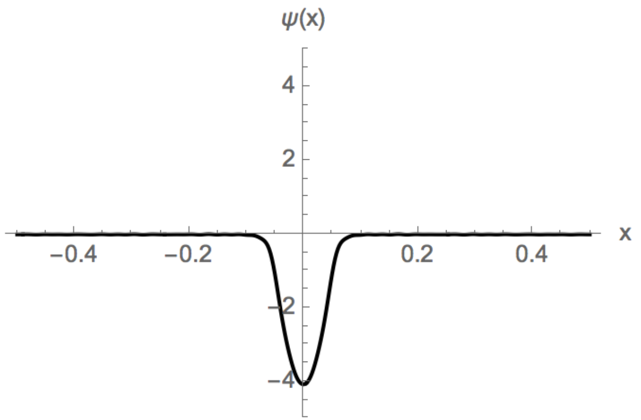
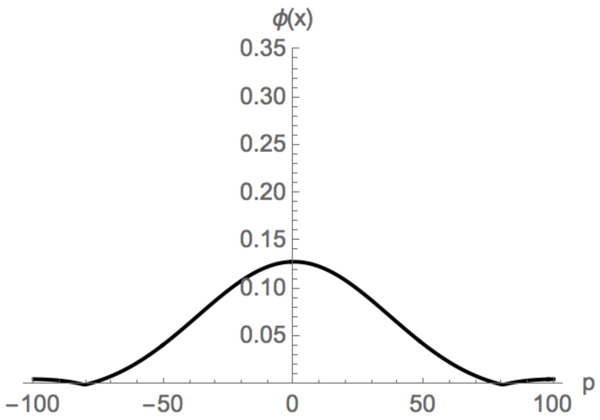
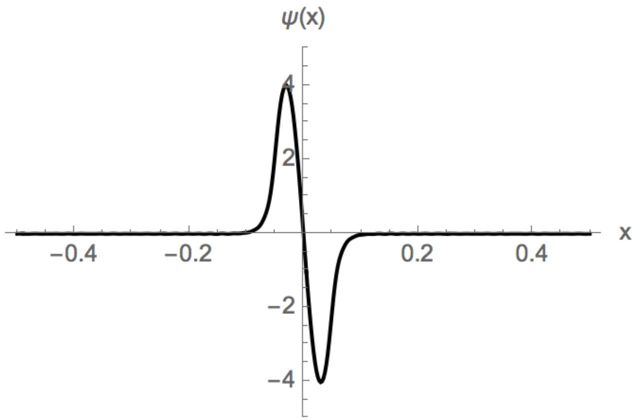
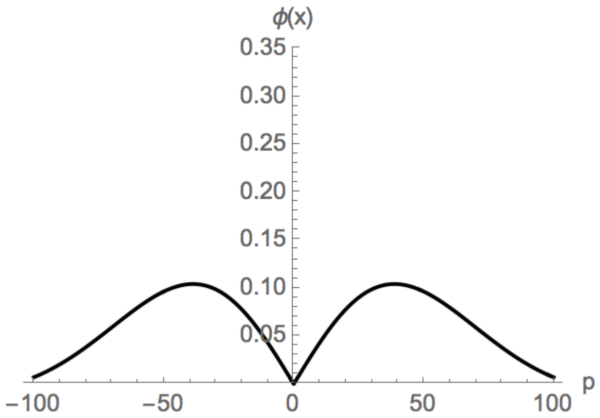
Eigenstates - Wells



