Below are solutions/hints on some of the questions. There is no guarantee of completeness or correctness; please watch out for typos.

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1. Show that an operator, when expressed as a matrix in the basis of its own eigenstates, is diagonal.

   Hint: Let's make this more specific: let $\{|w_n\rangle\}$ be the orthonormalized eigenstates of the operator $\hat{Y}$. Use the set $\{|w_n\rangle\}$ as basis set and express $\hat{Y}$ as a matrix in this representation. Show that this matrix is diagonal.

   Hints / Solution / Discussion →

   Let the corresponding eigenvalues be $\{y_n\}$, i.e., $\hat{Y}|w_n\rangle = y_n|w_n\rangle$ for every n.

   If the set $\{|w_n\rangle\}$ is used as basis set, then an operator $\hat{A}$ in this basis will be represented by a matrix whose matrix elements are

   $$A_{mn} = \langle w_m|\hat{A}|w_n\rangle$$

   (This is important, please make sure you know this, and go back to the first three questions of problem set 6 to see this in action.)

   Thus, if $\hat{Y}$ itself is expressed in this basis, then it is represented as a matrix whose elements are

   $$Y_{mn} = \langle w_m|\hat{Y}|w_n\rangle = \langle w_m|y_n|w_n\rangle = y_n\langle w_m|w_n\rangle = y_n\delta_{mn}$$

   i.e., Y_{mn} is only nonzero when $m = n$. In other words, only the diagonal matrix elements are nonzero, or, the matrix representing $\hat{Y}$ in this basis is diagonal.

   Concisely, a physicist would say: an operator is diagonal in its own eigenbasis.

   What if one represented the operator $\hat{Y}$ in a different basis? E.g., used the eigenstates of the Hamiltonian operator as the basis? Would $\hat{Y}$ be diagonal in that basis?

2. Consider a system of two spin-1/2 objects. (E.g., the spins of two ions trapped next to each other, or the electron and proton in a hydrogen atom, where we ignore spatial motion and concentrate on their spins.) The Hilbert space is 4-dimensional and is spanned by the basis

$$|{\uparrow\uparrow}\rangle \qquad |{\uparrow\downarrow}\rangle \qquad |{\downarrow\uparrow}\rangle \qquad |{\downarrow\downarrow}\rangle$$

with the obvious meanings: e.g., $|{\uparrow\downarrow}\rangle$ represents the state where the first spin has z-component up ($+\hbar/2$) and the second spin has z-component down ($-\hbar/2$).

Using these four states as the basis set, a general state can be written as

$$|\psi\rangle \;=\; \alpha\,|{\uparrow\uparrow}\rangle \;+\; \beta\,|{\uparrow\downarrow}\rangle \;+\; \gamma\,|{\downarrow\uparrow}\rangle \;+\; \delta\,|{\downarrow\downarrow}\rangle \;=\; \begin{pmatrix}\alpha\\ \beta\\ \gamma\\ \delta\end{pmatrix}$$

(a) In the state $|\psi\rangle$, what is the probability of finding the first spin to have z-component up?

Hints / Solution / Discussion →

Of the four basis states, the first two have z-up for the first spin. Therefore the probability of finding the first spin to have z-component up is the sum of the probabilities of $|{\uparrow\uparrow}\rangle$ and $|{\uparrow\downarrow}\rangle$:

$$|\alpha|^2 \;+\; |\beta|^2$$

(b) What is the probability of finding the second spin to have z-component down?

Hints / Solution / Discussion →

Same logic as above: $|\beta|^2 + |\delta|^2$

(c) In a simultaneous measurement of the z-components of both the spins, one finds the first spin to be spin-up, and the second to be spin-down. What is the state of the system immediately after the measurement?

Hints / Solution / Discussion →

The measurement has given results corresponding uniquely to the second basis state. Hence, after the measurement the system will be projected onto this state. If the measurement is done at time $t = t_0$, then

$$\left|\psi(t = t_0 + 0^+)\right\rangle \;=\; |\uparrow\downarrow\rangle$$

(d) Imagine instead a measurement of only the second spin. The result is found to be spin-up. What is the state of the system immediately after the measurement?

