PHYS 142: Assignment 2

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Question 1: Design an experiment to simulate the tunneling time in a double potential well.

For the potential I use the parameterization

$$V(x) = \alpha(x^2 - x_{min}^2)^2$$

where I choose $\alpha = .02$ and $x_{min} = 2.5$.

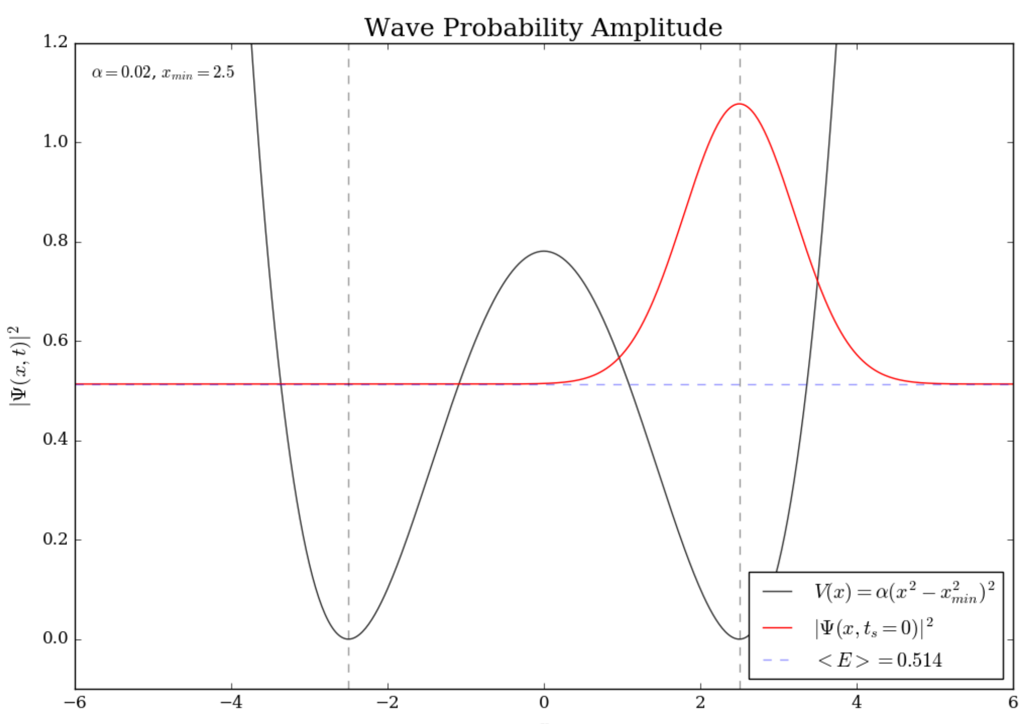
The initial condition is chosen to be the difference in the lowest two stationary stationary states for this potential:

$$|\psi_o\rangle = \frac{1}{\sqrt{2}}(|\phi_o\rangle - |\phi_1\rangle)$$

where $|\phi_o\rangle$ is the ground state and $|\phi_1\rangle$ is the first excited state. For simplification I use a gaussian approximation for the initial condition, choosing $\gamma = 1$ and the center to be at the the minimum of the potential well, x_{min}:

$$\psi_o(x) = e^{-\frac{\gamma}{2}(x-x_{min})^2}$$

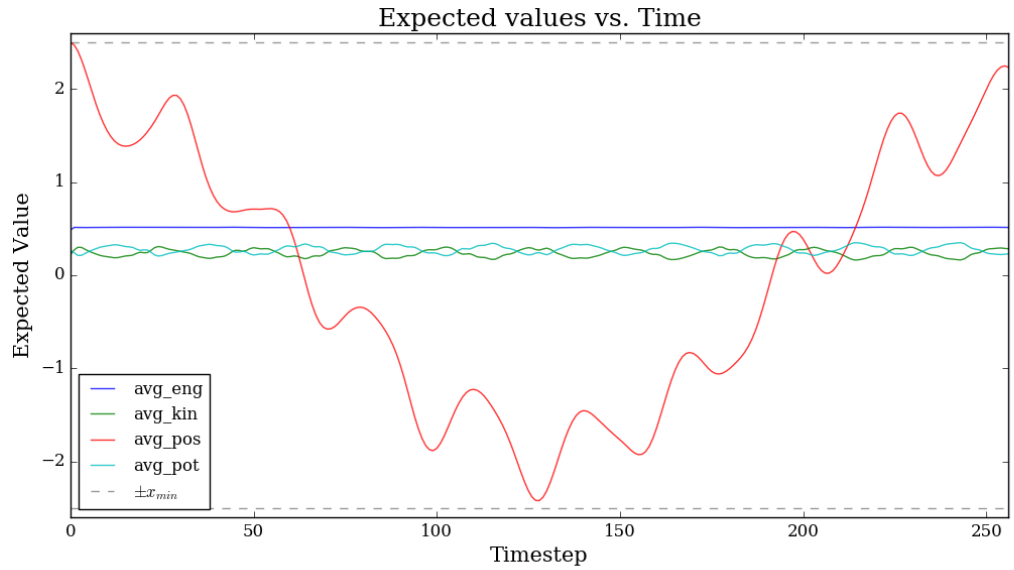
Plot of the normalized initial condition and double potential well:



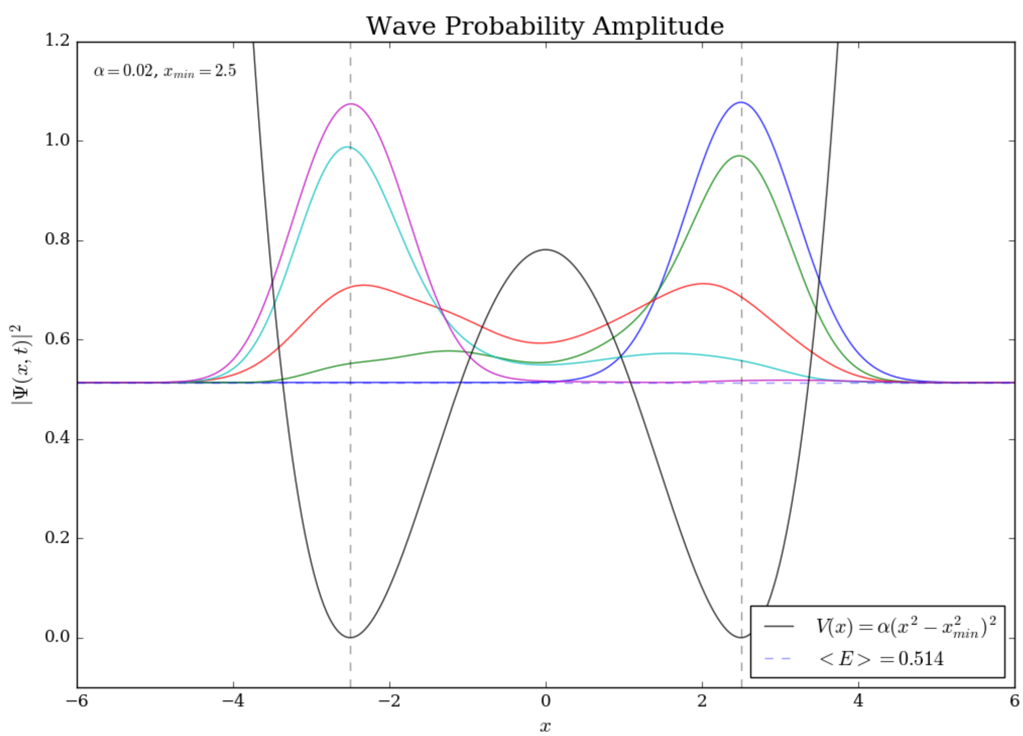
The tunneling time for this experiment can be numerically estimated as the time it takes the expected position to go from x_{min} to $-x_{min}$.

Question 2: Demonstrate how the wave function tunnels through the barrier with time.

Solution: Evolution of the wave function was taken over 256 time steps, with classical period of oscillation $T_o = 2\pi$, propagator caluclations in $T = \frac{T_o}{16}$ intervals, and N=8 time slices in each ($\Delta t = \frac{T_o}{128}$).