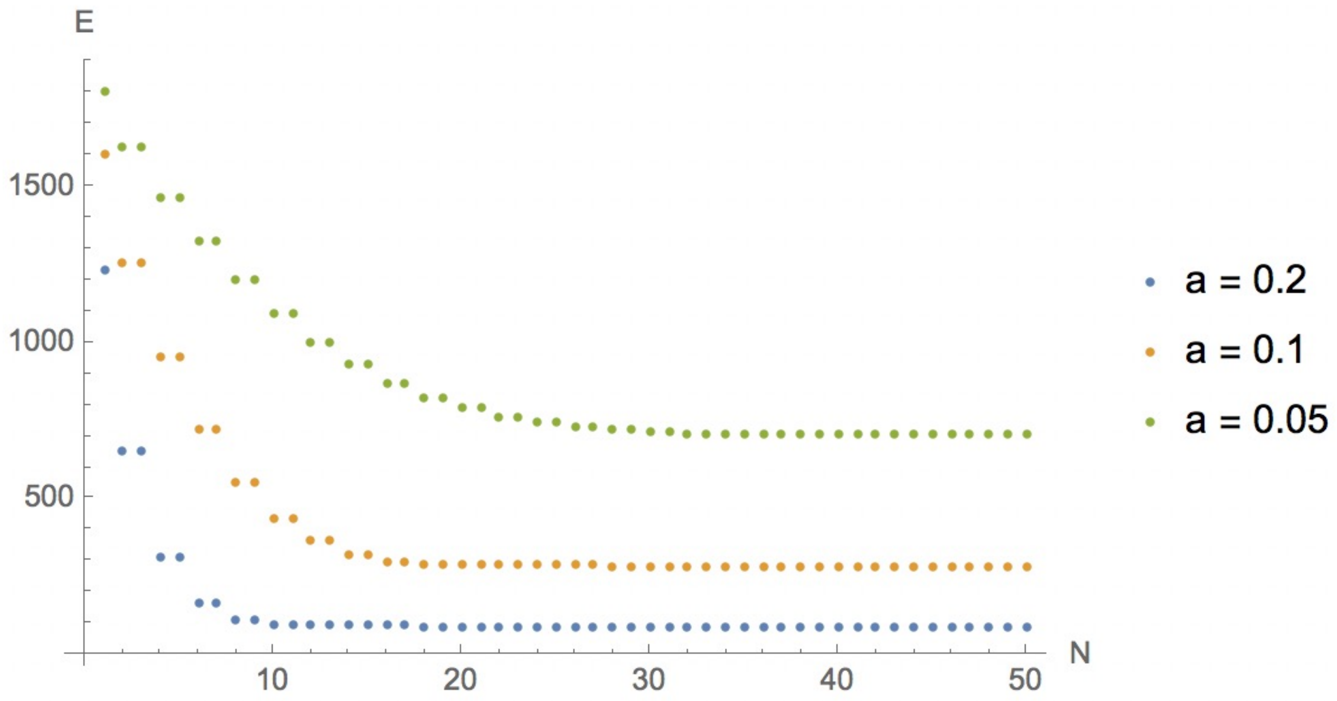






- Needs many extra states to plot bound states accurately
- No degeneracies

Eigenstates - Wells



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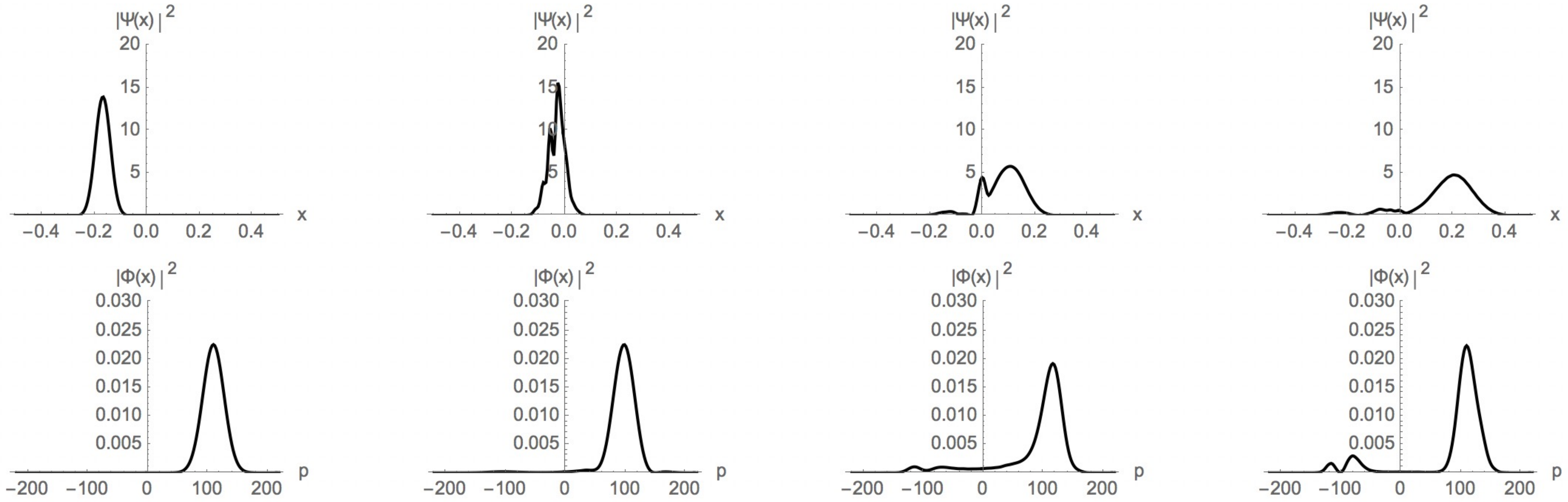
Wave Packet Scattering: Barriers