Hints / Solution / Discussion →

Trickier. The second spin is up in both the first and third basis states, $|\uparrow\uparrow\rangle$ and $|\downarrow\uparrow\rangle$. Hence the measurement will project the state of the system onto a linear combination of these two states:

$$|\psi\rangle \xrightarrow{\text{projection}} \alpha\,|\uparrow\uparrow\rangle \;+\; \gamma\,|\downarrow\uparrow\rangle$$

I've used the same coefficients for the two basis states (α and γ) as they had in the original state. A measurement on the second spin should not affect the relative weights of these two states, since they differ only through the value of the first spin.

However, the state written down above is not normalized. Normalizing, one gets

$$\frac{\alpha}{|\alpha|^2 + |\gamma|^2}\,|\uparrow\uparrow\rangle \;+\; \frac{\gamma}{|\alpha|^2 + |\gamma|^2}\,|\downarrow\uparrow\rangle$$

3. (a) Consider the operator $\hat{A} = \dfrac{d}{dx}$. Which of the following functions are eigenfunctions of $\hat{A}$? (Show your calculation/argument.)

$$f_1(x) = e^{ikx} \qquad f_2(x) = ax \qquad f_3(x) = \cos(kx) \qquad f_4(x) = e^{-ax^2}$$

Here k and a are real constants. For those functions that are eigenfunctions, give the eigenvalue.

Hints / Solution / Discussion →

A function $f(x)$ will be an eigenfunction of the operator $\hat{A}$ if

$$\hat{A}f(x) \;=\; (\text{a number}) \times f(x)$$

To find out if a function is an eigenfunction, apply the operator on it and see if you get back a number times the same function. If yes, then this number is the corresponding eigenvalue. Let's try the four functions, one by one.

$$\hat{A}f_1(x) \;=\; \frac{d}{dx}\left[e^{ikx}\right] \;=\; ike^{ikx} \;=\; ikf_1(x) \qquad \begin{cases}\text{Yes. The} \\ \text{eigenvalue is } ik.\end{cases}$$

$$\hat{A}f_2(x) \;=\; \frac{d}{dx}\left[ax\right] \;=\; a \qquad \text{No.}$$

$$\hat{A}f_3(x) \;=\; \frac{d}{dx}\left[\cos(kx)\right] \;=\; -\sin(kx) \qquad \text{No.}$$

$$\hat{A}f_4(x) \;=\; \frac{d}{dx}\left[e^{-ax^2}\right] \;=\; -2axe^{-ax^2}$$

No. the factor $(-2ax)$ multiplying $f_4(x) = e^{-ax^2}$ on the right is not just a number, it is itself a function of x.

(b) Consider the operator $\hat{B} = \dfrac{d^2}{dx^2}$. Which of the above functions are eigenfunctions of $\hat{B}$? For those functions that are eigenfunctions, give the eigenvalue.

Hints / Solution / Discussion →

Follow same procedure. You should find f_1 and f_3 to be eigenfunctions, and f_4 to be not an eigenfunction. The case of f_2 is a bit trickier.

$$\hat{B} f_1(x) \;=\; \frac{d^2}{dx^2}\big[e^{ikx}\big] \;=\; -k^2 e^{ikx} \;=\; -k^2 f_1(x) \qquad \begin{cases}\text{Yes. The} \\ \text{eigenvalue is } -k^2.\end{cases}$$

$$\hat{B} f_2(x) \;=\; \frac{d^2}{dx^2}\big[ax\big] \;=\; 0 \;=\; 0\big[ax\big] \;=\; 0 f_2(x)$$

Yes; an eigenfunction with eigenvalue zero. But admittedly confusing, since you might not immediately think of 0 as being 0 times the particular function $f_2(x)$.

