Problem 1: Expectation Value of Observable

(a) We need to explain why the expression

$$\sum_{n=0}^{\infty} \lambda_n |c_n|^2 \tag{1}$$

represents the average of the values one would observe, if one measured the observable corresponding to some operator $\hat{O}$. We know that λ_n corresponds to the eigenvalue of the basis function $u_n(x)$. The complex amplitude c_n is defined by

$$c_n \equiv \langle u_n|\psi\rangle = \int dx \; u_n^*(x) \; \psi(x) \; ; \tag{2}$$

the modulus squared of this amplitude $|c_n|^2$ gives the probability of finding the quantum state $|\psi\rangle$ in the state $|u_n\rangle$. Therefore the probability of observing the eigenvalue λ_n is just $|c_n|^2$. The average value is just the sum of all the possible values multiplied by their corresponding probabilities, which is just expression (1).

(b) Proving that $\langle\psi|\,\hat{O}\,|\psi\rangle$ is equivalent to (1) is an exercise in using Dirac notation. By now we are used to writing wave functions as a sum of basis wave functions, such as above:

$$\psi(x) = \sum_{n=0}^{\infty} c_n \; u_n(x) \; . \tag{3}$$

In the same way, we can write quantum mechanical state vectors as linear combinations of basis kets:

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n \; |u_n\rangle \; . \tag{4}$$

If we take the hermitian adjoint of (4), we get

$$\langle\psi| = \sum_{n=0}^{\infty} \langle u_n| \; c_n^* \; . \tag{5}$$

Now take operator $\hat{O}$ and operate on (4), yielding

$$\begin{aligned} \hat{O}\,|\psi\rangle &= \hat{O}\sum_{n=0}^{\infty} c_n \; |u_n\rangle \\ &= \sum_{n=0}^{\infty} c_n \; \hat{O}\,|u_n\rangle \\ &= \sum_{n=0}^{\infty} c_n \; \lambda_n \, |u_n\rangle \; . \end{aligned} \tag{6}$$

Finally, multiply (5) and (6) to get

$$\begin{aligned}
\langle\psi|\,\hat{O}\,|\psi\rangle &= \sum_{n=0}^{\infty} \langle u_n|\; c_n^* \sum_{m=0}^{\infty} c_m\;\lambda_m\,|u_m\rangle \\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_n^* c_m\;\lambda_n\,\langle u_n|u_m\rangle \\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_n^* c_m\;\lambda_n \delta_{nm} \\
&= \sum_{n=0}^{\infty} c_n^* c_n\;\lambda_n \\
&= \sum_{n=0}^{\infty} |c_n|^2\;\lambda_n\;. \qquad (7)
\end{aligned}$$

Problem 2: Harmonic Oscillator Again

A particle in a harmonic oscillator potential starts out at $t = 0$ in a linear combination of stationary states of the oscillator. Its wave function at time $t = 0$ is

$$\psi(x, 0) = \frac{1}{4}\phi_0(x) + \frac{i}{2}\phi_1(x) + \frac{\sqrt{11}}{4}\phi_2(x) \qquad (8)$$

where the $\phi_n(x)$'s are the stationary states of the harmonic oscillator with energies $E_n = \hbar\omega(n + 1/2)$.

(a) As we've seen several times before, stationary states evolve in time by picking up a phase factor of $\exp(-iE_n t/\hbar)$, where E_n is the energy of that particular stationary state. Hence the wave function at time t is just

$$\psi(x, t) = \frac{1}{4}e^{-iE_0 t/\hbar}\phi_0(x) + \frac{i}{2}e^{-iE_1 t/\hbar}\phi_1(x) + \frac{\sqrt{11}}{4}e^{-iE_2 t/\hbar}\phi_2(x)\;. \qquad (9)$$

(b) An energy of $\frac{3}{2}\hbar\omega$ corresponds to the energy eigenvalue of $|u_1\rangle$. Therefore the probability of measuring energy $\frac{3}{2}\hbar\omega$ is equal to the probability of finding the quantum system in state $|u_1\rangle$. That probability is just the norm squared of the coefficient $c_1 = i/2$, so the probability is $1/4$.