- Rectangular barrier, $V_0 = 3000, a = 0.05.$

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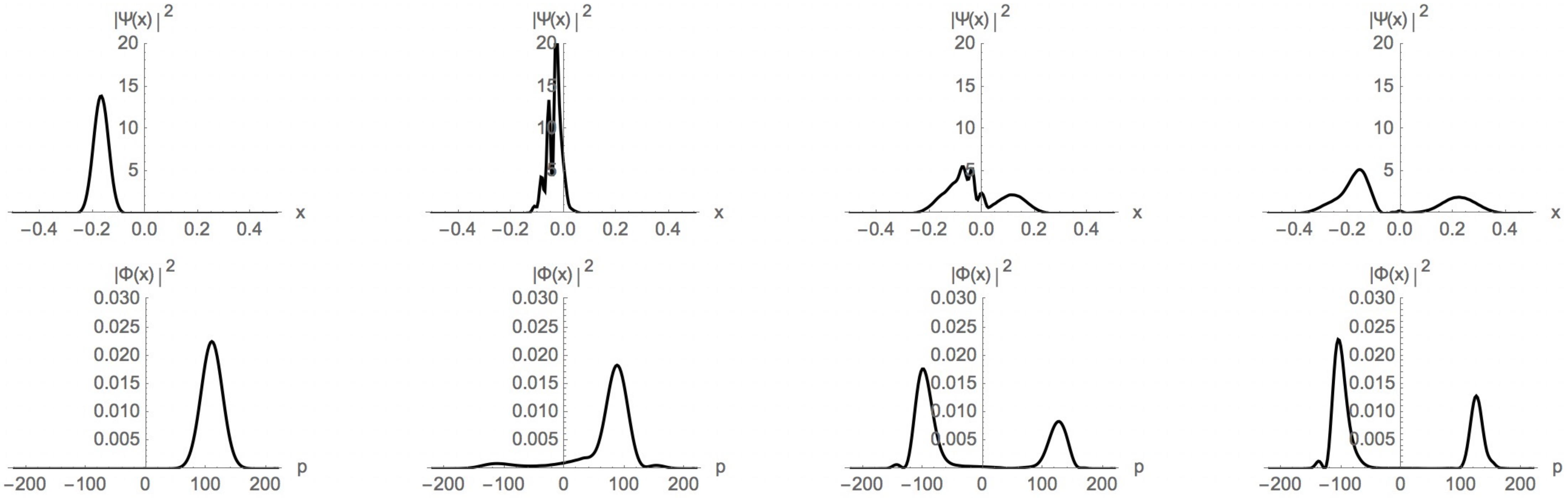