Snapshots of the wave function at timesteps $t_s = 0, 32, 64, 96, 128$:



Since the expected position reaches a minimum at $t_s = 128$, the tunneling time for this experiment is $t_s = 128$. For animation, see plots/wave_evolution.gif.

Question 3: Determine an approximate relation between the tunneling gap and tunneling time.

Solution:
Let ϕ_o and ϕ_1 be the two lowest energy stationary states for the solution for the double potential well, and let us define $|a\rangle$ and $|b\rangle$ as the normalized sum and difference of these two energy states:

$$|a\rangle = \frac{1}{\sqrt{2}}\left(|\phi_o\rangle + |\phi_o\rangle\right)$$
$$|b\rangle = \frac{1}{\sqrt{2}}\left(|\phi_o\rangle - |\phi_o\rangle\right)$$

where $|b\rangle$ looks like $t_s = 0$ and $|a\rangle$ looks like $t_s = 128$ in the last figure, and the tunneling time is the time it takes to get from $|b\rangle$ to $|a\rangle$.

$$\begin{aligned}
\langle b|e^{-iHt}|a\rangle &= \langle b|\frac{1}{\sqrt{2}}\left(e^{-iE_o t}|\phi_o\rangle + e^{-iE_1 t}|\phi_1\rangle\right) \\
&= \frac{1}{2}\left(e^{-iE_o t} - e^{-iE_1 t}\right) \\
||\langle b|e^{-iHt}|a\rangle|| &= \frac{1}{4}||1 - e^{-i(E_1 - E_o)t}||^2 \\
&= \frac{1}{2}\left[1 - \cos\left(\frac{(E_1 - E_o)t}{\hbar}\right)\right]
\end{aligned}$$

So $\frac{(E_1-E_o)t}{\hbar} = \omega\tau$ is the time period it takes the wave function to evolve between $|b\rangle$ to $|a\rangle$, where τ is the tunneling time. Thus as the tunneling gap $(E_1 - E_o)$ increases, the tunneling time decreases.

Question 4: For a free particle, show K(b,a) satisfies the Schrödinger Equation:

$$\frac{\hbar}{i}\frac{\partial K(b,a)}{\partial t_b} = \frac{-\hbar^2}{2m}\frac{\partial^2 K(b,a)}{\partial x_b^2}$$

where K(b,a) is:

$$K(b,a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}\, e^{\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}}$$

Solution:
For simplification, let $\alpha = \frac{m}{2i\hbar}$.

$$K(b,a) = \sqrt{\frac{\alpha}{\pi(t_b - t_a)}}\, e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}}$$

The partial derivatives for K(b,a) are:

$$\begin{aligned}
\frac{\partial K(b,a)}{\partial t_b} &= -\sqrt{\frac{\alpha}{\pi}}\left[\frac{1}{2(t_b - t_a)^{3/2}}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}} + \sqrt{\frac{\alpha}{\pi}}\left[-\frac{1}{2(t_b - t_a)^{1/2}}\right]\left[\frac{\alpha(x_b - x_a)^2}{(t_b - t_a)^2}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}} \\
&= \sqrt{\frac{\alpha}{\pi}}\left[-\frac{1}{2(t_b - t_a)^{3/2}} + \frac{\alpha(x_b - x_a)^2}{(t_b - t_a)^{5/2}}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}} \\
\frac{\partial K(b,a)}{\partial x_b} &= \sqrt{\frac{\alpha}{\pi}}\left[\frac{1}{(t_b - t_a)^{1/2}}\right]\left[\frac{-2\alpha(x_b - x_a)}{(t_b - t_a)}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}} \\
&= -\sqrt{\frac{\alpha}{\pi}}\left[\frac{2\alpha(x_b - x_a)}{(t_b - t_a)^{3/2}}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}} \\
\frac{\partial^2 K(b,a)}{\partial x_b^2} &= -\sqrt{\frac{\alpha}{\pi}}\left[\frac{2\alpha}{(t_b - t_a)^{3/2}}\right]\left[1 - \frac{2\alpha(x_b - x_a)^2}{(t_b - t_a)}\right] e^{\frac{-\alpha(x_b - x_a)^2}{(t_b - t_a)}}
\end{aligned}$$