(c) Here's a cute little demonstration of why the the stationary states $|\phi_n\rangle$ are orthogonal. The hamiltonian operator can operator either to the right, on a ket, or to the left, on a bra. That means that

$$\hat{H}\,|\phi_n\rangle = E_n\,|\phi_n\rangle \qquad (10)$$

and

$$\langle \phi_n | \hat{H} = \langle \phi_n | E_n \ . \tag{11}$$

Now if we let $\hat{H}$ operate to the left and to the right in the expression $\langle \phi_n | \hat{H} | \phi_m \rangle$, and realize that these two expressions must be equal to each other, we find:

$$\begin{aligned} \langle \phi_n | \hat{H} | \phi_m \rangle &= E_m \langle \phi_n | \phi_m \rangle \ ; & (12) \\ \langle \phi_n | \hat{H} | \phi_m \rangle &= E_n \langle \phi_n | \phi_m \rangle \ ; \ \text{therefore} & (13) \\ (E_m - E_n) \langle \phi_n | \phi_m \rangle &= 0 \ . & (14) \end{aligned}$$

But we know that the energy eigenvalues for the harmonic oscillator are nondegenerate; that is, if $n \neq m$ then $E_n \neq E_m$. Hence the $|\phi_n\rangle$'s are orthogonal to each other. Moreover, we are free to normalize them any way we please since the expression we just derived places no restriction on the normalization constant.

Thus the functions $\phi_n(x)$, which are just the position-space representation of the corresponding kets $\langle x | \phi_n \rangle \equiv \phi_n(x)$, can be made orthonormal.

(d) To evaluate the expectation value of x, we could write out the wave functions for $\phi_0(x)$, $\phi_1(x)$, and $\phi_2(x)$, then do a bunch of integrals. But it's algebraically simpler (though entire equivalent) to work with the raising and lowering operators. When we work with these operators, in a sense we are using a shorthand notation for integration by parts.

Using the definitions of $\hat{a}$ and $\hat{a}\dagger$, we find that the position operator $\hat{x}$ can be written as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \, (a + a\dagger) \tag{15}$$

where a and $a\dagger$ are the lowering and raising (annihilation and creation) operators. Operating on $\psi(x,t)$ with a, we get

$$a \ \psi(x,t) = \frac{i}{2} e^{-iE_1 t/\hbar} + \frac{\sqrt{22}}{4} e^{-iE_2 t/\hbar} \phi_2(x) \ , \tag{16}$$

and operating with $a\dagger$ gives us

$$a\dagger \ \psi(x,t) = \frac{1}{4} e^{-iE_0 t/\hbar} \phi_1(x) + \frac{i\sqrt{2}}{2} e^{-iE_1 t/\hbar} \phi_2(x) + \ldots \phi_3(x) \ . \tag{17}$$

We may as well ignore the $\phi_3(x)$ part because when we take the scalar product with $\psi(x,t)$, which contains no $\phi_3(x)$ term, that part will just drop out. So, combining the above two expressions,

$$\begin{aligned} \sqrt{\frac{\hbar}{2m\omega}} \, (a + a\dagger) \, \psi(x,t) &= \sqrt{\frac{\hbar}{2m\omega}} \left[\frac{i}{2} e^{-iE_1 t/\hbar} \phi_0(x) \right. \\ &+ \left(\frac{\sqrt{22}}{4} e^{-iE_2 t/\hbar} + \frac{1}{4} e^{-iE_0 t/\hbar} \right) \phi_1(x) \\ &+ \left. \frac{i\sqrt{2}}{2} e^{-iE_1 t/\hbar} \phi_2(x) + \ldots \right] \qquad (18) \end{aligned}$$

Now we take the dot product of this expression with $\langle\psi|$. This is equivalent to multiplying by $\psi^*(x)$ and integrating over all x. Either way, since the $\phi_n(x)$ are orthonormal, when we integrate (or take the dot product), we only keep the direct terms, which integrate to 1, and ignore the cross terms like $\phi_0(x)\phi_1(x)$, which are orthogonal to each other. The three terms that remain comprise the expectation value we are looking for.

