

22. A system is described by a Hamiltonian \mathcal{H} and by a second observable Ω where

$$\mathcal{H} = \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \quad \text{and} \quad \Omega = \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{for which} \quad |\psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix}.$$

- (a) Show that \mathcal{H} and Ω commute, *i.e.*, show that $[\mathcal{H}, \Omega] = 0$.
- (b) If the energy is measured, what results can be obtained and with what probabilities will these results be obtained? If Ω is measured, what results can be obtained and with what probabilities will these results be obtained?
- (c) Calculate the expectation values of the Hamiltonian $\langle \mathcal{H} \rangle$ and the Omega operator $\langle \Omega \rangle$ using the initial state vector. Then show that your expectation values agree with your part (b) probabilities and eigenvalues by using the general expression $\langle \Omega \rangle = \sum_i P(\omega_i) \omega_i$.
- (d) Calculate the time-dependent state vector $|\psi(t)\rangle$ in the energy eigenbasis.
- (e) Transform to the basis that simultaneously diagonalizes \mathcal{H} and Ω . Calculate the new form of the initial state vector $|\psi(0)\rangle$ in this diagonal basis.
- (f) Repeat parts (b) and (c) in the diagonal basis and compare your calculations.
- (g) Calculate the time evolution of the state vector in the diagonal basis. Calculate the possibilities and probabilities of measuring the energy, E_i , and the “omega-ness,” ω_j , at time t .
- (h) Describe the state vector immediately after each measurement and the result of each measurement if you do a gedanken experiment by alternating \mathcal{H} and Ω measurements starting with an \mathcal{H} measurement, *i.e.*, you measure $\mathcal{H}, \Omega, \mathcal{H}, \Omega, \mathcal{H}, \dots$, for the two possible cases:
 - 1) You find 5 when you first measure \mathcal{H} .
 - 2) You find 3 when you first measure \mathcal{H} .
- (i) Explain how the two-measurement process removes the degeneracy in \mathcal{H} .

This problem is a reminder that the members of a complex linear vector space are complex numbers. While the mathematical mechanics is likely clearest when components and elements are from the subset of real numbers, the development is incomplete if calculations are devoid of imaginary numbers. You should find that \mathcal{H} is degenerate so a second operator that commutes with \mathcal{H} , like Ω , is required to uniquely determine the state vector after a measurement involving the degenerate eigenvalue of \mathcal{H} . Together, \mathcal{H} and Ω form a complete set of commuting observables. These are the same operators used in problem 39 in part 2 of chapter 1.

These operators commute. Solve the eigenvalue/eigenvector problem for the non-degenerate operator Ω first so that you can take advantage of the common eigenbasis and use its eigenvectors in the solution of the eigenvalue/eigenvector problem for \mathcal{H} . You should find

$$|\omega = 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \quad |\omega = 1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad |\omega = 2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \quad \text{and}$$

$$|E_1 = 3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \quad |E_2 = 3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad |E = 5\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}.$$

Remember to conjugate when forming bras and remember also to transform the state vector in part (e) as $\mathcal{U}^\dagger |\psi\rangle$ when preparing to do calculations in the diagonal basis.

(a) The Hermitian operators \mathcal{H} and Ω commute, because

$$\begin{aligned} [\mathcal{H}, \Omega] &= \mathcal{H}\Omega - \Omega\mathcal{H} = \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \\ &= \begin{pmatrix} 4+1 & -4i-i & 0 \\ i+4i & 1+4 & 0 \\ 0 & 0 & 3 \end{pmatrix} - \begin{pmatrix} 4+1 & -i-4i & 0 \\ 4i+i & 1+4 & 0 \\ 0 & 0 & 3 \end{pmatrix} = \begin{pmatrix} 5 & -5i & 0 \\ 5i & 5 & 0 \\ 0 & 0 & 3 \end{pmatrix} - \begin{pmatrix} 5 & -5i & 0 \\ 5i & 5 & 0 \\ 0 & 0 & 3 \end{pmatrix} = 0. \end{aligned}$$

(b) Calculate the eigenvalues of \mathcal{H} ,

$$\begin{aligned} \det(\mathcal{H} - \beta\mathcal{I}) &= \det \begin{pmatrix} 4-\beta & -i & 0 \\ i & 4-\beta & 0 \\ 0 & 0 & 3-\beta \end{pmatrix} \\ &= (4-\beta)^2(3-\beta) - (3-\beta) = 0 \Rightarrow (16-8\beta+\beta^2)(3-\beta) - 3 + \beta = 0 \\ &\Rightarrow 48 - 24\beta + 3\beta^2 - 16\beta + 8\beta^2 - \beta^3 - 3 + \beta = 0 \\ &\Rightarrow -\beta^3 + 11\beta^2 - 39\beta + 45 = 0 \Rightarrow \beta^3 - 11\beta^2 + 39\beta - 45 = 0 \\ &\Rightarrow (\beta-3)(\beta-3)(\beta-5) = 0 \Rightarrow \beta = 3, 3, 5 \text{ are the eigenvalues of } \mathcal{H}. \end{aligned}$$

\mathcal{H} is degenerate at $E_i = 3$, so examine Ω in the hope that it is not degenerate.

$$\begin{aligned} \det(\Omega - \omega\mathcal{I}) &= \det \begin{pmatrix} 1-\omega & -i & 0 \\ i & 1-\omega & 0 \\ 0 & 0 & 1-\omega \end{pmatrix} = (1-\omega)^3 - (1-\omega) = 0 \\ &\Rightarrow 1 - 3\omega + 3\omega^2 - \omega^3 - 1 + \omega = 0 \Rightarrow -\omega^3 + 3\omega^2 - 2\omega = 0 \\ &\Rightarrow \omega(\omega^2 - 3\omega + 2) = 0 \Rightarrow \omega(\omega-1)(\omega-2) = 0 \\ &\Rightarrow \omega = 0, 1, 2 \text{ are the eigenvalues of } \Omega. \Omega \text{ is not degenerate so has conventionally determined eigenvectors, so find the eigenvectors of the non-degenerate operator first.} \end{aligned}$$

$$\omega = 0 \Rightarrow \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{lcl} a - bi & = & 0 \\ ai + b & = & 0 \\ c & = & 0 \end{array} \Rightarrow \begin{array}{lcl} b & = & -ai \\ b & = & -ai \\ c & = & 0 \end{array}$$

$$\Rightarrow |\omega = 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \text{ letting } a = 1 \text{ and normalizing. Next}$$

$$\omega = 1 \Rightarrow \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 1 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{lcl} a - bi & = & a \\ ai + b & = & b \\ c & = & c \end{array} \Rightarrow \begin{array}{lcl} b & = & 0 \\ a & = & 0 \\ c & = & c \end{array}$$

$$\Rightarrow |\omega = 1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \text{ letting } c = 1. \text{ This is already normalized. Then}$$

$$\omega = 2 \Rightarrow \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 2 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{lcl} a - bi & = & 2a \\ ai + b & = & 2b \\ c & = & 2c \end{array} \Rightarrow \begin{array}{lcl} b & = & ai \\ ai & = & b \\ c & = & 0 \end{array}$$

$$\Rightarrow |\omega = 2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \text{ when normalized if } a = 1. \text{ The non-degenerate eigenvalue of } \mathcal{H} \text{ is}$$

$$E = 5 \Rightarrow \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 5 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{lcl} 4a - bi & = & 5a \\ ai + 4b & = & 5b \\ 3c & = & 5c \end{array} \Rightarrow \begin{array}{lcl} b & = & ai \\ ai & = & b \\ c & = & 0 \end{array}$$

$$\Rightarrow |E = 5\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \text{ letting } a = 1 \text{ and normalizing. For } E = 3,$$

$$\begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 3 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{lcl} 4a - bi & = & 3a \\ ai + 4b & = & 3b \\ 3c & = & 3c \end{array} \Rightarrow \begin{array}{lcl} b & = & -ai \\ b & = & -ai \\ c & = & c \end{array}$$

and we need two eigenvectors from this one set of equations that are orthogonal to each other and to $|E = 5\rangle$. Since Ω and \mathcal{H} commute, they have a common set of eigenvectors. Examining the eigenvectors of Ω , $|E = 5\rangle = |\omega = 2\rangle$, and $|\omega = 0\rangle$ and $|\omega = 1\rangle$ both satisfy the one set of equations corresponding to the eigenvalue $E = 3$, so choose

$$|E_1 = 3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \text{ and } |E_2 = 3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The possibilities of a measurement are the eigenvalues per postulate 3. Probabilities are

$$P(\omega = 0) = \left| (1, i, 0) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \right|^2 = \left| \frac{1}{2} (i) \right|^2 = \frac{1}{4} (-i)(i) = \frac{1}{4} = P(E_1 = 3),$$

$$P(\omega = 1) = \left| (0, 0, 1) \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{2} |1|^2 = \frac{1}{2} = P(E_2 = 3),$$

$$P(\omega = 2) = \left| (1, -i, 0) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \right|^2 = \left| \frac{1}{2} (i) \right|^2 = \frac{1}{4} (-i)(i) = \frac{1}{4} = P(E = 5),$$

(c) The $t = 0$ expectation values of \mathcal{H} and Ω are $\langle \psi(0) | \mathcal{A} | \psi(0) \rangle$, or

$$\langle \mathcal{H} \rangle = (-i, 0, 1) \frac{1}{\sqrt{2}} \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2} (-i, 0, 1) \begin{pmatrix} 4i \\ -1 \\ 3 \end{pmatrix} = \frac{1}{2} (4 + 3) = \frac{7}{2},$$

$$\langle \Omega \rangle = (-i, 0, 1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2} (-i, 0, 1) \begin{pmatrix} i \\ -1 \\ 1 \end{pmatrix} = \frac{1}{2} (1 + 1) = 1.$$