$$\hat{B} f_3(x) \;=\; \frac{d^2}{dx^2}\big[\cos(kx)\big] \;=\; -k^2 \cos(kx) \;=\; -k^2 f_3(x) \qquad \begin{cases}\text{Yes. The} \\ \text{eigenvalue is } -k^2.\end{cases}$$

$$\hat{B} f_4(x) \;=\; \frac{d^2}{dx^2}\big[e^{-ax^2}\big] \;=\; \frac{d}{dx}\left(-2axe^{-ax^2}\right) \;=\; \left(4a^2x^2 - 2ax\right) e^{-ax^2}$$

No. the factor $(4a^2x^2 - 2ax)$ multiplying $f_4(x) = e^{-ax^2}$ on the right is not just a number, it is itself a function of x.

4. The quantum harmonic oscillator.

We denote the orthonormalized energy eigenstates of the harmonic oscillator by $|n\rangle$, on which the creation/annihilation operators act as follows:

$$\hat{a}\,|n\rangle \;=\; \sqrt{n}\,|n-1\rangle \qquad \hat{a}^\dagger\,|n\rangle \;=\; \sqrt{n+1}\,|n+1\rangle$$

(a) Express $\hat{x}^2$ in terms of $\hat{a}$ and $\hat{a}^\dagger$. Hence show that the uncertainty of the position in the state $|n\rangle$ is

$$\Delta x \;=\; \sigma\sqrt{n+\frac{1}{2}}$$

Hints / Solution / Discussion →
Remembering $\hat{x} = \dfrac{\sigma}{\sqrt{2}}(\hat{a}^\dagger + \hat{a})$, we obtain

$$\hat{x}^2 \;=\; \frac{\sigma^2}{2}\left(\hat{a}^\dagger + \hat{a}\right)\left(\hat{a}^\dagger + \hat{a}\right) \;=\; \frac{\sigma^2}{2}\left(\hat{a}^\dagger\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}\hat{a}\right) \tag{1}$$

CAUTION!! Since $\hat{a}$ and $\hat{a}^\dagger$ do not commute, $\hat{a}^\dagger\hat{a} \neq \hat{a}\hat{a}^\dagger$. The ordering of operators matter! Thus

$$\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger \neq 2\hat{a}^\dagger\hat{a} \qquad !!!!!!$$

Instead, you could convince yourself that

$$\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger = 2\hat{a}^\dagger\hat{a} + 1$$

where 1 stands for the operator $\hat{1}$. You can use this to simplify, or simply continue with Eq. (1), as we do below.
To evaluate the uncertainty $\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2}$ in the state $|n\rangle$, we need to calculate $\langle\hat{x}\rangle = \langle n|\,\hat{x}\,|n\rangle$ and $\langle\hat{x}^2\rangle = \langle n|\,\hat{x}^2\,|n\rangle$. We first calculate the expectation values of the required ladder operator combinations:

$$\langle n|\,\hat{a}\,|n\rangle = \sqrt{n}\langle n|n-1\rangle = 0 \qquad \langle n|\,\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\langle n|n+1\rangle = 0$$

Note we are using the orthonormality of the eigenstates, $\langle m|n+1\rangle = \delta_{mn}$. Extending this calculation, one sees that $\hat{a}^\dagger\hat{a}^\dagger$ and $\hat{a}\hat{a}$ have zero expectation value, but $\hat{a}^\dagger\hat{a}$ and $\hat{a}\hat{a}^\dagger$ give nonzero contributions.

$$\langle n|\,\hat{a}\hat{a}\,|n\rangle = \sqrt{n}\langle n|\,\hat{a}\,|n-1\rangle = \sqrt{n}\sqrt{n-1}\langle n|n-2\rangle = 0$$

$$\text{Similarly,}\qquad \langle n|\,\hat{a}^\dagger\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\sqrt{n+2}\langle n|n+2\rangle = 0$$

$$\langle n|\,\hat{a}^\dagger\hat{a}\,|n\rangle = \sqrt{n}\langle n|\,\hat{a}^\dagger\,|n-1\rangle = \sqrt{n}\sqrt{n}\langle n|n\rangle = n\times 1 = n$$

$$\langle n|\,\hat{a}\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\langle n|\,\hat{a}\,|n+1\rangle = \sqrt{n+1}\sqrt{n+1}\langle n|n\rangle = n+1$$