- Rectangular barrier, $V_0 = 6000, a = 0.05.$

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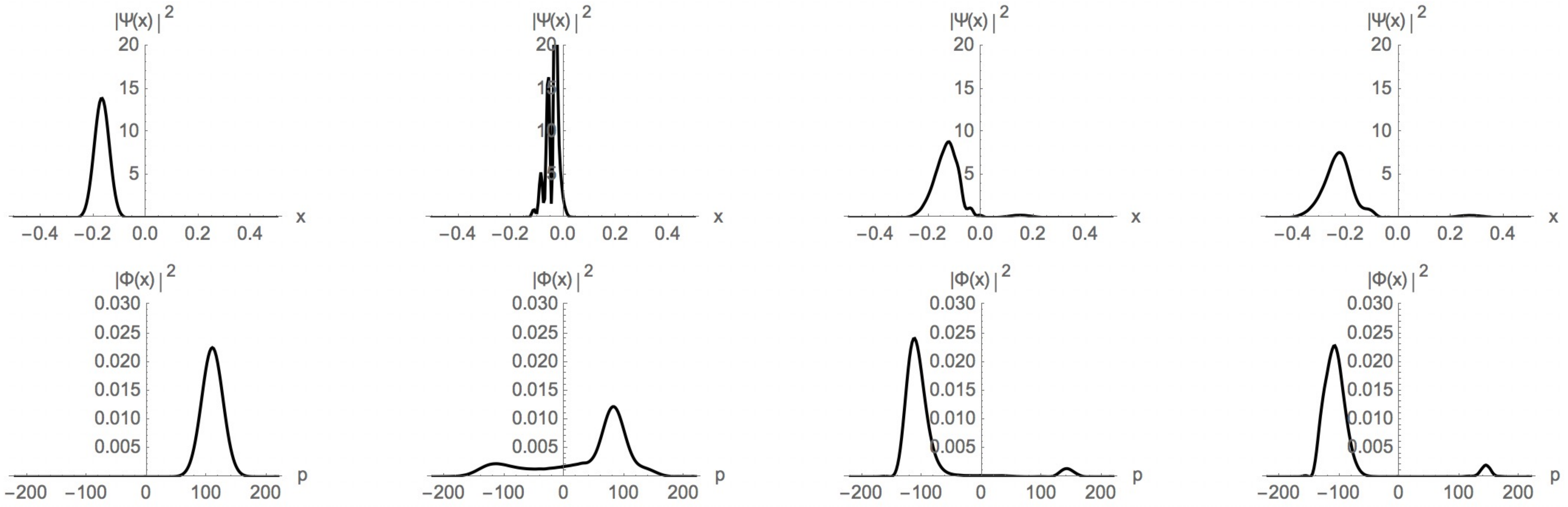
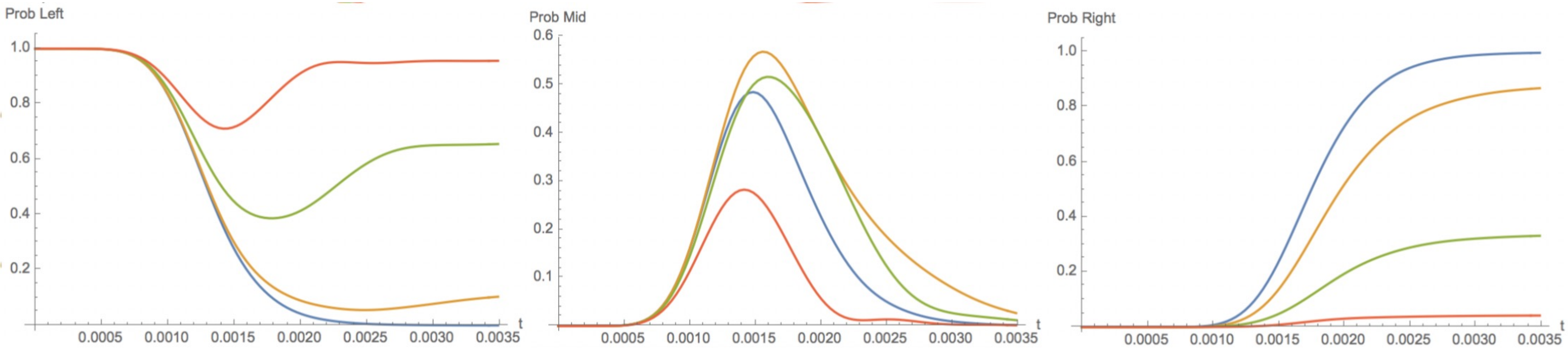


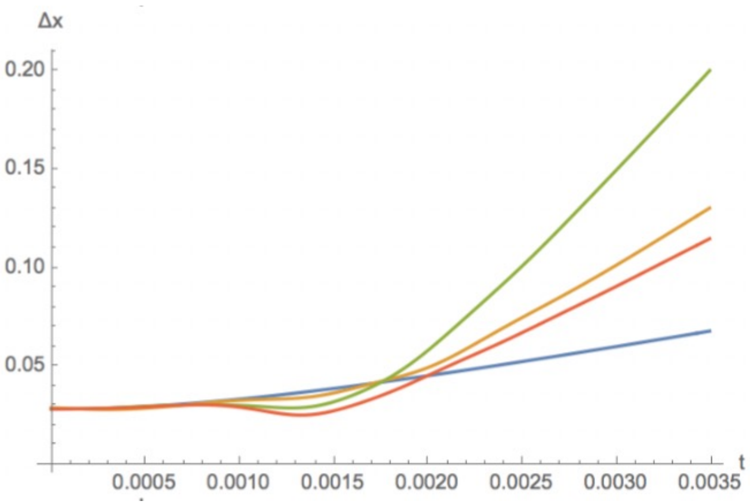
- Rectangular barrier, $V_0 = 9000, a = 0.05.$