The sums of the products of the probabilities and the corresponding eigenvalues yield

$$\langle \mathcal{H} \rangle = \sum_i P(E_i) E_i = \frac{1}{4} (3) + \frac{1}{2} (3) + \frac{1}{4} (5) = \frac{3+6+5}{4} = \frac{14}{4} = \frac{7}{2},$$

$$\text{and } \langle \Omega \rangle = \sum_i P(\omega_i) \omega_i = \frac{1}{4} (0) + \frac{1}{2} (1) + \frac{1}{4} (2) = \frac{1}{2} + \frac{1}{2} = 1.$$

(d) Expanding the initial state in terms of the eigenvectors of \mathcal{H} ,

$$\begin{aligned} |\psi(0)\rangle &= \sum_j |j\rangle \langle j| \psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} (1, i, 0) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (0, 0, 1) \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} (1, -i, 0) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} \\ &= \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} (i) + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (1) + \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} (i) \\ &= \frac{1}{2\sqrt{2}} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \frac{1}{2\sqrt{2}} \begin{pmatrix} i \\ -1 \\ 0 \end{pmatrix}, \end{aligned}$$

$$\begin{aligned} \Rightarrow |\psi(t)\rangle &= \sum_j |j\rangle \langle j| \psi(0)\rangle e^{-iE_j t/\hbar} \\ &= \frac{1}{2\sqrt{2}} \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix} e^{-i3t/\hbar} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i3t/\hbar} + \frac{1}{2\sqrt{2}} \begin{pmatrix} i \\ -1 \\ 0 \end{pmatrix} e^{-i5t/\hbar} = \frac{1}{2\sqrt{2}} \begin{pmatrix} ie^{-i3t/\hbar} + ie^{-i5t/\hbar} \\ e^{-i3t/\hbar} - e^{-i5t/\hbar} \\ 2e^{-i3t/\hbar} \end{pmatrix} \end{aligned}$$

(e) Per part (a), $[\Omega, \mathcal{H}] = [\mathcal{H}, \Omega] = 0$. The unitary matrix \mathcal{U} formed from the eigenvectors of \mathcal{H} by placing them from left to right in order of ascending eigenvalue is

$$\mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ -i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \Rightarrow \mathcal{U}^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix}.$$

The diagonal operators are

$$\begin{aligned} \mathcal{U}^\dagger \Omega \mathcal{U} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ -i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 2i \\ 0 & \sqrt{2} & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \end{aligned}$$

$$\begin{aligned}\mathcal{U}^\dagger \mathcal{H} \mathcal{U} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} \begin{pmatrix} 4 & -i & 0 \\ i & 4 & 0 \\ 0 & 0 & 3 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ -i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} \begin{pmatrix} 3 & 0 & 5 \\ -3i & 0 & 5i \\ 0 & 3\sqrt{2} & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 6 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 10 \end{pmatrix} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}.\end{aligned}$$

The state vector transforms $\mathcal{U}^\dagger |\psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix}.$

(f) Probabilities and expectation values using the diagonal basis are

$$\begin{aligned}P(\omega = 0) &= P(E_1 = 3) = \left| (1, 0, 0) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} \right|^2 = \frac{1}{4} |i|^2 = \frac{1}{4} (-i)(i) = \frac{1}{4}, \\ P(\omega = 1) &= P(E_2 = 3) = \left| (0, 1, 0) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} \right|^2 = \frac{1}{4} |\sqrt{2}|^2 = \frac{2}{4} = \frac{1}{2}, \\ P(\omega = 2) &= P(E = 5) = \left| (0, 0, 1) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} \right|^2 = \frac{1}{4} |i|^2 = \frac{1}{4} (-i)(i) = \frac{1}{4},\end{aligned}$$

$$\langle \Omega \rangle = (-i, \sqrt{2}, -i) \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} = \frac{1}{4} (-i, \sqrt{2}, -i) \begin{pmatrix} 0 \\ \sqrt{2} \\ 2i \end{pmatrix} = \frac{1}{4} (2 + 2) = 1,$$

$$\langle \mathcal{H} \rangle = (-i, \sqrt{2}, -i) \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} = \frac{1}{4} (-i, \sqrt{2}, -i) \begin{pmatrix} 3i \\ 3\sqrt{2} \\ 5i \end{pmatrix} = \frac{3 + 6 + 5}{4} = \frac{7}{2}.$$

All results are identical to those calculated previously.

(g) The time dependence of the state vector in the diagonal basis is

$$\begin{aligned}|\psi(t)\rangle &= \sum_j |j\rangle \langle j| \psi(0)\rangle e^{-iE_j t/\hbar} \\ &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1, 0, 0) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} e^{-i3t/\hbar} + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0, 1, 0) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} e^{-i3t/\hbar} \\ &\quad + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (0, 0, 1) \frac{1}{2} \begin{pmatrix} i \\ \sqrt{2} \\ i \end{pmatrix} e^{-i5t/\hbar} \\ &= \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (i) e^{-i3t/\hbar} + \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \sqrt{2} e^{-i3t/\hbar} + \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (i) e^{-i5t/\hbar} = \frac{1}{2} \begin{pmatrix} i e^{-i3t/\hbar} \\ \sqrt{2} e^{-i3t/\hbar} \\ i e^{-i5t/\hbar} \end{pmatrix}.\end{aligned}$$

The probabilities $P(E_1 = 3) = P(\omega = 0)$ are

$$\left| (1, 0, 0) \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} i e^{-i3t/\hbar} \right|^2 = \frac{1}{4} \left| i e^{-i3t/\hbar} \right|^2 = \frac{1}{4} (-i e^{+i3t/\hbar}) (i e^{-i3t/\hbar}) = \frac{1}{4}.$$

The probabilities $P(E_2 = 3) = P(\omega = 1)$ are

$$\left| (0, 1, 0) \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \sqrt{2} e^{-i3t/\hbar} \right|^2 = \frac{1}{4} \left| \sqrt{2} e^{-i3t/\hbar} \right|^2 = \frac{1}{4} (\sqrt{2} e^{+i3t/\hbar}) (\sqrt{2} e^{-i3t/\hbar}) = \frac{1}{2}.$$

The final set of probabilities $P(E = 5) = P(\omega = 2)$ are

$$\left| (0, 0, 1) \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} i e^{-i5t/\hbar} \right|^2 = \frac{1}{4} \left| i e^{-i5t/\hbar} \right|^2 = \frac{1}{4} (-i e^{+i5t/\hbar}) (i e^{-i5t/\hbar}) = \frac{1}{4},$$

identical to $t = 0$ probabilities. We have used only the pertinent component from $|\psi(t)\rangle$ which is a convenience inherent in the eigenstates being unit vectors, that is, in a diagonal basis.

(h) When you measure $E = 5$ the state vector is $|\psi(t > 0)\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ in the diagonal basis so the probability of measuring $\omega = 2$ is 1 with a zero probability of measuring $\omega = 0$ or $\omega = 1$. The state vector remains $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ for all $t > 0$ so a subsequent measurement of \mathcal{H} is necessarily $E = 5$, a subsequent measurement of Ω is necessarily $\omega = 2$. If the result of an initial measurement is $E = 3$, the state vector is

$$|\psi(t > 0)\rangle = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \Rightarrow |\psi(t > 0)\rangle \rightarrow A \begin{pmatrix} i \\ \sqrt{2} \\ 0 \end{pmatrix}$$

$$\Rightarrow (-i, \sqrt{2}, 0) A^* A \begin{pmatrix} i \\ \sqrt{2} \\ 0 \end{pmatrix} = |A|^2 (1+2) = 1 \Rightarrow A = \frac{1}{\sqrt{3}} \Rightarrow |\psi(t > 0)\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} i \\ \sqrt{2} \\ 0 \end{pmatrix}.$$

$$\Rightarrow P(\omega = 0) = \left| (1, 0, 0) \frac{1}{\sqrt{3}} \begin{pmatrix} i \\ \sqrt{2} \\ 0 \end{pmatrix} \right|^2 = \frac{1}{3} |i|^2 = \frac{1}{3} (-i)(i) = \frac{1}{3},$$

$$P(\omega = 1) = \left| (0, 1, 0) \frac{1}{\sqrt{3}} \begin{pmatrix} i \\ \sqrt{2} \\ 0 \end{pmatrix} \right|^2 = \frac{2}{3}.$$

A subsequent measurement of $\omega = 0$ puts the system into the unique state $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \Rightarrow E = 3$, $\omega = 0$, $E = 3$, $\omega = 0$, ad infinitum for further measurements of \mathcal{H} and Ω , or a subsequent

measurement of $\omega = 1$ puts the system into the unique state $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \Rightarrow E = 3, \omega = 1$, $E = 3, \omega = 1$, ad infinitum for further measurements of \mathcal{H} and Ω .

(i) The degeneracy at $E = 3$ is removed because

$$E = 3 \text{ and } \omega = 0 \Rightarrow |\psi\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \text{ and } E = 3 \text{ and } \omega = 1 \Rightarrow |\psi\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

The state vector is not uniquely determined by a measurement of $E = 3$ but the state vector is uniquely determined by a measurement of $E = 3$ and $\omega = 0$ or 1 .

Postscript: The finality of the “ad infinitum” of part (h) is moderated by the fact that the system under study can and likely will interact with another system, collision with another particle for instance, so that the state vector can change. Until it does interact with another system, however, it will remain in the state that corresponds to the eigenvalue measured during any measurement.