Employing these, we obtain

$$\begin{aligned}
\langle\hat{x}\rangle &= \frac{\sigma}{\sqrt{2}}\left(\langle\hat{a}^\dagger\rangle + \langle\hat{a}\rangle\right) = 0 \\
\langle\hat{x}^2\rangle &= \frac{\sigma^2}{2}\left(\langle\hat{a}^\dagger\hat{a}^\dagger\rangle + \langle\hat{a}^\dagger\hat{a}\rangle + \langle\hat{a}\hat{a}\rangle^\dagger + \langle\hat{a}\hat{a}\rangle\right) = \frac{\sigma^2}{2}\left[0 + n + (n+1) + 0\right] \\
\Longrightarrow \qquad \langle\hat{x}^2\rangle &= \sigma^2\left(n + \frac{1}{2}\right)
\end{aligned}$$

Thus the unceratinty is

$$\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2} = \sigma\sqrt{n + \frac{1}{2}}$$

(b) Express $\hat{p}^2$ in terms of $\hat{a}$ and $\hat{a}^\dagger$. Hence calculate the uncertainty of the momentum, Δp, in the state $|n\rangle$.

Hints / Solution / Discussion →
Using $\hat{p} = \frac{i}{\sqrt{2}}\frac{\hbar}{\sigma}(\hat{a}^\dagger - \hat{a})$, we obtain

$$\hat{p}^2 = -\frac{\hbar^2}{2\sigma^2}\left(\hat{a}^\dagger - \hat{a}\right)\left(\hat{a}^\dagger - \hat{a}\right) = -\frac{\hbar^2}{2\sigma^2}\left(\hat{a}^\dagger\hat{a}^\dagger - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}\hat{a}\right)$$

The rest of the calculation is very similar to the one above.
The result is

$$\Delta p = \frac{\hbar}{\sigma}\sqrt{n + \frac{1}{2}}$$

Note that this is dimensionally correct, because $\hbar$ has the dimensions

$$\boxed{\left[\hbar\right] = \left[\text{position}\right] \times \left[\text{momentum}\right] = \left[\text{energy}\right] \times \left[\text{time}\right]}$$

This might be worth remembering, so I put it in a box. ($\hbar$ is the fundamental constant of quantum mechanics, so you might want to know what type of quantity it is, i.e., what it's dimensions are.) I remember these two ways of expressing the dimensions of $\hbar$, because I remember the uncertainty relations

$$\Delta x \Delta p \sim \hbar/2\,, \qquad \Delta E \Delta t \sim \hbar/2\,.$$

(c) Find the uncertainty product $\Delta x \Delta p$ in the state $|n\rangle$. Also express this quantity as a function of the eigenenergy E_n.

Hints / Solution / Discussion →
Multiplying the expressions for the two uncertainties:

$$\Delta x \Delta p \;=\; \hbar\left(n+\frac{1}{2}\right) \;=\; \frac{E_n}{\omega}$$

(d) If the system wavefunction at time $t = 0$ is

$$|\psi(0)\rangle \;=\; \frac{\sqrt{3}}{2}\,|2\rangle - \frac{i}{2}\,|3\rangle$$

then what is the wavefunction at a later time $t = T$? Your answer should contain the oscillator frequency ω.