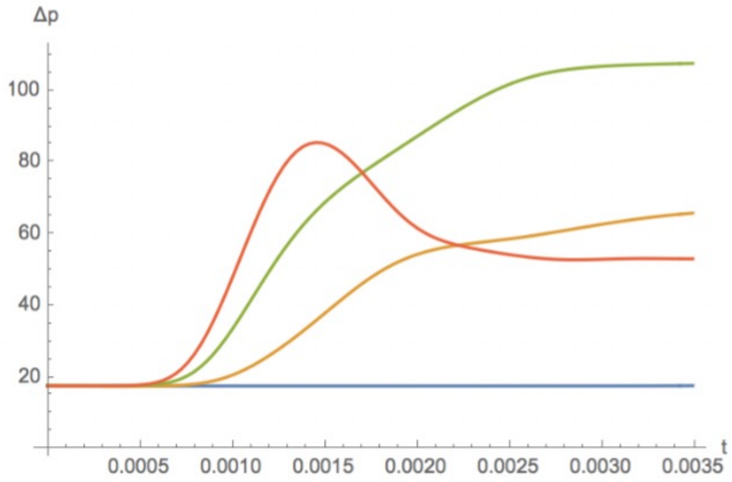
Analysis: Probabilities

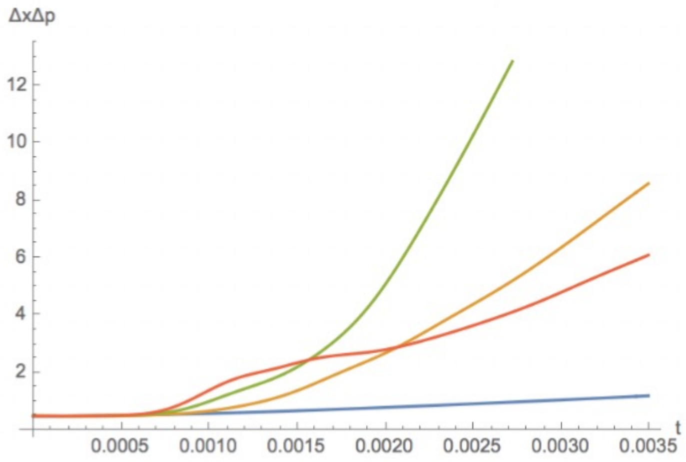


- Rectangular barrier: $a = 0.05$. $V_o = 0$ (Blue), $V_o = 3{,}000$ (Orange), $V_o = 6{,}000$ (Green), $V_o = 9{,}000$ (Red)

Analysis: Uncertainties







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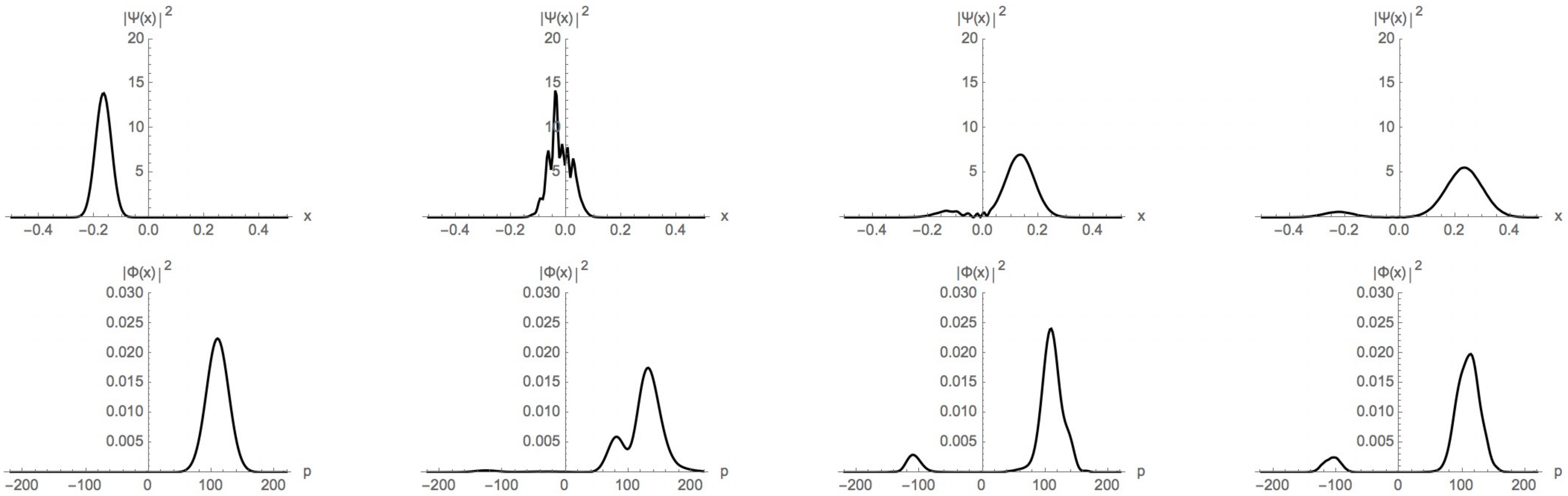
Wave Packet Scattering: Wells



