Policies

- You are free to collaborate on all of the problems, subject to the collaboration policy stated in the syllabus.
- You should submit all code used in the homework. You are free to use Python, C/C++, Julia, or any other code **within reason** as long as you comment your code such that the TA can follow along and run it without any issues.
- Please submit your report as a single .pdf file to Gradescope under "Assignment 2" or "Assignment 2 Corrections". **In the report, include any images generated by your code along with your answers to the questions.** For instructions specifically pertaining to the Gradescope submission process, see `https://www.gradescope.com/get_started#student-submission`.
- Please submit your code as a .zip archive to Gradescope under "Assignment 2 Code" or "Assignment 2 Code Corrections". The .zip file should contain all of your source code files.

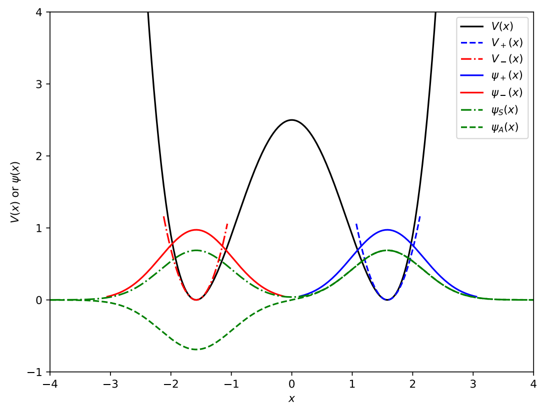
1 Tunneling in the Double Potential Well [40 Points]

Relevant materials: Week 4 lectures

Consider the double potential well,

$$V(x) = \alpha x^4 - 2x^2 + + \frac{1}{\alpha} \tag{1}$$

where x is the position of the particle, and we set $m = \hbar = 1$. For parts 1A, 1B, and 1C, you may set $\alpha = 0.4$. For the last part, you will need to vary α. The minima of the potential are at $x^2_{\text{min}} = \pm\frac{1}{\alpha}$ and the barrier height is $V(0) = \frac{1}{\alpha}$. The potential is shown in the figure below.



As discussed in lecture 9, we can approximate the potential by a harmonic potential near the minima.

$$V_+(x) = 4(x - x_{\text{min}})^2 \tag{2}$$
$$V_-(x) = 4(x + x_{\text{min}})^2, \tag{3}$$

which implies $\omega = 2\sqrt{2}$. The ground state wave functions for those approximate potential wells are

$$\psi_+(x) = \left(\frac{\omega}{\pi}\right)^{1/4} \exp\left(-\frac{\omega}{2}(x - x_{\text{min}})^2\right) \tag{4}$$
$$\psi_-(x) = \left(\frac{\omega}{\pi}\right)^{1/4} \exp\left(-\frac{\omega}{2}(x + x_{\text{min}})^2\right) \tag{5}$$

We can approximate the ground state and first excited state as the symmetric and antisymmetric combinations of these wave functions, respectively.

$$\psi_0(x) \approx \psi_S(x) = \frac{1}{\sqrt{2}}\left(\psi_+(x) + \psi_-(x)\right) \tag{6}$$

$$\psi_1(x) \approx \psi_A(x) = \frac{1}{\sqrt{2}}\left(\psi_+(x) - \psi_-(x)\right) \tag{7}$$

The energy gap between the ground state and first excited state is $\Delta E = E_1 - E_0$.

Problem A [10 points]: Demonstrate tunneling between the two wells using the Feynman path integral. Start with the particle in the right well

$$\psi(x, 0) = \psi_+(x), \tag{8}$$

and evolve the wave function at each time step using the elementary propagator.

Numerically, you may use discretization parameters similar to Assignment 1: $\epsilon = \Delta t = \pi/128$, $x_0 = -4$, $x_{N_D} = +4$, and $N_D = 600$. You will have to simulate a long enough period $T > t_{\text{tunnel}}$ that is longer than the tunneling time. As a reminder, the tunneling time is defined as the time it takes for the particle to reach the left well.

Plot the mean position $\langle x \rangle$ as a function of time t. How can you estimate the tunneling time t_{tunnel} from this plot?

Hint: *You may approximate the propagator as*

$$\tilde{\mathcal{K}}(x_b, \epsilon; x_a, 0) \sim \exp\left(i\left(\frac{1}{2}\frac{(x_b - x_a)^2}{\epsilon} - V\left(\frac{x_a + x_b}{2}\right)\epsilon\right)\right), \tag{9}$$

where x_a and x_b are the initial and final positions, respectively, and ϵ is the time step. Note, we lack the normalization factor in this approximation so you will need to normalize the wave function at each time step

$$\psi(x, t) \leftarrow \frac{\psi(x, t)}{\sqrt{\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx}}. \tag{10}$$

Problem B [10 points]: Estimate the energy gap ΔE between the ground state and first excited state.

Hint: *To estimate E_0 and E_1, you can use the expectation value of the Hamiltonian operator,*

$$E_0 \approx \int \psi_{\mathrm{S}}^*(x)\hat{H}\psi_{\mathrm{S}}(x)dx, \tag{11}$$

$$E_1 \approx \int \psi_{\mathrm{A}}^*(x)\hat{H}\psi_{\mathrm{A}}(x)dx, \tag{12}$$

where $\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$. This method may not agree with the numerical result shared in lecture 9.

Problem C [10 points]: Animate the evolution of the real and imaginary parts of the wave function $\psi(x, t)$ and the probability $|\psi(x, t)|^2$ as a function of time t over a period $T > t_{\text{tunnel}}$ and save it as a `.gif` or `.mp4` file.

Problem D [10 points]: Determine an approximate relationship between the tunneling time t_{tunnel} and the energy gap ΔE between the ground state and first excited state.

Hint: *Vary α and calculate the energy gap ΔE and tunneling time t_{tunnel} for each α as you did in parts 1A and 1B.*