PHYS-C0252 - Quantum Mechanics

Exercise set 2 - model solutions

Due date: May 8, 2024 by 23:59 on MyCourses
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You can write by hand and take pictures, use digital note-taking or LaTeX etc.

1. A quantum system described by a Hamiltonian $\hat{H}$ is in the state

$$|\psi\rangle = N\left[\frac{\mathrm{i}}{\sqrt{3}}|\phi_1\rangle - \frac{1}{\sqrt{2}}(-3+5\mathrm{i})|\phi_2\rangle + \frac{2}{\sqrt{5}}|\phi_3\rangle + \sqrt{7}|\phi_4\rangle\right],$$

where $|\phi_n\rangle$ are the eigenstates of energy such that $\hat{H}|\phi_n\rangle = nE_0|\phi_n\rangle$, E_0 has units of energy, and $N \in \mathbb{R}$.

(a) Find a suitable scalar N such that $|\psi\rangle$ is normalized.

(b) Let the energy of $|\psi\rangle$ be measured. Give all possible measurement results and their corresponding probabilities. Assume that the measurement is ideal, i.e., no measurement errors occur.

(c) What is the expectation value of the energy when the system is in the state $|\psi\rangle$? Is it a possible measurement result if the energy is measured?

(d) Consider an operator $\hat{X}$, the action of which on $|\phi_n\rangle$ ($n = 1, 2, 3, 4$) is defined by $\hat{X}|\phi_n\rangle = (n-3)x_0|\phi_n\rangle$, where x_0 is a real-valued scalar. Suppose that a measurement of the energy of the above-defined $|\psi\rangle$ yields $2E_0$. Assume that immediately afterwards, we ideally measure the physical quantity corresponding to $\hat{X}$. What is the value for the quantity obtained in the latter measurement?

Solution:

(a)

$$\langle\psi|\psi\rangle = 1$$

$$\Leftrightarrow N^2\Big[\underbrace{\frac{|\mathrm{i}|^2}{3}}_{=\frac{1}{3}}\langle\phi_1|\phi_1\rangle + \underbrace{\frac{1}{2}|-3+5\mathrm{i}|^2}_{=17}\langle\phi_2|\phi_2\rangle + \frac{4}{5}\langle\phi_3|\phi_3\rangle + 7\langle\phi_4|\phi_4\rangle\Big] = N^2\cdot\frac{377}{15} = 1$$

$$\Rightarrow N = \sqrt{\frac{15}{377}}.$$

(b)

$$E_1 = E_0, \quad E_2 = 2E_0, \quad E_3 = 3E_0, \quad E_4 = 4E_0.$$

$$P(E_1) = |\langle\phi_1|\psi\rangle|^2 = \left|\sqrt{\frac{15}{377}}\cdot\frac{\mathrm{i}}{\sqrt{3}}\right|^2 = \frac{5}{377},$$

$$P(E_2) = |\langle\phi_2|\psi\rangle|^2 = \left|\sqrt{\frac{15}{377}} \cdot -\frac{1}{\sqrt{2}}(-3+5\mathrm{i})\right|^2 = \frac{255}{377},$$

$$P(E_3) = |\langle\phi_3|\psi\rangle|^2 = \left|\sqrt{\frac{15}{377}} \cdot \frac{2}{\sqrt{5}}\right|^2 = \frac{12}{377},$$

$$P(E_4) = |\langle\phi_4|\psi\rangle|^2 = \left|\sqrt{\frac{15}{377}} \cdot \sqrt{7}\right|^2 = \frac{105}{377}.$$

(c) The expectation value of the energy is

$$\begin{aligned}\langle\hat{H}\rangle_\psi &= \sum_{n=1}^{4} E_n P(E_n) = \frac{5}{377}\underbrace{E_0}_{E_1} + \frac{255}{377}\underbrace{2E_0}_{E_2} + \frac{12}{377}\underbrace{3E_0}_{E_3} + \frac{105}{377}\underbrace{4E_0}_{E_4} \\ &= \frac{971}{377}E_0 \approx 2.58E_0.\end{aligned}$$

This isn't any of the eigenenergies E_n, so it is not possible to obtain the expectation value $\frac{971}{377}E_0$ if the energy is measured.

(d) An energy measurement that yields $2E_0$ implies that the system collapses to the state $|\phi_2\rangle$, and

$$\hat{X}|\phi_2\rangle = (2-3)x_0|\phi_2\rangle = -x_0\,|\phi_2\rangle\,.$$

Thus if we measure $\hat{X}$ immediately afterwards, we obtain $-x_0$.

2. Consider the raising and lowering operators of a one-dimensional harmonic oscillator, $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p})$ and $\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p})$, which satisfy

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

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

Show that $[\hat{N}, \hat{a}] = -\hat{a}$ and $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$, where $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator.