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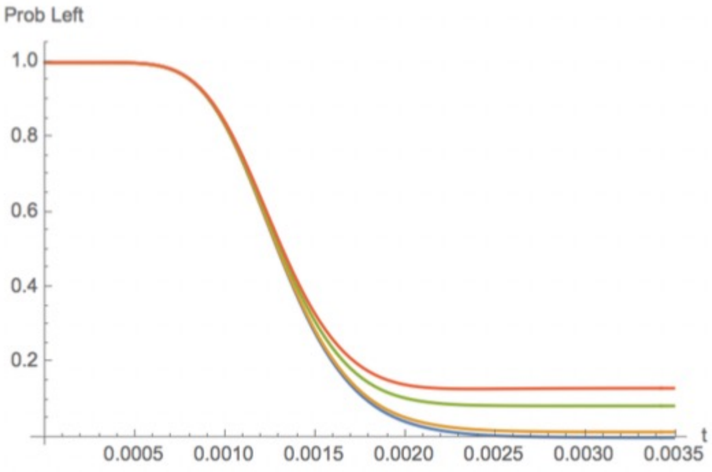

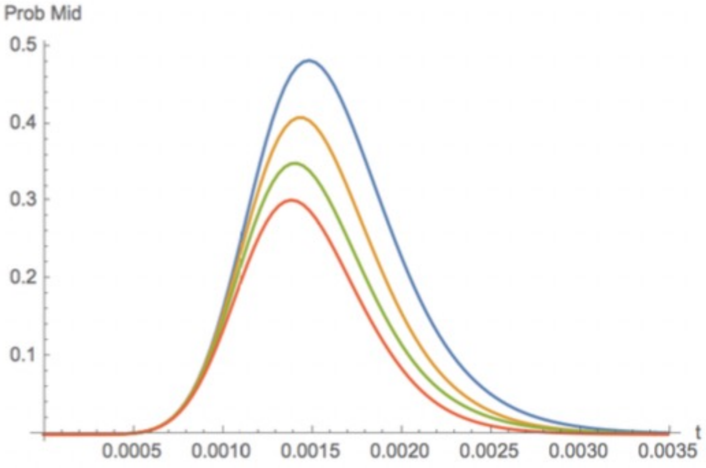

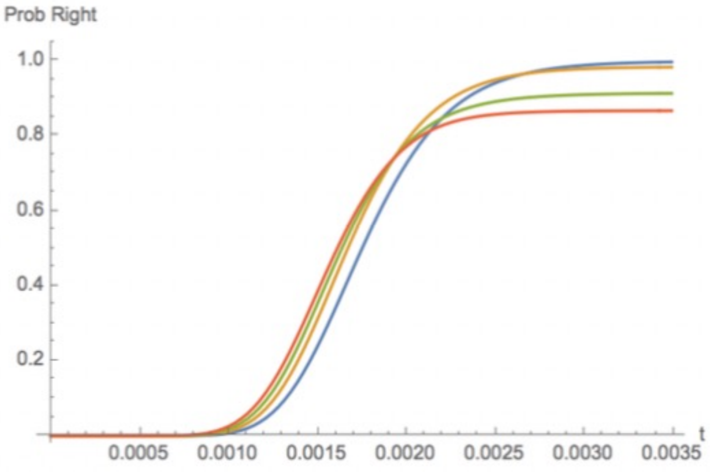

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