Plugging in $\frac{\partial K(b,a)}{\partial t_b}$ and $\frac{\partial^2 K(b,a)}{\partial x_b^2}$ to the Schrödinger Equation:

$$\begin{aligned}
\sqrt{\frac{\alpha}{\pi}}\left[-\frac{1}{2(t_b-t_a)^{3/2}}+\frac{\alpha(x_b-x_a)^2}{(t_b-t_a)^{5/2}}\right]e^{\frac{-\alpha(x_b-x_a)^2}{(t_b-t_a)}} &= -\sqrt{\frac{\alpha}{\pi}}\left(\frac{-i\hbar}{2m}\right)\left[\frac{2\alpha}{(t_b-t_a)^{3/2}}\right]\left[1-\frac{2\alpha(x_b-x_a)^2}{(t_b-t_a)}\right]e^{\frac{-\alpha(x_b-x_a)^2}{(t_b-t_a)}} \\
\left[-\frac{1}{2(t_b-t_a)^{3/2}}+\frac{\alpha(x_b-x_a)^2}{(t_b-t_a)^{5/2}}\right] &= \left(\frac{-i\hbar}{2m}\right)\left[\frac{2\alpha}{(t_b-t_a)^{3/2}}\right]\left[1-\frac{2\alpha(x_b-x_a)^2}{(t_b-t_a)}\right] \\
\left[-\frac{1}{2(t_b-t_a)}+\frac{\alpha(x_b-x_a)^2}{(t_b-t_a)^{2}}\right] &= \left(\frac{-i\hbar}{2m}\right)\left[\frac{2\alpha}{(t_b-t_a)}\right]\left[1-\frac{2\alpha(x_b-x_a)^2}{(t_b-t_a)}\right] \\
&= \underbrace{\left(\frac{2i\hbar}{m}\right)\alpha}_{1}\left[-\frac{1}{2(t_b-t_a)}+\frac{\alpha(x_b-x_a)^2}{(t_b-t_a)^2}\right] \\
&= \left[-\frac{1}{2(t_b-t_a)}+\frac{\alpha(x_b-x_a)^2}{(t_b-t_a)^2}\right]
\end{aligned}$$

Hence K(b,a) satisfies the Schrödinger Equation for a free particle (V(x) = 0).

Question 5: Using the equation for K show that the wavefunction

$$\psi(x',t')=\int_{-\infty}^{\infty}K(x',t',x,t)\psi(x,t)dx$$

satisfies the Schrödinger equation.

Solution:
Using the action for a free particle $S_{cl}=\int_t^{t'}dt\frac{1}{2}m\dot{x}(t)^2$, K becomes:

$$K(x',t',x,t)=\sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{im(x'-x)^2}{2\hbar(t'-t)}}$$

as stated in the lecture notes. Let $\beta=\sqrt{\frac{m}{2\pi i\hbar t}}$, $\gamma=x'-x$, and $\alpha=t'-t$. So K can be rewritten as

$$K=\beta e^{\frac{im}{2\alpha}\gamma^2}$$

Considering an initial condition $|\psi(x,t)\rangle$ evolved by some small amount of time α later, the wave function can then be described as

$$\psi(x,t+\alpha)=\int_{-\infty}^{\infty}K(x+\gamma,t+\alpha,x,t)\psi(x+\gamma,t)d\gamma$$

Taylor expanding the equation for ψ gives us

$$\psi(x+\gamma,t)=\psi(x,t)+\gamma\frac{d\psi(x,t)}{dx}+\frac{1}{2}\gamma^2\frac{d^2\psi(x,t)}{dx^2}+...$$

$$\psi(x,t+\alpha)\approx\beta\int_{-\infty}^{\infty}d\gamma\left[\psi(x,t)+\underbrace{\gamma\frac{d\psi(x,t)}{dx}}_{0\Rightarrow\text{odd function}}+\frac{1}{2}\gamma^2\frac{d^2\psi(x,t)}{dx^2}\right]e^{\frac{im}{2\alpha}\gamma^2}$$