23. (a) Find the position space form of an inner product,
 (b) the momentum space form of an inner product, and
 (c) comment on the consequence of the two kets of part (a) being dual state vectors.
-

Dirac notation is independent of basis so is particularly useful for exploiting the advantages of abstract Hilbert space. Conversion to a specific subspace, such as position space, is often the most expedient way to address specific physical problems. The key techniques in transitioning from Hilbert space to a specific representation are the insertion of the identity and the choice of the form for that identity. Representations described in problems 9 and 10 in part 3 of chapter 1 are pertinent. Limits are not used on integrals where the integration is to be done over all space, meaning from $-\infty$ to ∞ in each dimension. Excluding limits over all space is a common practice.

$$(a) \quad \langle \psi | \psi' \rangle = \langle \psi | \mathcal{I} | \psi' \rangle \quad (1)$$

$$= \langle \psi | \left(\int |x\rangle \langle x| dx \right) | \psi' \rangle \quad (2)$$

$$= \int \langle \psi | x \rangle \langle x | \psi' \rangle dx, \quad (3)$$

$$\text{but } \langle \psi | x \rangle = \psi^*(x) \text{ and } \langle x | \psi' \rangle = \psi'(x) \Rightarrow \langle \psi | \psi' \rangle = \int \psi^*(x) \psi'(x) dx$$

is the position space form of an inner product. The identity is inserted in line (1) and the position space form of the identity is explicitly denoted in line (2). The bra and ket may be moved as indicated in line (3) since the variable of integration is not inherent in either abstract vector.

(b) Proceeding as in the previous example but choosing a momentum space form of the identity,

$$\langle \psi | \psi' \rangle = \langle \psi | \mathcal{I} | \psi' \rangle = \langle \psi | \int | p \rangle \langle p | dp | \psi' \rangle = \int \langle \psi | p \rangle \langle p | \psi' \rangle dp = \int \hat{\psi}^*(p) \hat{\psi}'(p) dp.$$

(c) If the two vectors of part (a) are dual vectors, the result becomes

$$\langle \psi | \psi \rangle = \int \psi^*(x) \psi(x) dx, \quad \text{and since} \quad \langle \psi | \psi \rangle = 1 \quad \text{for a normalized vector,}$$

$$\int \psi^*(x) \psi(x) dx = 1 \quad \text{is the normalization condition in one spatial dimension in position space.}$$

Postscript: Integral forms are used to describe continuous systems or systems populated so heavily that they may be treated as continuous.

24. Show that (a) $\langle x | \mathcal{X} | x' \rangle = x \delta(x - x')$ and (b) $\langle x | \mathcal{P} | x' \rangle = -i\hbar \delta'(x - x')$.

These relations are so useful in developing representation in position space that they have been stated as portions of the postulates of quantum mechanics².

Part (a) is a one-line application of the eigenvalue/eigenvector problem where you must recognize a delta function. Postulate 2 requires that \mathcal{X} is Hermitian. Hermitian operators can operate to the right or to the left. The eigenvalue/eigenvector relation is $\langle x | \mathcal{X} = \langle x | x$ when \mathcal{X} operates to the left. Unfortunately, the eigenvalue/eigenvector relation does not apply to part (b) because neither $\langle x |$ nor $| x' \rangle$ is an eigenbasis of \mathcal{P} .

For part (b), use the quantum mechanical Fourier transforms

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \hat{\psi}(p) e^{ipx/\hbar} dp, \quad \hat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

to form a Fourier integral for $\psi(x)$. You can write $\psi(x) = \int_{-\infty}^{\infty} \delta(x - x') \psi(x') dx'$, set the two expressions for $\psi(x)$ equal, and develop relations for $\delta(x - x')$ and finally $\delta'(x - x')$. Then

$$\langle x | \mathcal{P} | x' \rangle = \langle x | \mathcal{I} | \mathcal{P} | x' \rangle = \langle x | \left(\int | p \rangle \langle p | dp \right) | \mathcal{P} | x' \rangle,$$

and using the relations of $\langle x | p \rangle$ and $\langle p | x \rangle$ seen in the postscript of problem 28 from part 3 of chapter 1, you eventually arrive at expressions that you can recognize as $\delta'(x - x')$.

(a) Attaining the eigenvalue by letting \mathcal{X} operate to the left and recognizing $\langle x | x' \rangle = \delta(x - x')$,

$$\langle x | \mathcal{X} | x' \rangle = \langle x | x | x' \rangle = x \langle x | x' \rangle = x \delta(x - x').$$

² Shankar, *Principles of Quantum Mechanics* (Plenum Press, New York, 1994), 2nd ed., pp. 115-116.

(b) The quantum mechanical Fourier integral is

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \left(\frac{1}{\sqrt{2\pi\hbar}} \int \psi(x') e^{-ipx'/\hbar} dx' \right) e^{ipx/\hbar} dp = \frac{1}{2\pi\hbar} \int dp \int \psi(x') e^{ip(x-x')/\hbar} dx'.$$

The wavefunction in position space can be written $\psi(x) = \int \delta(x-x') \psi(x') dx'$ so

$$\begin{aligned} \int \delta(x-x') \psi(x') dx' &= \frac{1}{2\pi\hbar} \int dp \int \psi(x') e^{ip(x-x')/\hbar} dx' \\ \Rightarrow \delta(x-x') \psi(x') &= \frac{1}{2\pi\hbar} \int \psi(x') e^{ip(x-x')/\hbar} dp = \frac{1}{2\pi\hbar} \psi(x') \int e^{ip(x-x')/\hbar} dp \\ \Rightarrow \delta(x-x') &= \frac{1}{2\pi\hbar} \int e^{ip(x-x')/\hbar} dp \\ \Rightarrow \delta'(x-x') &= \frac{1}{2\pi\hbar} \int \frac{i}{\hbar} p e^{ip(x-x')/\hbar} dp. \end{aligned} \quad (1)$$

$$\begin{aligned} \langle x | \mathcal{P} | x' \rangle &= \langle x | \mathcal{I} | \mathcal{P} | x' \rangle = \langle x | \left(\int |p\rangle \langle p| dp \right) | \mathcal{P} | x' \rangle \\ &= \int \langle x | p \rangle \langle p | \mathcal{P} | x' \rangle dp \\ &= \int \langle x | p \rangle \langle p | p | x' \rangle dp = \int p \langle x | p \rangle \langle p | x' \rangle dp \end{aligned} \quad (2)$$

$$= \int p \left(\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \right) \left(\frac{1}{\sqrt{2\pi\hbar}} e^{-ipx'/\hbar} \right) dp \quad (3)$$

$$= \frac{1}{2\pi\hbar} \int p e^{ip(x-x')/\hbar} dp = \frac{\hbar}{i} \delta'(x-x') = -i\hbar \delta'(x-x'). \quad (4)$$

Line (1) is differentiation with respect to x . The first expression in line (2) is the result of the eigenvalue/eigenvector equation, $\langle p | \mathcal{P} = \langle p | p$. Line (3) employs the expressions developed for $\langle x | p \rangle$ and $\langle p | x \rangle$ in the postscript of problem 28 in part 3 of chapter 1. The second expression in line (4) is attained by comparing the first expression in line (4) with equation (1).

Postscript: The relations above are in the position basis. Analogous relations in the momentum basis are $\langle p | \mathcal{P} | p' \rangle = p \delta(p-p')$ and $\langle p | \mathcal{X} | p' \rangle = i\hbar \delta'(p-p')$. The absence of a negative sign in the last equation is a choice of phase. A choice of phase is necessary.

25. Find the form of an expectation value of the position operator in position space.

The expectation value of position is $\langle \psi | \mathcal{X} | \psi \rangle$ in Dirac notation. Insert the identity in terms of $|x'\rangle$ on the left and $|x\rangle$ on the right of the abstract position operator. Rearrange the expression to find a factor of $\langle x' | \mathcal{X} | x \rangle = x' \delta(x'-x)$. One of the two integrations can be done using this delta function to find $\langle \psi | \mathcal{X} | \psi \rangle = \int \psi^*(x) x \psi(x) dx$.

$$\langle \psi | \mathcal{X} | \psi \rangle = \langle \psi | \mathcal{I} | \mathcal{X} | \mathcal{I} | \psi \rangle \quad (1)$$

$$= \langle \psi | \left(\int |x'\rangle \langle x'| dx' \right) | \mathcal{X} | \left(\int |x\rangle \langle x| dx \right) | \psi \rangle \quad (2)$$

$$= \int \int \langle \psi | x' \rangle \langle x' | \mathcal{X} | x \rangle \langle x | \psi \rangle dx' dx$$

$$= \int \int \psi^*(x') x' \delta(x' - x) \psi(x) dx' dx \quad (3)$$

$$= \int \left(\int \psi^*(x') x' \delta(x' - x) \psi(x) dx' \right) dx = \int \psi^*(x) x \psi(x) dx.$$

The identity is inserted twice in line (1), two different forms of the identity are used in line (2), inner products and the bracket (per problem 24 a)) are represented in position space in line (3).

Postscript: We stated earlier that $\mathcal{X} \rightarrow x$ in position space and problem 25 demonstrates this fact. Similarly, if more than one spatial dimension is required, $\mathcal{Y} \rightarrow y$, and $\mathcal{Z} \rightarrow z$.

26. Find the form of the expectation value of the momentum operator in position space.

This problem is similar to the last problem except, of course, it addresses momentum. Start with $\langle \psi | \mathcal{P} | \psi \rangle$, insert identities in the same form as the last problem but you will need to use the relation $\langle x | \mathcal{P} | x' \rangle = -i\hbar \delta'(x - x')$ addressed in problem 24. The delta function is an even function but the derivative of the delta function is an odd function so $\langle x' | \mathcal{P} | x \rangle = i\hbar \delta'(x' - x)$ is the form that you want to use. Problem 17 of part 3 of chapter 1 may help you to evaluate the derivative of the delta function. You should find

$$\langle \psi | \mathcal{P} | \psi \rangle = -i\hbar \int \psi^*(x) \frac{d}{dx} \psi(x) dx.$$

$$\langle \psi | \mathcal{P} | \psi \rangle = \langle \psi | \mathcal{I} | \mathcal{P} | \mathcal{I} | \psi \rangle$$

$$= \langle \psi | \left(\int |x'\rangle \langle x'| dx' \right) | \mathcal{P} | \left(\int |x\rangle \langle x| dx \right) | \psi \rangle$$

$$= \int \int \langle \psi | x' \rangle \langle x' | \mathcal{P} | x \rangle \langle x | \psi \rangle dx' dx$$

$$= \int \int \psi^*(x') (i\hbar \delta'(x' - x)) \psi(x) dx' dx \quad (1)$$

$$= \int \psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) dx = -i\hbar \int \psi^*(x) \frac{d}{dx} \psi(x) dx. \quad (2)$$

The inner products and the derivative of the delta function are both represented in position space in line (1). Evaluating the derivative of the delta function results in the first expression in line (2).