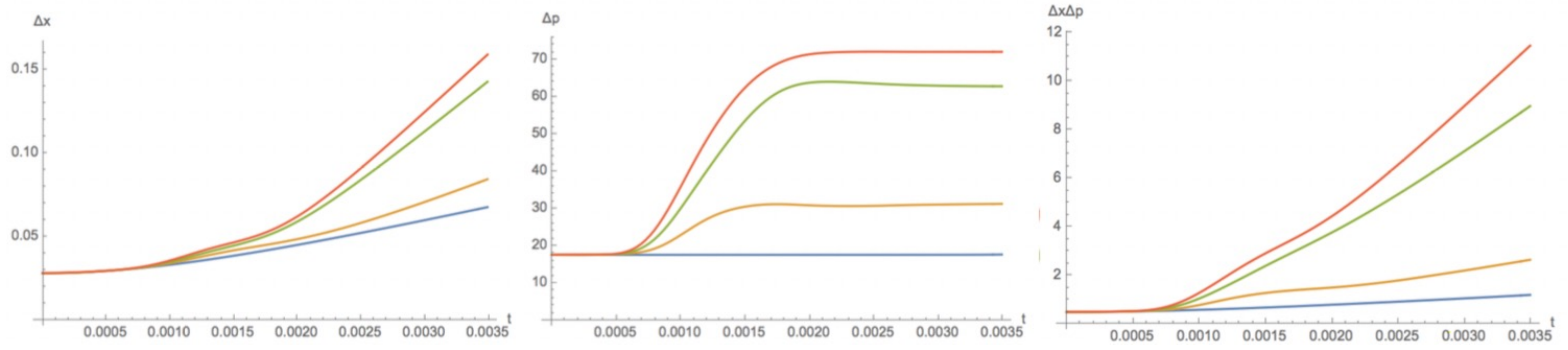

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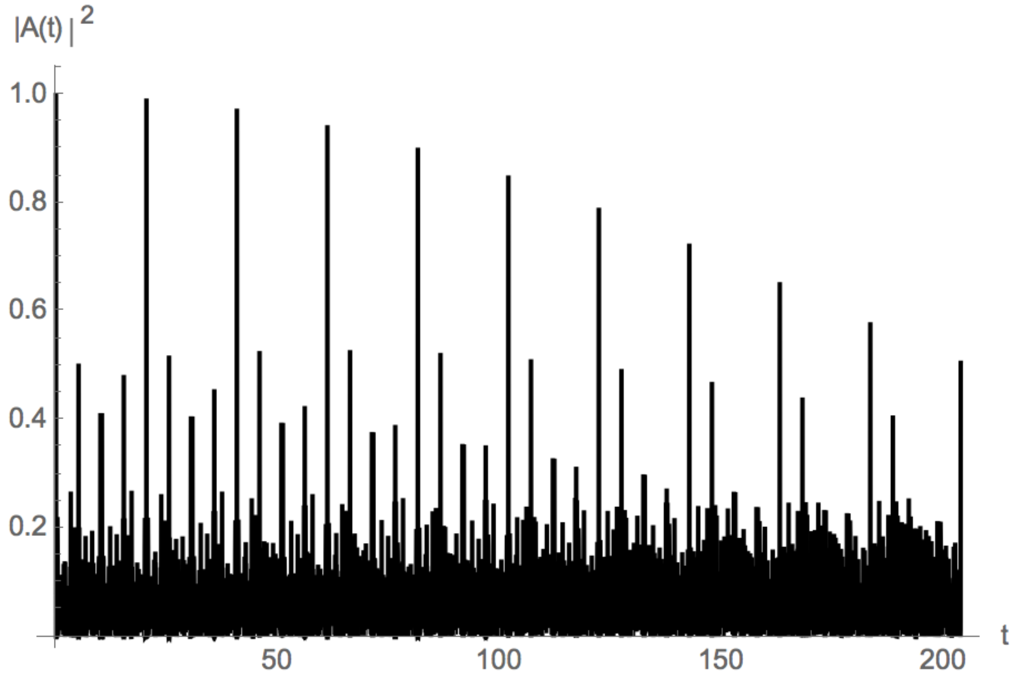
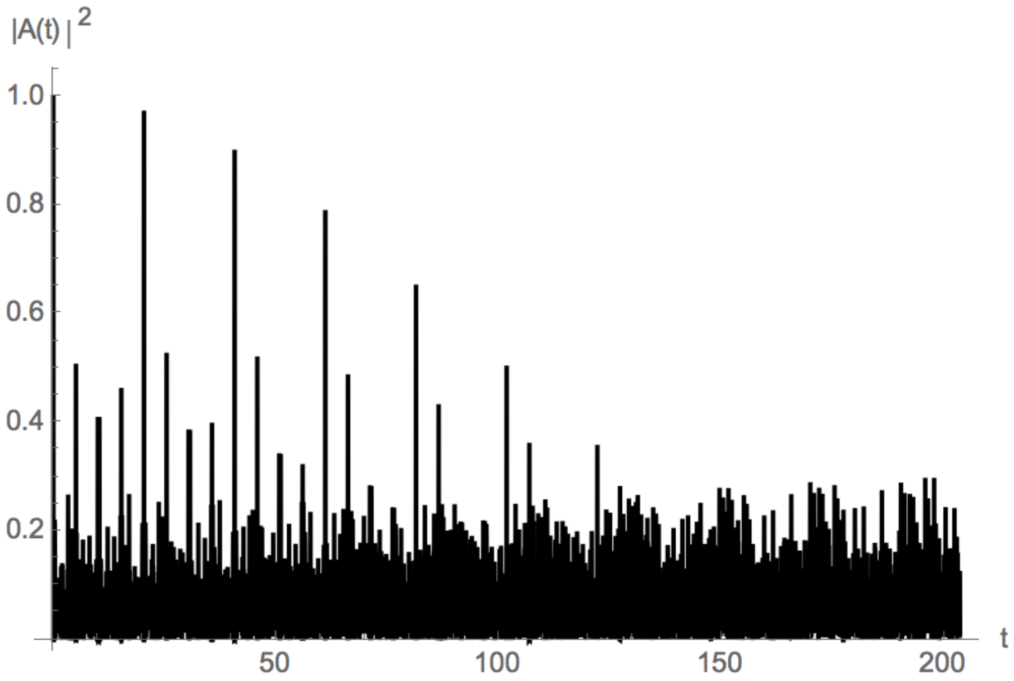
Wave Packet Revival Decay