Evaluating the gaussian integral gives

$$\psi(x,t+\alpha)\approx\underbrace{\beta\sqrt{\frac{2\hbar\pi\alpha}{im}}}_{1}\left[\psi+\frac{1}{2}\gamma^2\frac{d^2\psi}{dx^2}\right]=\left[1-\frac{\alpha}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\right]\psi(x,t)$$

For the limit as $\alpha \to 0$ we have
$$\frac{d\psi(x,t)}{dt} = \frac{\psi(x,t+\alpha) - \psi(x,t)}{\alpha}$$
Hence
$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\psi(x,t)$$

Question 6: For a harmonic oscillator, show that the exponent of the propagator matrix has the form
$$S_{cl} = \frac{m\omega}{2\sin\omega T}\left[(x_a^2 + x_b^2)\cos\omega T - 2x_a x_b\right]$$

Solution:
Solving for the action for the harmonic oscillator:
$$S_{cl} = \int_{t_a}^{t_b} \mathcal{L}(x,\dot{x},t)dt = \frac{m}{2}\int_{t_a}^{t_b}(\dot{x}^2 - \omega^2 x^2)dt$$
For the first part of the integral
$$\int_{t_a}^{t_b}\dot{x}^2 dt = \int_{t_a}^{t_b}\dot{x}\dot{x}dt = x\dot{x}\Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} x\ddot{x}dt = x\dot{x}\Big|_{t_a}^{t_b} - \omega^2\int_{t_a}^{t_b} x^2 dt$$
using $\ddot{x} = -\omega^2 x$.
$$\begin{aligned} S_{cl} &= \frac{m}{2}\left[x\dot{x}\Big|_{t_a}^{t_b} + \omega^2\int_{t_a}^{t_b} x^2 dt - \omega^2\int_{t_a}^{t_b} x^2 dt\right] = \frac{m}{2}\left[x\dot{x}\right]_{t_a}^{t_b} \\ &= \frac{m}{2}\left[x(t_b)\dot{x}(t_b) - x(t_a)\dot{x}(t_a)\right] \end{aligned}$$
Now we need to plug in $x(t)$ and $\dot{x}(t)$ for $t_a = 0$ and $t_b = T$. Recall that a harmonic oscillator m$\ddot{x} = -kx$ has the general solution
$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$
where $\omega = \sqrt{k/m}$. Applying boundary condtions $x(0) = x_a$ and $x(T) = x_b$:
$$x(0) = B = x_a$$
$$x(T) = A\sin(\omega T) + x_a\cos(\omega T) = x_b$$
we determine the solutions for the constants:
$$A = \frac{x_b - x_a\cos(\omega T)}{\sin(\omega T)}$$
$$B = x_a$$
So the particular solution for x is:
$$\begin{aligned} x(t) &= \left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\sin\omega T + x_a\cos\omega T \\ \dot{x}(t) &= \left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\omega\cos\omega t - x_a\omega\sin\omega t \end{aligned}$$

Now plugging in $t_a = 0$ and $t_b = T$ we get:

$$
\begin{aligned}
x(0) &= x_a \\
x(T) &= x_b \\
\dot{x}(0) &= \left(\frac{x_b - x_a \cos\omega T}{\sin\omega T}\right)\omega \\
\dot{x}(T) &= \left(\frac{x_b - x_a \cos\omega T}{\sin\omega T}\right)\omega\cos\omega T - x_a\omega\sin\omega T
\end{aligned}
$$

Finally, the action can be reduced to the solution above:

$$
\begin{aligned}
S_{cl} &= \frac{m}{2}\omega\left[x_b\left(\frac{x_b - x_a \cos\omega T}{\sin\omega T}\right)\cos\omega T - x_b x_a \sin\omega T - x_a x_b\left(\frac{x_b - x_a \cos\omega T}{\sin\omega T}\right)\right] \\
&= \frac{m\omega}{2\sin\omega T}\left[x_b^2\cos\omega T - x_a x_b\cos^2\omega T - x_a x_b \sin^2\omega T - x_a x_b + x_a^2\cos\omega T\right] \\
S_{cl} &= \frac{m\omega}{2\sin\omega T}\left[(x_a^2 + x_b^2)\cos\omega T - 2x_a x_b\right]
\end{aligned}
$$