Problem Set 3

Particle in a Box

1. Prove that $\Psi_n(x)$ is an eigenfunction of the Hamiltonian ($\hat{H}$). What are the eigenvalues?

2. What is the expectation value of the position of the particle in a box, $\langle \hat{x} \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

3. What is the expectation value of the square of the position of the particle in a box, $\langle \hat{x}^2 \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

4. What is the expectation value of the momentum operator of the particle in a box, $\langle \hat{p}_x \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

5. What is the expectation value of the square of the momentum operator of the particle in a box, $\langle \hat{p}_x^2 \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

6. What is the expectation value of the potential energy operator of the particle in a box, $\langle \hat{V} \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

7. What is the expectation value of the kinetic energy operator of the particle in a box, $\langle \hat{T} \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

8. What is the expectation value of the Hamiltonian operator (total energy operator) of the particle in a box, $\langle \hat{H} \rangle$, corresponding to the energy eigenfunction, $\Psi_n(x)$?

9. Prove that the particle in a box eigenfunctions are orthonormal, meaning:

   $$\int_{-\infty}^{\infty} \Psi_m^*(x)\Psi_n(x)\mathrm{d}x = \delta_{mn},$$

   where δ_{mn} is the Kronecker delta.

10. Graph the lowest few particle in a box wavefunctions, $\Psi_n(x)$, as a function of x.

11. Graph the square of lowest few particle in a box wavefunctions, $|\Psi_n(x)|^2$, as a function of x.

Some Potentially Useful Equations

Energy eigenfunctions:	$\Psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right),\ n = 1, 2, 3, \ldots & \text{if } 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}$
Energy eigenvalues:	$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2},\ n = 1, 2, 3, \ldots$
Expectation value:	$\langle \hat{A} \rangle = \frac{\int_{-\infty}^{\infty} \Psi^*(x)\hat{A}\Psi(x)\mathrm{d}x}{\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\mathrm{d}x}$
Position operator:	$\hat{x} = x$
Momentum operator:	$\hat{p}_x = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$
Kinetic energy operator:	$\hat{T} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$
Potential energy operator:	$\hat{V} = V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$
Hamiltonian operator:	$\hat{H} = \hat{T} + \hat{V}$
Kronecker delta:	$\delta_{mn} = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$