Solution: Using the identities

$$[\hat{a}, \hat{a}^\dagger] = 1, \qquad [\hat{a}^\dagger, \hat{a}] = -1, \qquad [\hat{a}^\dagger, \hat{a}^\dagger] = [\hat{a}, \hat{a}] = 0,$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \quad \forall \hat{A}, \hat{B}, \hat{C} \in \mathcal{L}(\mathcal{H}),$$

we have

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger\hat{a}, \hat{a}] = \hat{a}^\dagger[\hat{a}, \hat{a}] + [\hat{a}^\dagger, \hat{a}]\hat{a} = -\hat{a}$$
$$[\hat{N}, \hat{a}^\dagger] = [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}^\dagger]\hat{a} = \hat{a}^\dagger$$

3. Let's have another swing at the one-dimensional harmonic oscillator. Suppose that the oscillator is prepared in one of the eigenstates of the Hamiltonian, $|\psi\rangle = |n\rangle$, where $n \in \{0, 1, 2, \ldots\}$.

   (a) What is the variance in the energy of the system in the state $|\psi\rangle$? Hint: Recall that the Hamiltonian operator is an observable that corresponds to the total energy of the system.

(b) Express the position operator $\hat{q}$ and the momentum operator $\hat{p}$ in terms of the ladder operators $\hat{a}$ and $\hat{a}^\dagger$.

(c) Verify the validity of the Heisenberg uncertainty relation by evaluating the product $\Delta q \Delta p$. Hint: Use the expressions found in part (b) and take advantage of the rules that the ladder operators obey when acting on the eigenstates $|n\rangle$ (see Exercise 2). Also note that $\langle n|m\rangle = \delta_{nm}$.

(d) For which n is the Heisenberg uncertainty minimized, i.e. $\Delta q \Delta p = \hbar/2$?

Solution:

(a) Since Hamiltonian operator $\hat{H}$ is an observable that corresponds to the total energy of the system, we may obtain the energy variance as:

$$\Delta E^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = \langle \psi | \hat{H}^2 | \psi \rangle - \langle \psi | \hat{H} | \psi \rangle^2 .$$

Hamiltonian for the one-dimensional harmonic oscillator is given by

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) = \hbar\omega \left(\hat{N} + \frac{1}{2} \right),$$

where $\hat{N}$ is the so-called number operator that acts on the Hamiltonian eigenstates $|n\rangle$ as $\hat{N}|n\rangle = n|n\rangle$. Noting that we have prepared the oscillator in one of the eigenstates of the Hamiltonian, action of the Hamiltonian on $|\psi\rangle = |n\rangle$ is simply

$$\begin{aligned} \hat{H}|\psi\rangle = \hat{H}|n\rangle &= \hbar\omega \left(\hat{N} + \frac{1}{2} \right)|n\rangle = \hbar\omega\hat{N}|n\rangle + \frac{1}{2}\hbar\omega|n\rangle \\ &= \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle . \end{aligned}$$

By noting that $\hat{H}^2 = \hat{H}\hat{H}$, we can also compute action of $\hat{H}^2$ on $|\psi\rangle$ quite straightforwardly using the above result:

$$\begin{aligned} \hat{H}^2|\psi\rangle = \hat{H}^2|n\rangle &= \hat{H}\left(\hat{H}|n\rangle\right) = \hat{H}\hbar\omega\left(n + \frac{1}{2}\right)|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)\left(\hat{H}|n\rangle\right) \\ &= \left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2 |n\rangle . \end{aligned}$$

Putting everything together and recalling that $\langle m|n\rangle = \delta_{mn} \Rightarrow \langle n|n\rangle = 1$ we finally compute the desired energy variance:

$$\begin{aligned} \Delta E^2 = \langle n|\hat{H}^2|n\rangle - \langle n|\hat{H}|n\rangle^2 &= \langle n|\left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2|n\rangle - \left[\langle n|\hbar\omega\left(n + \frac{1}{2}\right)|n\rangle\right]^2 \\ &= \left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2\langle n|n\rangle - \left[\hbar\omega\left(n + \frac{1}{2}\right)\langle n|n\rangle\right]^2 \\ &= \left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2 \cdot 1 - \left[\hbar\omega\left(n + \frac{1}{2}\right) \cdot 1\right]^2 \\ &= \left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2 - \left[\hbar\omega\left(n + \frac{1}{2}\right)\right]^2 = 0. \end{aligned}$$

Thus we conclude that the energy variance associated with the state prepared in the eigenstate of the Hamiltonian is zero!

More generally, given an observable $\hat{\Lambda}$ with a *non-degenerate* spectrum $\{\lambda_i\}$ and the corresponding set of orthonormal eigenstates $\{|\lambda_i\rangle\}$, the variance associated with an outcome of the measurement of $\hat{\Lambda}$ provided that the system is in one of the eigenstates $|\lambda_i\rangle$ immediately prior to the measurement will be exactly zero.