Hints / Solution / Discussion →
The two eigenstates appearing in the wavefunction correspond to eigenenergies

$$\epsilon_2 = \frac{5}{2}\hbar\omega\,; \qquad \epsilon_3 = \frac{7}{2}\hbar\omega\,.$$

Hence the wavefunction at time $t = T$ is

$$\begin{aligned}|\psi(T)\rangle \;&=\; \frac{\sqrt{3}}{2}\,|2\rangle e^{-i\epsilon_2 T/\hbar} - \frac{i}{2}\,|3\rangle e^{-i\epsilon_3 T/\hbar}\\ &=\; \frac{\sqrt{3}}{2}\,|2\rangle e^{-i5\omega T/2} - \frac{i}{2}\,|3\rangle e^{-i7\omega T/2}\end{aligned}$$

(e) Given that the initial system wavefunction is

$$|\psi(0)\rangle \;=\; \frac{\sqrt{3}}{2}\,|2\rangle - \frac{i}{2}\,|3\rangle,$$

calculate the expectation value of position in the state $|\psi(t)\rangle$ as a function of time. Sketch a plot of $\langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle$ against time.

Hints / Solution / Discussion →

The state at time t is

$$|\psi(t)\rangle \;=\; \frac{\sqrt{3}}{2}\,|2\rangle e^{-i5\omega t/2} - \frac{i}{2}\,|3\rangle e^{-i7\omega t/2}$$

Therefore

$$\langle\hat{x}\rangle \;=\; \langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle$$
$$=\; \left(\frac{\sqrt{3}}{2}\langle 2|\,e^{+i5\omega t/2} - \frac{(-i)}{2}\langle 3|\,e^{+i7\omega t/2}\right)\hat{x}\left(\frac{\sqrt{3}}{2}\,|2\rangle e^{-i5\omega t/2} - \frac{i}{2}\,|3\rangle e^{-i7\omega t/2}\right)$$

with

$$\hat{x} = \frac{\sigma}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right) \ .$$

In the expression for $\langle\hat{x}\rangle$ we have the following eight matrix elements appearing:

$$\langle 2|\,\hat{a}\,|2\rangle \qquad \langle 2|\,\hat{a}\,|3\rangle \qquad \langle 3|\,\hat{a}\,|2\rangle \qquad \langle 3|\,\hat{a}\,|3\rangle$$
$$\langle 2|\,\hat{a}^\dagger\,|2\rangle \qquad \langle 2|\,\hat{a}^\dagger\,|3\rangle \qquad \langle 3|\,\hat{a}^\dagger\,|2\rangle \qquad \langle 3|\,\hat{a}^\dagger\,|3\rangle$$

Of these, only the following two are nonzero:

$$\langle 2|\,\hat{a}\,|3\rangle = \sqrt{3}\langle 2|2\rangle \;=\; \sqrt{3}\,, \qquad \langle 3|\,\hat{a}^\dagger\,|2\rangle = \sqrt{3}\langle 3|3\rangle \;=\; \sqrt{3}\,,$$

while the other matrix elements are all zero.

Please make sure you can figure out why the other matrix elements are zero. Remember that $\langle m|n\rangle = \delta_{mn}$. This means that $\langle m|\,\hat{a}\,|n\rangle$ can be nonzero only if $n = m-1$, and $\langle m|\,\hat{a}^\dagger\,|n\rangle$ can be nonzero only if $n = m+1$.

Thus

$$\langle\hat{x}\rangle \;=\; \frac{\sigma}{\sqrt{2}}\Bigg(\left[\frac{\sqrt{3}}{2}\right]e^{+i5\omega t/2}\langle 2|\,\hat{a}\,|3\rangle\left[-\frac{i}{2}\right]e^{-i7\omega t/2}$$
$$+\;\left[+\frac{i}{2}\right]e^{+i7\omega t/2}\langle 3|\,\hat{a}^\dagger\,|2\rangle\frac{\sqrt{3}}{2}e^{-i5\omega t/2}\Bigg)$$
$$=\; \frac{\sigma}{\sqrt{2}}\frac{3i}{4}\left(-e^{-i\omega t} + e^{i\omega t}\right) \;=\; \frac{\sigma}{\sqrt{2}}\frac{3i}{4}\times 2i\sin(\omega t)$$
$$=\; -\frac{3\sigma}{2\sqrt{2}}\sin(\omega t)$$

The required plot of $\langle\hat{x}\rangle$ versus time is a plot of the negative sine function.