Postscript: This problem demonstrates that $\mathcal{P} \rightarrow -i\hbar \frac{d}{dx}$ in position space as we have indicated in part 3 of chapter 1. The parentheses in line (2) are placed to identify this explicitly.

This position space relation and $\mathcal{X} \rightarrow x$ are easily generalized to two or three dimensions by working two or three one-dimensional problems. If more than one spatial component is required,

$$\mathcal{P} \rightarrow -i\hbar \nabla = -i\hbar \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right), \text{ in three spatial dimensions, for instance.}$$

The analogous relations in momentum space in one dimension are $\mathcal{X} \rightarrow i\hbar \frac{d}{dp}$ and $\mathcal{P} \rightarrow p$, and in three dimensions are

$$\mathcal{X} \rightarrow i\hbar \frac{d}{dp_x}, \quad \mathcal{Y} \rightarrow i\hbar \frac{d}{dp_y}, \quad \mathcal{Z} \rightarrow i\hbar \frac{d}{dp_z}, \quad \text{and} \quad \mathcal{P}_x \rightarrow p_x, \quad \mathcal{P}_y \rightarrow p_y, \quad \mathcal{P}_z \rightarrow p_z.$$

The absence of a negative sign in the relations for spatial operators in momentum space reflects the popular choice of phase, also mentioned in the postscript to problem 24.

27. Derive the position space form of the time-independent Schrodinger equation in one dimension. Assume that potential energy is a function of position only.

Basis-independent statements of the Schrodinger equation offer generality and flexibility and can provide physical insight, but they are not often useful to attain functional or numeric solutions to real problems. Representations of the Schrodinger equation in position space and momentum space are the tools generally used to address specific systems.

Start with the eigenvalue/eigenvector equation for the time-independent, quantum mechanical Hamiltonian, $\mathcal{H}|\psi\rangle = E|\psi\rangle$. Form the quantum mechanical Hamiltonian,

$$H_{\text{classical}} = T + V = \frac{p^2}{2m} + V \quad \longrightarrow \quad \mathcal{H} = \frac{\mathcal{P}^2}{2m} + \mathcal{V}.$$

Potential energy is given to be a function of position only $\Rightarrow \mathcal{V} \rightarrow \mathcal{V}(\mathcal{X})$ and $\mathcal{X} \rightarrow x \Rightarrow \mathcal{V}(\mathcal{X}) \rightarrow V(x)$ for this problem. Form a bracket of both sides using $\langle x|$. Assume that this bra commutes with the Hamiltonian. You should find

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x).$$

$$\begin{aligned} \mathcal{H}|\psi\rangle = E|\psi\rangle &\Rightarrow \left(\frac{\mathcal{P}^2}{2m} + \mathcal{V} \right) |\psi\rangle = E|\psi\rangle \\ &\Rightarrow \left(\frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}) \right) |\psi\rangle = E|\psi\rangle \end{aligned} \tag{1}$$

$$\Rightarrow \langle x | \left(\frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}) \right) | \psi \rangle = \langle x | E | \psi \rangle \quad (2)$$

$$\Rightarrow \left(\frac{1}{2m} \mathcal{P}^2 + \mathcal{V}(\mathcal{X}) \right) \langle x | \psi \rangle = E \langle x | \psi \rangle \quad (3)$$

$$\Rightarrow \left[\frac{1}{2m} \left(-i\hbar \frac{d}{dx} \right) \left(-i\hbar \frac{d}{dx} \right) + V(x) \right] \psi(x) = E \psi(x) \quad (4)$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x).$$

Equation (1) imbeds the assumption that potential energy is a function of position only. Brackets are formed with $\langle x |$ so as to eventually attain a position space representation in equation (2). The E on the right side of equation (3) is an eigenvalue and any constant can be removed from a bracket. The expression in parenthesis on the left side of equation (3) is treated as an eigenvalue. The position space representations of the momentum operator, the potential energy operator, and the inner products are substituted in equation (4).

Postscript: The assumption that $\langle x |$ commutes with the Hamiltonian is founded by the requirement for eigenstates to be unique, a property that results from the linear independence of the eigenstates. There are an infinite number of $\psi(x)$'s or $\psi_i(x)$'s. The right side of equation (2) becomes a constant times an eigenfunction. In order for the left side of equation (2) to be the same in an infinite number of cases, it also must become a constant times a function which is why $\langle x |$ commutes with \mathcal{H} in equation (3). In general, an arbitrary bra does not commute with a Hermitian operator.

28. Consider a particle described by the wavefunction

$$\psi(x) = A \quad \text{when} \quad -10 \text{ \AA} \leq x \leq +10 \text{ \AA}, \quad \psi(x) = 0 \quad \text{otherwise.}$$

- Calculate the normalization constant A .
 - Calculate the probability that the particle will be found between $x = -3 \text{ \AA}$ and $x = +5 \text{ \AA}$.
 - What are the possible results and the probability of each possible result of a measurement of position?
 - A measurement of position is made and the particle is found at $x = 3.5 \text{ \AA}$. Sketch the wavefunction immediately after the measurement.
 - Calculate the momentum space wavefunction $\hat{\psi}(p)$ that corresponds to the position space wavefunction $\psi(x)$ by calculating the Fourier transform of $\psi(x)$. Sketch $\hat{\psi}(p)$.
 - The momentum of the particle described by $\psi(x)$ is measured. What results can be obtained, and with what probabilities will they be obtained?
 - Suppose the momentum is measured and $p = 0$ is obtained. Sketch $\hat{\psi}(p)$ immediately after the measurement.
-

Integral forms are used to describe continuous systems or systems populated so heavily that they may be treated as continuous systems. This problem introduces the application of the postulates to such systems. It also introduces the methods of calculating the possible results of a measurement and the probabilities of these possible results for continuous systems. The term **probability density** is introduced. This problem also introduces the concept of the units of a wavefunction.

The normalization condition is given by

$$\langle \psi | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1,$$

as you found in problem 23. The wavefunction is zero everywhere except between -10\AA and $+10\text{\AA}$, and between these limits it is a constant. Substitute the constant wavefunction into this integral using limits where $\psi(x)$ is non-zero and solve for A to complete part (a). Integrate the probability, $P = \int \psi^*(x) \psi(x) dx$, between the given limits for part (b). It is same integration as part (a) except for the limits.

Write down the interval where the wavefunction is non-zero and you are done with part (c). This, however, is deeper than it might appear. The eigenvalues of the position operator are positions, x 's in one dimension. Any possible x_i is an eigenvalue in the same sense that an α_i is an eigenvalue of a matrix operator and the result of a measurement can be only an individual eigenvalue per postulate 3. There are two aspects to the physics of this situation. First, any measurement of position is limited by the quality of your equipment. A position measured to be 3.5\AA means only that you have measured to $3.5\text{\AA} \pm 0.05\text{\AA}$. This is an interval. Secondly, the probability of measuring any given eigenvalue x_i is zero because there are an infinite number of points on any continuous curve. It is like asking what is one divided by infinity? The mathematics answers this question since $\int_a^a f(x) dx = 0$, any integral with the same upper and lower limit is zero. That said, assume that you had ideal instruments that could measure individual eigenvalues (which is both mathematically and physically impossible, but assume it nevertheless). Assume that you have ideal instruments for part (d) also. Use postulate 5. Only ideal instruments could measure a delta function. If you measure $x = 3.5\text{\AA}$, then the state vector is the eigenvector of the position operator with eigenvalue 3.5\AA , which is a delta function centered at $x = 3.5\text{\AA}$. For part (e), you must calculate the Fourier transform

$$\hat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-10\text{\AA}}^{+10\text{\AA}} e^{-ipx/\hbar} \psi(x) dx,$$

where the integration is over only the region where the wavefunction is non-zero. The sinc function

$$\hat{\psi}(p) = \frac{1}{\sqrt{10\pi\hbar\text{\AA}}} \frac{\sin\left(\frac{p}{\hbar}(10\text{\AA})\right)}{p/\hbar},$$

is the result. The eigenvalues of the momentum operator are momenta for part (f). These are eigenvalues in the same sense as the eigenvalues of a matrix operator per postulate 3 so the possible results are momenta between $-\infty$ and $+\infty$. In contrast to part (c), all momenta are possible results of a measurement. Notice also that the **probability density**, $|\hat{\psi}(p)|^2$ diminishes as you go away from $p = 0$. Part (g) is very similar to part (d). If you could measure an individual eigenvalue (again you really cannot), you would get a delta function at $p = 0$...so sketch that.

(a) Calculate the normalization constant

$$\begin{aligned}
 \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1 &\Rightarrow \int_{-10 \text{ \AA}}^{+10 \text{ \AA}} A^* A dx = 1 \Rightarrow \int_{-10 \text{ \AA}}^{+10 \text{ \AA}} |A|^2 dx = 1 \\
 \Rightarrow |A|^2 \int_{-10 \text{ \AA}}^{+10 \text{ \AA}} dx = 1 &\Rightarrow |A|^2 x \Big|_{-10 \text{ \AA}}^{+10 \text{ \AA}} = 1 \Rightarrow |A|^2 (+10 \text{ \AA} - (-10 \text{ \AA})) = 1 \\
 \Rightarrow 20 \text{ \AA} |A|^2 = 1 &\Rightarrow |A|^2 = \frac{1}{20 \text{ \AA}} \Rightarrow A = \frac{1}{\sqrt{20 \text{ \AA}}}.
 \end{aligned}$$

The normalization constant will always have units of $1/\sqrt{\text{length}}$ in one dimension in position space. A popular procedure is to minimize clutter by excluding units during calculation, and then carefully placing the units back into the final answer.