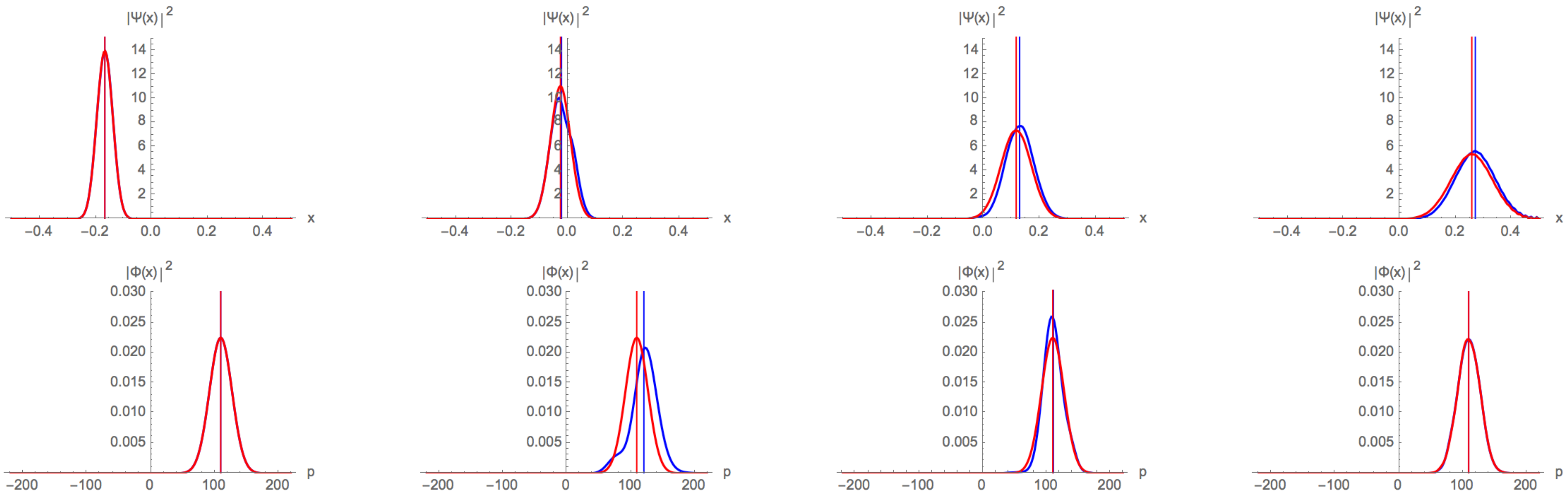




- First 10 revival periods
- Rectangular Barrier: $V_0 = 0.5$ (left), $V_0 = 1$ (right).

Example: Reflectionless Well

- Defined by a sech^2 potential function
- Total transmission for certain heights



Future Work

- Model supersymmetrical ISW
- Multiple barriers and wells
- 2-Dimensional Problems
- Use different basis potentials for other problems