5. (a) Show that for any three operators $\hat{A}$, $\hat{B}$, and $\hat{C}$,

$$[\hat{A}\hat{B}, \hat{C}] \;=\; \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$

Hints / Solution / Discussion →

$$\begin{aligned} \text{right side} &= \hat{A}\left(\hat{B}\hat{C} - \hat{C}\hat{B}\right) \;+\; \left(\hat{A}\hat{C} - \hat{C}\hat{A}\right)\hat{B} \\ &= \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} \;=\; \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} \\ &= \left(\hat{A}\hat{B}\right)\hat{C} - \hat{C}\left(\hat{A}\hat{B}\right) \;=\; [\hat{A}\hat{B}, \hat{C}] \;=\; \text{left side} \end{aligned}$$

(b) Use the relation $[\hat{x}, \hat{p}] = i\hbar$ and the result above to prove by mathematical induction the identity

$$[\hat{x}^n, \hat{p}] = in\hbar\hat{x}^{n-1}$$

for any positive integer n.

(If unfamiliar, please look up "mathematical induction", a standard technique for proving statements for all positive integers n.)

Hints / Solution / Discussion →

Mathematical induction (in the most common form) is a procedure for proving that a statement is true for all positive integers. It involves two steps:
(1) demonstrate the statement for $n = 1$, and
(2) show that if it is true for $n = k$ then it is also true for $n = k + 1$.
Together, these would prove the statement for all positive integers n.

First step: The statement we want to prove is clearly true for $n = 1$, since in that case it reduces to the known commutation relation between $\hat{x}$ and $\hat{p}$:

$$[\hat{x}^1, \hat{p}] \;=\; i(1)\hbar\hat{x}^0 \qquad \Longleftrightarrow \qquad [\hat{x}, \hat{p}] \;=\; i\hbar\hat{1} \;=\; i\hbar$$

Second step of mathematical induction:
Assume that the statement is true for $n = k$, i.e., that

$$[\hat{x}^k, \hat{p}] = in\hbar\hat{x}^{k-1}$$

This implies that

$$\begin{aligned}[\hat{x}^{k+1},\hat{p}] \;=\; [\hat{x}^k\hat{x},\hat{p}] \;=\; \hat{x}^k[\hat{x},\hat{p}]+[\hat{x}^k,\hat{p}]\hat{x} \;&=\; \hat{x}^k(i\hbar\hat{1})+\left(ik\hbar\hat{x}^{k-1}\right)\hat{x} \\ &=\; i\hbar\hat{x}^k+ik\hbar\hat{x}^k \;=\; i(k+1)\hbar\hat{x}^k\end{aligned}$$

i.e., that the statement is true also for $n=k+1$ if it is true for $n=k$. Hence statement is proved by mathematical induction.

Proof **without** mathematical induction:
Apply on an arbitrary function:

$$\begin{aligned}[\hat{x}^n,\hat{p}]f(x) \;&=\; \hat{x}^n\hat{p}]f(x)-\hat{p}\hat{x}^nf(x) \\ &=\; x^n\left(-i\hbar\partial_x\right)f(x)-\left(-i\hbar\partial_x\right)\left(x^nf(x)\right) \\ &=\; -i\hbar x^nf'(x)+i\hbar\left(x^nf'(x)+nx^{n-1}f(x)\right) \\ &=\; i\hbar nx^{n-1}f(x) \;=\; i\hbar n\hat{x}^{n-1}f(x)\end{aligned}$$

which indicates $[\hat{x}^n,\hat{p}]=i\hbar n\hat{x}^{n-1}$. Here we have used $\hat{x}^n=x^n$, which follows from $\hat{x}=x$.