(b) Calculate the probability

$$\begin{aligned}
 P(-3 \text{ \AA} < x < 5 \text{ \AA}) &= \int_{-3}^5 \psi^*(x) \psi(x) dx = \int_{-3}^5 |A|^2 dx \\
 &= \frac{1}{20 \text{ \AA}} x \Big|_{-3 \text{ \AA}}^{+5 \text{ \AA}} = \frac{1}{20 \text{ \AA}} (+5 \text{ \AA} - -3 \text{ \AA}) = \frac{8}{20} = \frac{2}{5} = 0.4.
 \end{aligned}$$

(c) The possible results of a position measurement are any x in the interval $-10 \text{ \AA} \leq x \leq 10 \text{ \AA}$.

(d) If we measure the position, and we find the particle at $x = 3.5 \text{ \AA}$, then the wavefunction is a delta function centered at $x = 3.5 \text{ \AA}$, which is sketched at the right.

(e) The wavefunction in momentum space is given by the Fourier transform

$$\begin{aligned}
 \hat{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-10}^{10} e^{-ipx/\hbar} A dx \\
 &= \frac{A}{\sqrt{2\pi\hbar}} \int_{-10}^{10} e^{-ipx/\hbar} dx = \frac{A}{\sqrt{2\pi\hbar}} \frac{\hbar}{(-ip)} (e^{-ip10/\hbar} - e^{+ip10/\hbar}) \\
 &= \frac{A\sqrt{2}}{\sqrt{\pi\hbar}} \frac{\hbar}{p} \left(\frac{e^{+ip10/\hbar} - e^{-ip10/\hbar}}{2i} \right) = \frac{\sqrt{2}}{\sqrt{20 \text{ \AA}}} \frac{1}{\sqrt{\pi\hbar}} \frac{\hbar}{p} \sin\left(\frac{p}{\hbar} 10 \text{ \AA}\right) \\
 &= \frac{1}{\sqrt{10\pi\hbar \text{ \AA}}} \frac{\sin\left(\frac{p}{\hbar} (10 \text{ \AA})\right)}{p/\hbar}.
 \end{aligned}$$

(f) The possible results of a momentum measurement are any p in the interval $-\infty \leq p \leq \infty$. The probability density in momentum space is $|\hat{\psi}(p)|^2$, and

$$P(p_a < p < p_b) = \frac{1}{10\pi\hbar \text{ \AA}} \int_{p_a}^{p_b} \frac{\sin^2\left(\frac{p}{\hbar} (10 \text{ \AA})\right)}{p^2/\hbar^2} dp$$

is a relation to calculate probability.

(g) If you find $p = 0$, the momentum wavefunction will be a delta function located at $p = 0$.

Postscript: The probability of measuring any individual x_i in parts (c) or (d) is zero. The probability of attaining a value between the limits a and b is $P(a < x < b) = \frac{1}{20 \text{ Å}} \int_a^b dx$, for this problem where a and b are in angstroms. The region of interest can be very small, for instance if $a = 3.499999 \text{ Å}$ and $b = 3.500001 \text{ Å}$. There is a small probability of finding the particle between these limits, and this is realistically what is meant by a measurement of $x = 3.5 \text{ Å}$.

29. For $\psi(x) = A e^{-x^2/4}$,

- (a) normalize $\psi(x)$,
- (b) find $P(-\infty < x < 0)$,
- (c) find $P(0 < x < 1)$, and
- (d) find $P(1 < x < \infty)$.

The given wavefunction is **Gaussian** because the exponent of Euler's number contains only the negative of the square of the independent variable and the "A" and 4 are constants. The Gaussian wavefunction or "**wave packet**" is dominantly the most popular description of the localized probability density that is associated with a particle. It is a primary topic of chapter three. Many realistic problems, including part (c) of this one, do not have a closed form solution. The solution to part (c) may remind you of a solution to a statistics problem using a normal distribution. A normal distribution is the same thing as a Gaussian distribution.

Refer to problem 20 of part 3 of chapter 1 to normalize $\psi(x)$. Part (b) is an application of form 15.3.29 from the *Handbook of Mathematical Formulas and Integrals* by Jeffrey,

$$\int_0^\infty e^{-q^2 t^2} dt = \frac{\sqrt{\pi}}{2q}, \quad q > 0.$$

You need to recognize that the given $\psi(x)$ is an even function to use this integral. Part (c) requires

$$\int_0^b e^{-at^2} dt = \frac{1}{2} \sqrt{\frac{\pi}{a}} \operatorname{erf}(b\sqrt{a}), \quad \text{where} \quad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,$$

and is known as the **error function**. The last integral is solved numerically and is used frequently enough that it is tabulated in standard tables, for instance,

| | | | | | | | | |
|-------------------------|--------|--------------|--------|------------|--------|--------|--------|--------|
| x | 0.5 | $1/\sqrt{2}$ | 1.0 | $\sqrt{2}$ | 1.5 | 2.0 | 2.5 | 3.0 |
| $\operatorname{erf}(x)$ | 0.5205 | 0.6827 | 0.8427 | 0.9546 | 0.9331 | 0.9772 | 0.9937 | 0.9986 |

is an abbreviated table. There are related functions such as the **normal probability function**. Values for the error function can be derived from tables of the normal probability function. Ensure

that you read the definitions of the functions before you start using tabulated data because different authors employ different conventions and different notation. Keep good track of your constants.

(a) Problem 20 of part 3 of chapter 1 found the normalization constant of

$$f(x) = A e^{-Bx^2} \quad \text{to be} \quad A = \left(\frac{2B}{\pi}\right)^{1/4}. \quad \text{For} \quad \psi(x) = A e^{-x^2/4}, \quad \text{we see that} \quad B = \frac{1}{4}$$

$$\Rightarrow \quad \psi(x) = \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4} \quad \text{is the normalized wavefunction.}$$

(b) Probability for the given wavefunction is

$$P(a < x < b) = \int_a^b \psi^*(x) \psi(x) dx = \int_a^b \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4} \left(\frac{1}{2\pi}\right)^{1/4} e^{-x^2/4} dx = \frac{1}{\sqrt{2\pi}} \int_a^b e^{-x^2/2} dx$$

$$\Rightarrow \quad P(-\infty < x < 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^0 e^{-x^2/2} dx = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{-x^2/2} dx$$

because $\psi(x)$ is an even function. Then

$$\int_0^{\infty} e^{-q^2 t^2} dt = \frac{\sqrt{\pi}}{2q} \quad \Rightarrow \quad \psi(x) = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{2\pi}}{2} = \frac{1}{2} \quad \text{since} \quad q = \frac{1}{\sqrt{2}} \quad \text{for our integral.}$$

$$(c) \quad P(0 < x < 1) = \frac{1}{\sqrt{2\pi}} \int_0^1 e^{-x^2/2} dx,$$

$$\int_0^b e^{-at^2} dt = \frac{1}{2} \sqrt{\frac{\pi}{a}} \operatorname{erf}(b \sqrt{a}) \quad \text{and} \quad a = \frac{1}{2}, \quad b = 1, \quad \text{for this integral,}$$

$$\Rightarrow \quad P(0 < x < 1) = \frac{1}{\sqrt{2\pi}} \int_0^1 e^{-x^2/2} dx = \frac{1}{\sqrt{2\pi}} \frac{1}{2} \sqrt{\frac{2\pi}{1}} \operatorname{erf}\left(\frac{1}{\sqrt{2}}\right) = \frac{1}{2} (0.6827) = 0.3414.$$

(d) Since $P(-\infty < x < \infty) = 1$,

$$P(1 < x < \infty) = 1 - P(-\infty < x < 0) - P(0 < x < 1) = 1 - 0.5 - 0.3414 = 0.1586.$$

Postscript: You may recognize the answers to part (c) to be the portion of a normal distribution that is one standard deviation greater than the mean and part (d) to be the percentage greater than one standard deviation above the mean. A general normal or Gaussian distribution is

$$f(x) = \frac{1}{\sqrt{2\pi} \sigma} \exp\left(-\frac{1}{2} \left[\frac{x - \mu}{\sigma}\right]^2\right), \quad \text{where } \mu \text{ is the mean and } \sigma \text{ is the standard deviation.}$$

The probability distribution for $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/4}$ is a Gaussian distribution with a mean of zero and a standard deviation of 1.

30. Consider the spin-1 angular momentum operators:

$$\mathcal{L}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{L}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \text{and} \quad \mathcal{L}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

- (a) What are the possible values one can obtain if \mathcal{L}_z is measured?
- (b) Consider the state for which $\mathcal{L}_z = 1$. What are $\langle \mathcal{L}_x \rangle$, $\langle \mathcal{L}_x^2 \rangle$, and $\Delta \mathcal{L}_x$ in this state?
- (c) Find the eigenvalues and eigenvectors of the \mathcal{L}_x operator in the \mathcal{L}_z basis.
- (d) If the particle is in the state with $\mathcal{L}_z = -1$ and \mathcal{L}_x is measured, what are the possible results of the measurement and with what probabilities will they be obtained?
- (e) Consider the initial state $|\psi\rangle = \frac{1}{\sqrt{21}} \begin{pmatrix} 4 \\ 1 \\ 2 \end{pmatrix}$ in the \mathcal{L}_z basis. If \mathcal{L}_z^2 is measured and the result $+1$ is obtained, what is the state immediately after the measurement? How probable was this result? What are the possible outcomes and their respective probabilities for a measurement of \mathcal{L}_z immediately after attaining a result of 1 for a measurement of \mathcal{L}_z^2 ?
- (f) Find the state vector for which the \mathcal{L}_z probabilities are

$$P(\mathcal{L}_z = 1) = \frac{1}{4}, \quad P(\mathcal{L}_z = 0) = \frac{1}{2}, \quad \text{and} \quad P(\mathcal{L}_z = -1) = \frac{1}{4}.$$

The given matrices are the spin-1 angular momentum operators (less a factor of \hbar). This problem highlights the postulates of quantum mechanics using these commonly encountered operators. Parts (c) and (e) of this problem introduce a consequence of operators that do not commute.