$$
\begin{aligned}
\langle x\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{1}{4}e^{+iE_0t/\hbar}\frac{i}{2}e^{-iE_1t/\hbar}\right. \\
&+ \frac{i}{2}e^{+iE_1t/\hbar}\left(\frac{\sqrt{22}}{4}e^{-iE_2t/\hbar}+\frac{1}{4}e^{-iE_0t/\hbar}\right) \\
&+ \left.\frac{\sqrt{11}}{4}e^{+iE_2t/\hbar}\frac{i\sqrt{2}}{2}e^{-iE_1t/\hbar}\right] \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{i}{8}e^{-i\omega t}-\frac{\sqrt{22}i}{8}e^{-i\omega t}-\frac{i}{8}e^{i\omega t}+\frac{\sqrt{22}i}{8}e^{i\omega t}\right] \\
&= \sqrt{\frac{\hbar}{2m\omega}}\frac{i}{8}(\sqrt{22}-1)(e^{i\omega t}-e^{-i\omega t}) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1-\sqrt{22}}{4}\right)\sin\omega t\ . \qquad (19)
\end{aligned}
$$

Problem 3: Electron in a Box

The electron starts out at time $t = 0$ with a wave function $\psi(x, t = 0)$ corresponding to the ground state wave function of a box of width a:

$$\psi(x,0)=\phi_0^a(x)=\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} \qquad 0<x<a\ . \tag{20}$$

When the wall at $x = a$ is suddenly moved to $x = 2a$, the electron's wave function no longer corresponds to a stationary state of the system. There will, therefore, be some nonzero probabilities for finding the electron in one of many different stationary states of the new system.

Denote the new stationary states by $\phi_n^{2a}(x)$. These have the form

$$\phi_n^{2a}(x)=\sqrt{\frac{1}{a}}\sin\frac{n\pi x}{2a} \qquad 0<x<2a\ . \tag{21}$$

Since the new basis states form a complete orthonormal basis, we can write $\psi(x, 0)$ as a linear combination of the these states in the usual way. Then, by multiplying by one of the basis states, integrating, and applying the orthonormality property, we find that the amplitude c_n for finding the the electron in the n^{th} state is

$$
\begin{aligned}
c_n &= \int_0^{2a} \phi_n^{2a}(x)\ \phi_0^a(x)\ dx \\
&= \int_0^a \left(\sqrt{\frac{1}{a}}\sin\frac{n\pi x}{2a}\right)\left(\sqrt{\frac{2}{a}}\ \sin\frac{\pi x}{a}\right) dx\ . \qquad (22)
\end{aligned}
$$

We only integrate up to $x = a$ because $\phi_0^a(x)$ equals 0 for $x > a$. Now we have a formula for each of the c_n's, and hence the probabilities for finding the electron in any particular state.

(a) The ground state correponds to $n = 1$. Applying Eq. 22, we get $c_1 = 4\sqrt{2}/3\pi$, so that the probability of finding the electron in the ground state is $32/9\pi^2 \approx 0.36$.

(b) For the first excited state, $n = 2$. The result is $c_2 = 1/\sqrt{2}$, so that the corresponding probability is $1/2$.

(c) Notice that the first few stationary states of the box with width a are

$$
\begin{aligned}
\phi_n^a(x) &\propto \sin\frac{n\pi x}{a} \\
&= \sin\frac{\pi x}{a},\ \sin\frac{2\pi x}{a},\ \sin\frac{3\pi x}{a}\ldots \qquad (23)
\end{aligned}
$$

while the stationary state wave functions of the $2a$-width box are

$$
\begin{aligned}
\phi_n^{2a}(x) &\propto \sin\frac{n\pi x}{2a} \\
&= \sin\frac{1\pi x}{2a},\ \sin\frac{2\pi x}{2a},\ \sin\frac{3\pi x}{2a},\ \sin\frac{4\pi x}{2a}\ \sin\frac{5\pi x}{2a},\ \sin\frac{6\pi x}{2a}\ldots \qquad (24)
\end{aligned}
$$

Notice that the 4^{th}, 6^{th}, etc. states of the new basis are equal, up to a normalization constant, to the 2^{nd}, 3^{rd}, etc. states of the old basis. But each of these states must be orthogonal to the the ground state of the old basis, which is exactly what $\psi(x, 0)$ is. Therefore, the coefficients $c_4, c_6, c_8, \ldots$ must all equal zero, so that the probability of finding the electron in these states is also zero.