Computational Physics II — UCSD PHYS 142/242
Assignment 1 — Due: Friday, January 24, 2025, 8:00pm
Corrections due: Wednesday, January 29, 2025, 8:00pm

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 1" or "Assignment 1 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 1 Code" or "Assignment 1 Code Corrections". The .zip file should contain all of your source code files.

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1 Harmonic Oscillator Path Integral [50 Points]

Relevant materials: Week 1 lectures

Consider the harmonic oscillator with Lagrangian,

$$L(x, \dot{x}) = K(\dot{x}) - V(x) = \frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2, \tag{1}$$

where x is the position of the oscillator and $\dot{x}$ is its velocity. Note this is expressed in units where the mass $m = 1$ and angular frequency $\omega = 1$, so the classical oscillator period $T_0 = 2\pi$. For this problem, you can work in units $m = \omega = \hbar = 1$, so the classical oscillator period $T_0 = 2\pi$.

We will use the discrete approximation to the path integral for the harmonic oscillator, where the time step is $\epsilon = \Delta t = T_0/128$. The electron position is also discretized into $N_D + 1$ possible points, $x_0 = -4, x_1, x_2, \ldots, x_{N_D} = +4$, where $N_D = 600$. The initial probability amplitude (sometimes called the wave-function) of the electron is a Gaussian centered at x_{start},

$$\Psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha}{2}(x - x_{\text{start}})^2\right), \tag{2}$$

where $\alpha = 2$ and $x_{\text{start}} = 3/4$. The amplitude can be represented as a vector ψ_0 with $N_D + 1$ components, $\psi_0 = (\Psi_0(x_0), \Psi_0(x_1), \ldots, \Psi_0(x_{N_D}))$. We recommend using complex NumPy arrays, e.g. `np.array([1+2j, 3+4j])` and `np.zeros((10, 10), dtype=np.complex64))`.

Problem A [10 points]: Calculate the propagator matrix $\mathcal{K}_{8\epsilon}$ for a time period $T_0/16 = 8\epsilon$ (8 time steps) built from the elementary propagator matrix $\mathcal{K}_\epsilon$ for a single $\epsilon = \Delta t = T_0/128$ time step.

Recall we gave the general form of the propagator in lecture as

$$\mathcal{K}(x_b, t_b; x_a, t_a) = \left(\frac{m\omega}{2\pi i\hbar \sin(\omega(t_b - t_a))}\right)^{1/2} \exp\left(\frac{im\omega}{2\hbar \sin(\omega(t_b - t_a))}[(x_a^2 + x_b^2)\cos(\omega(t_b - t_a)) - 2x_a x_b]\right) \tag{3}$$

where x_a and x_b are the initial and final positions, respectively, and t_a and t_b are the initial and final times, respectively.

Use NumPy to print the matrix (default truncated output) and copy the (truncated) output into your report. Note by default if `K_8eps` is a large NumPy array, `print(K_8eps)` prints the first 3 and last 3 elements along each axis.

Hint: *The elementary propagator matrix $\mathcal{K}_\epsilon$ is an $(N_D + 1) \times (N_D + 1)$-dimensional complex matrix that time evolves the state ψ by one time step, and*

$$\mathcal{K}_t = (\Delta x)^{N-1}\mathcal{K}_\epsilon^N \tag{4}$$

time evolves the state by N time steps, where $N\epsilon = t$.

Problem B [10 points]: Evolve the probability amplitude of the electron with $T_0/16$ time steps and measure its mean position $\langle x \rangle$ as a function of time. Make a graph showing $\langle x \rangle$ versus time t. Label the axes.

Hint: *Recall*

$$\langle x \rangle = \int x P_t(x) dx \tag{5}$$

where $P_t(x) = |\Psi_t(x)|^2$ *is the probability density function at time* t.

Problem C [10 points]: Calculate the mean energy $\langle E \rangle$, mean kinetic energy $\langle K \rangle$, and mean potential energy $\langle V \rangle$ as a function of time. Make one graph showing all three with a legend labeling them.

Hint: *Recall* $E = K + V$ *and for the mean value of* V, *we have*

$$\langle V \rangle = \int \frac{1}{2} x^2 P_t(x) dx. \tag{6}$$

For the mean value of K, there are a few different ways to calculate it. Edit: As discussed in lecture, we will use another form of $\langle K \rangle$, *which is simpler, assuming we know some quantum mechanics*

$$\langle K \rangle = \int \Psi_t^*(x) \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial x^2} \right) \Psi_t(x) dx = \frac{\hbar^2}{2} \int \left| \frac{\partial \Psi_t}{\partial x} \right|^2 dx \tag{7}$$

Problem D [10 points]: Calculate the time evolution of the probability amplitude at times $mT_0/16$ for $m = 1, \ldots, 8$. Make a single graph showing the probability amplitudes initially and at those eight times, with a legend labeling them. Optional: Superimpose the potential $V(x)$ and amplitudes at those eight times on the same graph as the probability density function $P_t(x) = |\Psi_t(x)|^2$ at those eight times.

Problem E [10 points]: Animate the time evolution of the probability amplitude over the full time period $T_0 = 2\pi$. Each frame should correspond to one time step of $\epsilon = T_0/128$ (so $128 + 1$ frames total). Save the animation as a `.gif` or `.mp4` file.