Notice first that postulate 2 is satisfied because all three operators are Hermitian. Part (a) is an application of postulate 3. Notice that it concerns only \mathcal{L}_z . If an eigenvalue of \mathcal{L}_z has been measured, you can ascertain the system's eigenstate from postulate 5 for part (b). The calculation of the expectation values $\langle \mathcal{L}_z = 1 | \mathcal{L}_x | \mathcal{L}_z = 1 \rangle$, $\langle \mathcal{L}_z = 1 | \mathcal{L}_x \mathcal{L}_x | \mathcal{L}_z = 1 \rangle$, and

$$\sqrt{\langle \mathcal{L}_z = 1 | (\mathcal{L}_x \mathcal{L}_x - \langle \mathcal{L}_x \rangle^2) | \mathcal{L}_z = 1 \rangle} \quad \text{are extensions of postulate 4.}$$

None of the three spin-1 angular momentum operators commute. You can diagonalize any one of them (see problems 19 and 24 of part 2 of chapter 1) and express the other two in that basis. \mathcal{L}_z is the usual choice of the three operators to be expressed as a diagonal matrix. The given \mathcal{L}_z is diagonal which means that the operators are given in the \mathcal{L}_z basis. Part (c) directs you only to solve the eigenvalue/eigenvector problem for the given \mathcal{L}_x for which problem 24 of part 2 of chapter 1 may be of interest. Postulate 5 provides the eigenstate corresponding to a measurement

of $\mathcal{L}_z = -1$ for part (d). Postulate 3 and the results of part (c) provide the possible results of a measurement of \mathcal{L}_x . Postulate 4 tells you how to calculate probabilities for each possibility.

Construct the operator \mathcal{L}_z^2 to start part (e). You will find that it is two-fold degenerate at $\mathcal{L}_z^2 = 1$, therefore, the state vector following the measurement is a superposition of the two possible eigenstates per postulate 1. The projection operator $\mathcal{P} = |\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta|$, where $|\alpha\rangle$ and $|\beta\rangle$ represent the two $\mathcal{L}_z^2 = 1$ eigenstates, operating on the given state vector, $\mathcal{P}|\psi\rangle$, provides the state vector that is the superposition. Normalize this state vector so that an equality may be used in applying postulate 4 to attain probabilities. You have the eigenvectors and the probabilities but the state vector is unknown for part (f), for instance $|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$. Use postulate 4 to solve for each component.

(a) The eigenvalues are on the principal diagonal in the diagonal matrix \mathcal{L}_z so are 1, 0, and -1 .

(b) Measurement forces the system into the eigenstate corresponding to the measured eigenvalue.

Therefore $\mathcal{L}_z = 1 \Rightarrow |\psi\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$. The expectation values and the uncertainty are

$$\langle \mathcal{L}_x \rangle_\psi = (1, 0, 0) \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (1, 0, 0) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (0) = 0.$$

$$\mathcal{L}_x^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$\Rightarrow \langle \mathcal{L}_x^2 \rangle_\psi = (1, 0, 0) \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} (1, 0, 0) \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{2},$$

$$\Delta \mathcal{L}_x = \langle (\mathcal{L}_x - \langle \mathcal{L}_x \rangle)^2 \rangle^{1/2} = \langle (\mathcal{L}_x - 0)^2 \rangle^{1/2} = \langle \mathcal{L}_x^2 \rangle^{1/2} = \langle \frac{1}{2} \rangle^{1/2} = \frac{1}{\sqrt{2}}.$$

(c) This is the standard eigenvalue/eigenvector problem for \mathcal{L}_x because \mathcal{L}_z is diagonal meaning that the three operators are given in the \mathcal{L}_z basis. Referring to problem 24 of part 2 of chapter 1,

$$\mathcal{U}^\dagger \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \mathcal{U} = \begin{pmatrix} -\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$$

$$\Rightarrow \mathcal{U}^\dagger \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

so -1 , 0 and 1 are the eigenvalues. The eigenvectors in the original \mathcal{L}_z basis were found to be

$$|-1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}, \quad |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \text{and} \quad |1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}.$$

(d) The measurement $\mathcal{L}_z = -1 \Rightarrow |\psi\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ per postulate 5. Then per postulate 4,

$$P(\mathcal{L}_x = -1) = \left| \langle \mathcal{L}_x = -1 | \psi \rangle \right|^2 = \left| \frac{1}{2} (1, -\sqrt{2}, 1) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \left(\frac{1}{2} \right)^2 = \frac{1}{4},$$

$$P(\mathcal{L}_x = 0) = \left| \langle \mathcal{L}_x = 0 | \psi \rangle \right|^2 = \left| \frac{1}{\sqrt{2}} (1, 0, -1) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \left(\frac{-1}{\sqrt{2}} \right)^2 = \frac{1}{2},$$

$$P(\mathcal{L}_x = 1) = \left| \langle \mathcal{L}_x = 1 | \psi \rangle \right|^2 = \left| \frac{1}{2} (1, \sqrt{2}, 1) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \left(\frac{1}{2} \right)^2 = \frac{1}{4}.$$

(e) The operator \mathcal{L}_z^2 is

$$\mathcal{L}_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and the eigenvalues of 1, 0, and -1 are on the principal diagonal. A measurement of $\mathcal{L}_z^2 = +1$ forces the system into a superposition of *both* eigenvectors that have eigenvalue 1, meaning

$$|\psi\rangle = \alpha \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha \\ 0 \\ \beta \end{pmatrix}.$$

The projection operator constructed from the states existing in the superposition is

$$\mathcal{P} = |1\rangle\langle 1| + |1'\rangle\langle 1'| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

So the unnormalized state vector immediately after a measurement that yields $\mathcal{L}_z^2 = 1$ is

$$\mathcal{P}|\psi\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix}.$$

The new state vector will have to be normalized if eigenstates are missing from the original state vector so the original normalization constant is an unnecessary complication and is excluded. Then

$$(4, 0, 2) A^* A \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix} = |A|^2 (16 + 4) = |A|^2 (20) = 1 \Rightarrow A = \frac{1}{2\sqrt{5}}$$

$$\Rightarrow |\psi\rangle = \frac{1}{2\sqrt{5}} \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix} \text{ is normalized, and } \alpha = \frac{2}{\sqrt{5}}, \quad \beta = \frac{1}{\sqrt{5}}, \quad \text{if you want}$$

to resolve the state into individual vectors. To find the probability of measuring $\mathcal{L}_z^2 = +1$, add the probabilities corresponding to each of the ways that we can obtain $\mathcal{L}_z^2 = 1$,

$$\begin{aligned} P(\mathcal{L}_z^2 = +1) &= \left| \langle 1 | \psi \rangle \right|^2 + \left| \langle 1' | \psi \rangle \right|^2 \\ &= \left| (1, 0, 0) \frac{1}{\sqrt{21}} \begin{pmatrix} 4 \\ 1 \\ 2 \end{pmatrix} \right|^2 + \left| (0, 0, 1) \frac{1}{\sqrt{21}} \begin{pmatrix} 4 \\ 1 \\ 2 \end{pmatrix} \right|^2 \\ &= \left| \frac{4}{\sqrt{21}} \right|^2 + \left| \frac{2}{\sqrt{21}} \right|^2 = \frac{16}{21} + \frac{4}{21} = \frac{20}{21}. \end{aligned}$$

If \mathcal{L}_z is measured for the state vector prepared by measuring $\mathcal{L}_z^2 = 1$, the possible outcomes are 1 or -1 because the new state vector is a linear combination of the $|\mathcal{L}_z = +1\rangle$ and $|\mathcal{L}_z = -1\rangle$ eigenvectors. The $|\mathcal{L}_z = 0\rangle$ eigenvector is absent, so there is no possibility of measuring $\mathcal{L}_z = 0$. The probabilities of measurements of \mathcal{L}_z following a measurement of $\mathcal{L}_z^2 = 1$ are

$$\begin{aligned} P(\mathcal{L}_z = 1) &= \left| \langle \mathcal{L}_z = 1 | \psi \rangle \right|^2 = \left| (1, 0, 0) \frac{1}{2\sqrt{5}} \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix} \right|^2 = \left| \frac{4}{2\sqrt{5}} \right|^2 = \frac{4}{5}, \\ P(\mathcal{L}_z = -1) &= \left| \langle \mathcal{L}_z = -1 | \psi \rangle \right|^2 = \left| (0, 0, 1) \frac{1}{2\sqrt{5}} \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix} \right|^2 = \left| \frac{2}{2\sqrt{5}} \right|^2 = \frac{1}{5}. \end{aligned}$$

(f) The eigenvectors are the unit vectors in the \mathcal{L}_z basis and the state vector is unknown, so

$$\begin{aligned} P(\mathcal{L}_z = 1) &= \left| \langle \mathcal{L}_z = 1 | \psi \rangle \right|^2 = \left| (1, 0, 0) \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \right|^2 = |\alpha|^2 = \frac{1}{4} \Rightarrow \alpha = \frac{1}{2}, \\ P(\mathcal{L}_z = 0) &= \left| \langle \mathcal{L}_z = 0 | \psi \rangle \right|^2 = \left| (0, 1, 0) \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \right|^2 = |\beta|^2 = \frac{1}{2} \Rightarrow \beta = \frac{1}{\sqrt{2}}, \\ P(\mathcal{L}_z = -1) &= \left| \langle \mathcal{L}_z = -1 | \psi \rangle \right|^2 = \left| (0, 0, 1) \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \right|^2 = |\gamma|^2 = \frac{1}{4} \Rightarrow \gamma = \frac{1}{2}, \end{aligned}$$

and the state vector is $|\psi\rangle = \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ 1/2 \end{pmatrix}$ which is normalized.

