Problem Set 4

Operators and Dirac Notation

1. Determine the matrix elements of the identity operator in a basis of particle in a box energy eigenfunctions. $I_{ij} = \langle \Psi_i | \hat{I} | \Psi_j \rangle$

2. Determine the matrix elements of the position operator in a basis of particle in a box energy eigenfunctions. $X_{ij} = \langle \Psi_i | \hat{x} | \Psi_j \rangle$

3. Determine the matrix elements of the square of the position operator in a basis of particle in a box energy eigenfunctions. $Y_{ij} = \langle \Psi_i | \hat{x}^2 | \Psi_j \rangle$

4. Determine the matrix elements of the momentum operator in a basis of particle in a box energy eigenfunctions. $P_{ij} = \langle \Psi_i | \hat{p}_x | \Psi_j \rangle$

5. Determine the matrix elements of the square of the momentum operator in a basis of particle in a box energy eigenfunctions. $Q_{ij} = \langle \Psi_i | \hat{p}_x^2 | \Psi_j \rangle$

6. Determine the matrix elements of the kinetic energy operator in a basis of particle in a box energy eigenfunctions. $T_{ij} = \langle \Psi_i | \hat{T} | \Psi_j \rangle$

7. Determine the matrix elements of the Hamiltonian (total energy) operator in a basis of particle in a box energy eigenfunctions. $H_{ij} = \langle \Psi_i | \hat{H} | \Psi_j \rangle$

8. Determine the commutator of the position and momentum operators. $[\hat{x}, \hat{p}_x] = ?$

9. Determine the commutator of the square of the position and momentum operators. $[\hat{x}^2, \hat{p}_x] = ?$

10. Determine the commutator of the position and square of the momentum operators. $[\hat{x}, \hat{p}_x^2] = ?$

11. Determine the commutator of the square of the position and square of the momentum operators. $[\hat{x}^2, \hat{p}_x^2] = ?$

12. Determine the commutator of the position and kinetic energy operators. $[\hat{x}, \hat{T}] = ?$

13. Determine the commutator of the momentum and kinetic energy operators. $[\hat{p}_x, \hat{T}] = ?$

14. Show that, $\Delta\hat{x}\Delta\hat{p}_x \geq \frac{\hbar}{2}$, in general, using the commutator of position and momentum.

15. Show that, $\Delta\hat{x}\Delta\hat{p}_x \geq \frac{\hbar}{2}$, for a particle in a box energy eigenfunction using the RMSD of the position and momentum operators.

For each of the superposition states,

$$\Phi_1(x) = N_1\left(\Psi_1(x) + \Psi_2(x)\right)$$
$$\Phi_2(x) = N_2\left(3\Psi_1(x) - \Psi_2(x)\right)$$
$$\Phi_3(x) = N_3\left(2\Psi_1(x) + \sqrt{2}\Psi_2(x) + \sqrt{3}\Psi_3(x)\right)$$
$$\Phi_4(x) = N_4\left(\Psi_1(x) + 0.7\Psi_2(x) + 0.4\Psi_3(x)\right)$$
$$\Phi_5(x) = N_5\left(3\Psi_1(x) + \Psi_2(x) + 2\Psi_3(x) + \sqrt{2}\Psi_4(x)\right)$$

do the following.

1. Normalize the superposition state wavefunction, $\Phi(x)$.
2. Calculate the expectation value of the position operator, $\langle \hat{x} \rangle$, corresponding to the following particle in a box superposition state, $\Phi(x)$,
3. Calculate the expectation value of the square of the position operator, $\langle \hat{x}^2 \rangle$, corresponding to the following particle in a box superposition state, $\Phi(x)$,
4. Calculate the expectation value of the momentum operator, $\langle \hat{p}_x \rangle$, corresponding to the following particle in a box superposition state, $\Phi(x)$,
5. Calculate the expectation value of the square of the momentum operator, $\langle \hat{p}_x^2 \rangle$, corresponding to the following particle in a box superposition state, $\Phi(x)$,
6. Calculate the expectation value of the Hamiltonian (total energy) operator, $\langle \hat{H} \rangle$, corresponding to the following particle in a box superposition state, $\Phi(x)$,
7. Graph the superposition state wavefunction, $\Phi(x)$, as a function of x.
8. Graph the square of the superposition state wavefunction, $|\Phi(x)|^2$, 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:	$\delta_{mn} = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$
Ket:	$\vert n\rangle = \Psi_n(x)$
Bra:	$\langle n\vert = \Psi_n^*(x)$
Bra-ket:	$\langle m\vert\hat{A}\vert n\rangle = \int_{-\infty}^{\infty} \Psi_m^*(x)\hat{A}\Psi_n(x)\mathrm{d}x$
Matrix form of an operator	$A_{mn} = \langle \Psi_m\vert\hat{A}\vert\Psi_n\rangle = \int_{-\infty}^{\infty} \Psi_m^*(x)\hat{A}\Psi_n(x)\mathrm{d}x$
Resolution of the identity	$\hat{I} = \sum_{n=1}^{\infty} \vert\Psi_n\rangle\langle\Psi_n\vert$
Commutator:	$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Root-mean-square deviation:	$\Delta\hat{A} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$
Heisenberg uncertainty principle	$\Delta A \Delta B \geq \frac{1}{2}\vert\langle[\hat{A}, \hat{B}]\rangle\vert$