31. Use the normalized state vector of part (f) of problem 30 to demonstrate that components of a state vector having different phases lead to variable probabilities.

Phase is not a focal issue because results are independent of multiplication by the same $e^{i\phi}$. It can, however, be an important consideration. For instance, if the components of a state vector differ in phase, the probabilities are generally phase dependent.

A general form of the phase-dependent state vector from part (f) of the last problem is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |\mathcal{L}_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |\mathcal{L}_z = 0\rangle + \frac{e^{i\delta_3}}{2} |\mathcal{L}_z = -1\rangle = \begin{pmatrix} \frac{1}{2} e^{i\delta_1} \\ \frac{1}{\sqrt{2}} e^{i\delta_2} \\ \frac{1}{2} e^{i\delta_3} \end{pmatrix}$$

Show that the state vector with components having different phases is still normalized. Then calculate the probability of measuring $\mathcal{L}_x = 0$, for instance. You will get non-vanishing exponential terms which depend on the difference between the phases.

The phase-dependent form of the state vector is normalized because

$$|\langle\psi|\psi\rangle|^2 = \left| \left(\frac{e^{-i\delta_1}}{2}, \frac{e^{-i\delta_2}}{\sqrt{2}}, \frac{e^{-i\delta_3}}{2} \right) \begin{pmatrix} \frac{1}{2} e^{i\delta_1} \\ \frac{1}{\sqrt{2}} e^{i\delta_2} \\ \frac{1}{2} e^{i\delta_3} \end{pmatrix} \right|^2 = \left| \frac{1}{4} + \frac{1}{2} + \frac{1}{4} \right|^2 = 1,$$

so component phase dependence is not consequential to normalization. However,

$$\begin{aligned} P(\mathcal{L}_x = 0) &= |\langle\mathcal{L}_x = 0|\psi\rangle|^2 = \left| \frac{1}{\sqrt{2}} (1, 0, -1) \begin{pmatrix} \frac{1}{2} e^{i\delta_1} \\ \frac{1}{\sqrt{2}} e^{i\delta_2} \\ \frac{1}{2} e^{i\delta_3} \end{pmatrix} \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} \left(\frac{e^{i\delta_1}}{2} - \frac{e^{i\delta_3}}{2} \right) \right|^2 = \frac{1}{2} \left(\frac{e^{-i\delta_1}}{2} - \frac{e^{-i\delta_3}}{2} \right) \left(\frac{e^{i\delta_1}}{2} - \frac{e^{i\delta_3}}{2} \right) \\ &= \frac{1}{8} (e^{-i\delta_1+i\delta_1} - e^{-i\delta_1+i\delta_3} - e^{-i\delta_3+i\delta_1} + e^{-i\delta_3+i\delta_3}) \\ &= \frac{1}{8} (2 - e^{i(\delta_1-\delta_3)} - e^{-i(\delta_1-\delta_3)}) = \frac{1}{4} \left(\frac{2}{2} - \frac{e^{i(\delta_1-\delta_3)} + e^{-i(\delta_1-\delta_3)}}{2} \right) \\ &= \frac{1}{4} (1 - \cos(\delta_1 - \delta_3)). \end{aligned}$$

The probability of measuring $\mathcal{L}_x = 0$ varies from a maximum of $1/2$ to a minimum of 0 as a function of $\delta_1 - \delta_3$. A relative phase difference between the components of the state vector is, therefore, physically significant.

Postscript: We expect all of the probabilities for any of the eigenvalues of \mathcal{L}_x and \mathcal{L}_y to be phase dependent. This is because the spin-1 angular momentum operators do not commute. In fact, we expect this sort of behavior whenever the operators under consideration do not commute. It is a consequence of multiple operators describing the same system that do not commute. Picture

a vector representing angular momentum in three dimensions. In establishing the three spin-1 angular momentum operators in the \mathcal{L}_z basis, we have effectively fixed the z -component of angular momentum but since the operators do not commute, the projection of the angular momentum vector onto the xy plane varies as the angular momentum vector precesses around the z -axis. We will address this “semi-classical” picture when discussing angular momentum.

Practice Problems

32. (a) What are the dimensions of $\psi(x, y)$?
- (b) What are the dimensions of $\psi(x, y, z)$?
- (c) What are the dimensions of $\psi(r, \theta, \phi)$?
- (d) What are the dimensions of $\hat{\psi}(p)$?
- (e) What are the dimensions of $\hat{\psi}(p_x, p_y)$?
- (f) What physical quantity does the units of \hbar represent?

Dimensional consistency is a valuable tool in physics and the field of quantum mechanics is no exception. It is helpful to have a simple procedure to derive the dimensions of a state vector or wavefunction. A general statement of probability useful for extension to larger dimension is

$$P = \int_V |\psi|^2 dV$$

so probability is $|\psi(x, y)|^2 dx dy$ in two dimensions, and $|\psi(x, y, z)|^2 dx dy dz$ in three dimensions. In spherical coordinates, probability is $|\psi(r, \theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi$, where the additional factors are from the differential volume element. Probability is a dimensionless number, so ψ must have the dimensions of $(1/dV)^{1/2}$. Planck’s constant is the fundamental constant of quantum mechanics. If an expression contains some form of Planck’s constant, it is necessarily a quantum mechanical result. Planck’s constant has dimensions of energy multiplied by time. What physical quantity does energy multiplied by time represent?

33. Consider a system described by the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad \text{which at } t = 0 \text{ is in the state } |\psi(0)\rangle = \frac{1}{\sqrt{17}} \begin{pmatrix} 2 \\ 3 \\ -2 \end{pmatrix}.$$

- (a) What results can be obtained for a measurement of energy and with what probabilities will these results be obtained?

- (b) Calculate the expectation value of the Hamiltonian $\langle \mathcal{H} \rangle$ for the state $|\psi(0)\rangle$ using $\langle \mathcal{H} \rangle = \langle \psi(0) | \mathcal{H} | \psi(0) \rangle$. Show that your expectation value agrees with your calculations from part (a) using $\langle \mathcal{H} \rangle = \sum_i P(E_i) E_i$.
- (c) Expand the initial state vector $|\psi(0)\rangle$ in the energy eigenbasis to calculate the time dependent state vector $|\psi(t)\rangle$.
- (d) If the energy is measured at time t what results can be obtained and with what probabilities will these results be obtained? Compare your probabilities with the $t = 0$ case in part (a).
- (e) Suppose that you measure the energy of the system at $t = 0$ and you find $E = -1$. What is the state vector of the system immediately after your measurement? Now let the system evolve without any additional measurements until $t = 10$. What is the state vector $|\psi(10)\rangle$ at $t = 10$? What energies will you measure if you repeat the energy measurement at $t = 10$?

See problem 19.

34. Consider a system described by the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}, \quad \text{which at } t = 0 \text{ is in the state } |\psi(0)\rangle = \frac{1}{\sqrt{29}} \begin{pmatrix} 2 \\ 5 \end{pmatrix}.$$

- (a) Is \mathcal{H} Hermitian?
- (b) Attain the eigenvalues and eigenvectors of \mathcal{H} by solving the eigenvalue/eigenvector problem.
- (c) If the energy is measured what results can be obtained and with what probabilities will these results be obtained?
- (d) Calculate the expectation value of the Hamiltonian using both

$$\langle \mathcal{H} \rangle_{\psi(0)} = \langle \psi(0) | \mathcal{H} | \psi(0) \rangle \quad \text{and} \quad \langle \mathcal{H} \rangle = \sum_i P(E_i) E_i.$$

- (e) Expand the initial state vector $|\psi(0)\rangle$ in the energy eigenbasis and use the time evolution of the energy eigenvectors, *i.e.*, $|E_i(t)\rangle = e^{-iE_i t/\hbar} |E_i(0)\rangle$, to calculate the time dependent state vector $|\psi(t)\rangle$.
- (f) If the energy is measured at time t , what results can be obtained and with what probabilities will these results be obtained? Compare your answer with the $t = 0$ case in part (c).
- (g) Diagonalize \mathcal{H} using a unitary transformation. Transform $|\psi(0)\rangle$ and both eigenvectors to be consistent with this unitary transformation.
- (h) Calculate $|\psi(t)\rangle$ and both $t > 0$ probabilities in the basis in which \mathcal{H} is diagonal.
- (i) Suppose that you measure the energy of the system at $t = 0$ and you find $E = 2$. Find the state vector of the system immediately after your measurement and at time $t = 10$ in both the basis in which \mathcal{H} is diagonal and in the basis of part (b). What energies will you measure if you repeat the energy measurement at $t = 10$?

See problem 20.

35. Given the arbitrary diagonal operator and the arbitrary state vector

$$\Omega = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \quad \text{and} \quad |\psi\rangle = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \text{show that} \quad \langle \psi | \Omega | \psi \rangle = \sum_i P(\omega_i) \omega_i.$$

This problem reinforces problem 9. The two methods of calculating expectation values yield identical results. First, normalize the state vector to find that $1/\sqrt{|x|^2 + |y|^2 + |z|^2}$ is the normalization constant. Then calculate $\langle \psi | \Omega | \psi \rangle$. Calculate the probabilities for each eigenvalue using the unit vectors appropriate to a diagonal operator. You then have the probabilities and the eigenvalues to calculate $\sum_i P(\omega_i) \omega_i$. This problem is relatively simple in the basis of a diagonal operator. Think about how you would do this in the basis of an arbitrary operator... which may make you appreciate more fully the utility of diagonal operators.

36. Consider the operator

$$\Omega = \begin{pmatrix} 0 & 4i & 0 \\ -4i & 0 & -3i \\ 0 & 3i & 0 \end{pmatrix} \quad \text{and the state vector} \quad |\psi\rangle = \begin{pmatrix} 1 \\ i \\ -1 \end{pmatrix}.$$

(a) Verify that the eigenvalues and eigenvectors of Ω are

$$|\omega = -5\rangle = \frac{4}{5\sqrt{2}} \begin{pmatrix} 1 \\ i5/4 \\ 3/4 \end{pmatrix}, \quad |\omega = 0\rangle = \frac{3}{5} \begin{pmatrix} 1 \\ 0 \\ -4/3 \end{pmatrix}, \quad \text{and} \quad |\omega = 5\rangle = \frac{4}{5\sqrt{2}} \begin{pmatrix} 1 \\ -i5/4 \\ 3/4 \end{pmatrix}.$$

Using Ω , $|\psi\rangle$, and the given eigenvalues and eigenvectors,

(b) find the probabilities of each possibility,

(c) find the expectation value using both $\langle \psi | \Omega | \psi \rangle$ and $\sum_i P(\omega_i) \omega_i$,

(c) calculate the uncertainty using $\Delta\Omega_\psi = \langle \psi | \left(\Omega - \langle \Omega \rangle \mathcal{I} \right)^2 | \psi \rangle^{1/2}$,

(e) and calculate the uncertainty using $\Delta\Omega_\psi = \langle \psi | \Omega^2 - \langle \Omega \rangle^2 \mathcal{I} | \psi \rangle^{1/2}$. Compare this answer with your result from part (c).

Uncertainty is the primary point of this problem. What is called “standard deviation” in many fields is called uncertainty in quantum mechanics. This is uncertainty in the same sense of the word used in the term “Heisenberg uncertainty principle.” Also, you can never leave the possibilities and probabilities behind so this problem is practice in a three dimensional case where selected elements and components are imaginary.

First, normalize the state vector. Remember to conjugate components when forming bra’s for probabilities. You have already attained the eigenvalues and eigenvectors if you completed

problem 34 of part 2 of chapter 1. You also diagonalized Ω in that problem. Using the diagonal basis will be the easier path and we address that method in the next problem. Your probabilities, $P(\omega_i) = |\langle \omega_i | \psi \rangle|^2$, must sum to 1 and the expectation values must be the same using both methods. You do not have to carry the square root in your calculations if you compute variance and then take a square root to attain uncertainty. We get $\Delta\Omega = \sqrt{74}/3$.

37. The diagonal form of the Ω operator used in the last problem is $\Omega = \begin{pmatrix} -5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 5 \end{pmatrix}$.

- (a) Transform $|\psi\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ i \\ -1 \end{pmatrix}$ used in the previous problem to the diagonal basis.
- (b) Calculate the probability of each possibility of a measurement of Ω .
- (c) Calculate the expectation value using both $\langle \psi | \Omega | \psi \rangle$ and $\sum_i P(\omega_i) \omega_i$.
- (d) Calculate the uncertainty using $\Delta\Omega_\psi = \langle \psi | (\Omega - \langle \Omega \rangle)^2 | \psi \rangle^{1/2}$.
- (e) Calculate the uncertainty using $\Delta\Omega_\psi = \langle \psi | \Omega^2 - \langle \Omega \rangle^2 | \psi \rangle^{1/2}$. Compare this answer with your result from part (d).
-

You will likely find the calculations of the last problem easier in the diagonal basis. You need to understand the concepts surrounding diagonal operators to understand the techniques that are employed frequently in realistic problems.

You need to calculate $\mathcal{U}^\dagger |\psi\rangle$ to transform the state vector to the same basis as the diagonal Ω . Calculations yield nonsense if the operator and state vector are not in the same basis. You calculated \mathcal{U}^\dagger using the eigenvectors of in problem 34 of part 2 of chapter 1,

$$\mathcal{U}^\dagger = \begin{pmatrix} 4/5\sqrt{2} & -i/\sqrt{2} & 3/5\sqrt{2} \\ 3/5 & 0 & -4/5 \\ 4/5\sqrt{2} & i/\sqrt{2} & 3/5\sqrt{2} \end{pmatrix}.$$

The probabilities of measuring any eigenvalue, the expectation value, and the uncertainty must be the same as the last problem.

38. Find the possible outcomes of a measurement, the probabilities of each possible outcome, the expectation value, and the uncertainty for

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{given that} \quad |\psi\rangle = \begin{pmatrix} 2 \\ i \end{pmatrix}.$$

Support your answers with alternative calculations or consistency checks where possible.

This problem features one of the Pauli spin matrices. This problem is posed without parts because realistic problems do not come with parts though it still leads you down the necessary path. Would you know to travel this path at this point if asked only for uncertainty?

You want to normalize the state vector, solve the eigenvalue/eigenvector problem, and use the eigenvectors and the state vector to attain probabilities. The sum of the probabilities must be 1. Calculate $\langle \sigma_y \rangle = \langle \psi | \sigma_y | \psi \rangle$ and check this result using $\langle \sigma_y \rangle = \sum P(\sigma_{y_i}) \sigma_{y_i}$. Calculate the uncertainty using $\Delta \sigma_{y\psi} = \langle \psi | (\sigma_y - \langle \sigma_y \rangle \mathcal{I})^2 | \psi \rangle^{1/2}$ and check the uncertainty using $\Delta \sigma_{y\psi} = \langle \psi | \sigma_y^2 - \langle \sigma_y \rangle^2 \mathcal{I} | \psi \rangle^{1/2}$.

39. Consider the operator $\Lambda = \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$, which has eigenvalues and normalized eigenvectors

$$|\lambda = 2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad |\lambda = 3\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}. \quad \text{Given the state vector} \quad |\psi\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix},$$

the inner product $\langle \lambda | \psi \rangle$ is 9/10 using the eigenvector that corresponds to 2, and 16/25 using the eigenvector that corresponds to 3. These should be probabilities but their sum is not 1. There is, in fact, an error present. Can you determine what the error is?

This counter example is meant to highlight an error and thus increase the chance that you will avoid it. If you perform the mathematical mechanics you will find that there is not an error in the given information. Consider postulate 2. Also, are these eigenvectors orthogonal?

40. (a) Represent the expectation value of the momentum operator in momentum space.

(b) Represent the expectation value of the position operator in momentum space.

Use procedures similar to those seen in problems 25 and 26. Use the relations

$$\langle p | \mathcal{P} | p' \rangle = p \delta(p - p') \quad \text{and} \quad \langle p | \mathcal{X} | p' \rangle = i\hbar \delta'(p - p')$$

discussed in the postscript to problem 24. You should find that

$$\langle \psi | \mathcal{P} | \psi \rangle = \int \hat{\psi}^*(p) p \hat{\psi}(p) dp \Rightarrow \mathcal{P} \rightarrow p \text{ in momentum space, and}$$

$$\langle \psi | \mathcal{X} | \psi \rangle = \int \hat{\psi}^*(p) \left(i\hbar \frac{d}{dp} \right) \hat{\psi}(p) dp \Rightarrow \mathcal{X} \rightarrow i\hbar \frac{d}{dp} \text{ in momentum space.}$$

41. For $\psi(x) = A x$, $0 \leq x \leq 1$,

(a) Find the normalization constant A ,

(b) calculate $P(1/2 < x < 3/4)$,

(c) calculate $P(0 < x < 1/2)$,

(d) calculate $P(3/4 < x < 1)$.

This is a straightforward application of the normalization procedure and probability calculation for a continuous wavefunction that is easy to integrate.

42. For $\psi(x) = A(2 - x^2)$, $-1 < x < 1$,

- (a) find the normalization constant,
 - (b) calculate $P(-1 < x < 0)$,
 - (c) calculate $P(0 < x < 1/2)$,
 - (d) calculate $P(1/2 < x < 1)$.
-

This is another toy problem with the same intent as the last. The sum of the probabilities over all space where the wavefunction is non-zero must be 1 as in problem 41.

43. Consider a particle described by the wavefunction $\psi(x) = \frac{A}{x^2 + 1}$.

- (a) Find the normalization constant A .
 - (b) Calculate $P(0 < x < 1)$.
 - (c) What are the possible results and the probability of each possible result of a measurement of position?
 - (d) A measurement of position is made and the particle is found at $x = \pi$. Sketch the wavefunction immediately after the measurement.
 - (e) Calculate the momentum space wavefunction $\hat{\psi}(p)$ that corresponds to the position space wavefunction $\psi(x)$ by calculating the Fourier transform of $\psi(x)$. Sketch $\hat{\psi}(p)$.
 - (f) The momentum of the particle described by $\psi(x)$ is measured. What results can be obtained, and with what probabilities will they be obtained?
 - (g) Suppose the momentum is measured and $p = 0$ is obtained. Sketch $\hat{\psi}(p)$ immediately after the measurement.
-

Follow the procedures of problem 28. The wavefunction is a Lorentzian curve which is used frequently in spectral analysis. Problem 39 of part 3 of chapter 1 may be of interest. The integrals

$$\int \frac{dx}{(a^2 + b^2x^2)^2} = \frac{x}{2a^2(a^2 + b^2x^2)} + \frac{1}{2a^3b} \arctan\left(\frac{bx}{a}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \frac{e^{-iqx}}{x^2 + a^2} dx = \frac{\pi}{a} e^{-|aq|}$$

will also be of interest. You should find

$$P(0 < x < 1) = \frac{1}{2\pi} + \frac{1}{4} \approx 0.4092 \quad \text{for part (b), and} \quad \hat{\psi}(p) = \frac{e^{-|p|/\hbar}}{\sqrt{\hbar}} \quad \text{for part (e).}$$

44. For $\psi(x) = e^{-x^2}$,

- (a) normalize $\psi(x)$,
- (b) find $P(-\infty < x < 0)$,
- (c) find $P(0 < x < 1)$, and
- (d) find $P(1 < x < \infty)$.

This is also a Gaussian wavefunction so there is little to add to the comments for problem 29. The interpretation of $\langle \psi | \psi \rangle$ as a probability is due to Max Born and exists in postulate 4. This interpretation defies explanation in terms of macroscopic experience which is essentially why it is one of the postulates.