(b) To construct position and momentum operators from the ladder operators given by $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p})$ and $\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p})$, note that one can isolate $\hat{q}$ by adding $\hat{a}$ and $\hat{a}^\dagger$:

$$\hat{a} + \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}) + \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p}) = 2\sqrt{\frac{m\omega}{2\hbar}}\hat{q} = \sqrt{\frac{2m\omega}{\hbar}}\hat{q}$$
$$\Rightarrow \hat{q} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right).$$

Similarly, one can isolate $\hat{p}$ by subtracting $\hat{a}^\dagger$ from $\hat{a}$:

$$\hat{a} - \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}) - \sqrt{\frac{m\omega}{2\hbar}}(\hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p}) = \frac{2\mathrm{i}}{m\omega}\sqrt{\frac{m\omega}{2\hbar}}\hat{p} = \mathrm{i}\sqrt{\frac{2}{\hbar m\omega}}\hat{p}$$
$$\Rightarrow \hat{p} = \frac{1}{\mathrm{i}}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right) = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right).$$

(c) We proceed by direct computation:

$$\begin{aligned}
\langle\hat{q}\rangle &= \langle\psi|\,\hat{q}\,|\psi\rangle = \langle n|\,\hat{q}\,|n\rangle = \langle n|\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right)|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\hat{a}^\dagger + \hat{a}\right)|n\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\hat{a}^\dagger|n\rangle + \hat{a}|n\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,|n-1\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\langle n|n+1\rangle + \sqrt{n}\,\langle n|n-1\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\cdot 0 + \sqrt{n}\cdot 0\right) \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\langle\hat{p}\rangle &= \langle\psi|\,\hat{p}\,|\psi\rangle = \langle n|\,\hat{p}\,|n\rangle = \langle n|\,\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right)|n\rangle = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\langle n|\left(\hat{a}^\dagger - \hat{a}\right)|n\rangle \\
&= \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\langle n|\left(\hat{a}^\dagger|n\rangle - \hat{a}|n\rangle\right) = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\langle n|\left(\sqrt{n+1}\,|n+1\rangle - \sqrt{n}\,|n-1\rangle\right) \\
&= \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\,\langle n|n+1\rangle - \sqrt{n}\,\langle n|n-1\rangle\right) = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\cdot 0 - \sqrt{n}\cdot 0\right) \\
&= 0
\end{aligned}$$

$$
\begin{aligned}
\langle \hat{q}^2 \rangle = \langle \psi | \hat{q}^2 | \psi \rangle = \langle n | \hat{q}^2 | n \rangle = \langle n | \left[\sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}^\dagger + \hat{a} \right) \right]^2 | n \rangle = \frac{\hbar}{2m\omega} \langle n | \left(\hat{a}^\dagger + \hat{a} \right)^2 | n \rangle \\
&= \frac{\hbar}{2m\omega} \langle n | \left(\hat{a}^\dagger \hat{a}^\dagger + \hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}\hat{a} \right) | n \rangle \\
&= \frac{\hbar}{2m\omega} \langle n | \left(\hat{a}^\dagger \hat{a}^\dagger | n \rangle + \hat{a}^\dagger \hat{a} | n \rangle + \hat{a}\hat{a}^\dagger | n \rangle + \hat{a}\hat{a} | n \rangle \right) \\
&= \frac{\hbar}{2m\omega} \langle n | \left(\hat{a}^\dagger \sqrt{n+1} | n+1 \rangle + \hat{a}^\dagger \sqrt{n} | n-1 \rangle + \hat{a}\sqrt{n+1} | n+1 \rangle + \hat{a}\sqrt{n} | n-1 \rangle \right) \\
&= \frac{\hbar}{2m\omega} \langle n | \left(\sqrt{n+2}\sqrt{n+1} | n+2 \rangle + \sqrt{n}\sqrt{n} | n \rangle + \sqrt{n+1}\sqrt{n+1} | n \rangle + \sqrt{n-1}\sqrt{n} | n-2 \rangle \right) \\
&= \frac{\hbar}{2m\omega} \left(\sqrt{n+2}\sqrt{n+1} \langle n | n+2 \rangle + n \langle n | n \rangle + (n+1) \langle n | n \rangle + \sqrt{n-1}\sqrt{n} \langle n | n-2 \rangle \right) \\
&= \frac{\hbar}{2m\omega} \left(\sqrt{n+2}\sqrt{n+1} \cdot 0 + n \cdot 1 + (n+1) \cdot 1 + \sqrt{n-1}\sqrt{n} \cdot 0 \right) \\
&= \frac{\hbar}{2m\omega} (2n+1)
\end{aligned}
$$

$$
\begin{aligned}
\langle \hat{p}^2 \rangle = \langle \psi | \hat{p}^2 | \psi \rangle = \langle n | \hat{p}^2 | n \rangle = \langle n | \left[\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}} \left(\hat{a}^\dagger - \hat{a} \right) \right]^2 | n \rangle = -\frac{\hbar m\omega}{2} \langle n | \left(\hat{a}^\dagger - \hat{a} \right)^2 | n \rangle \\
&= -\frac{\hbar m\omega}{2} \langle n | \left(\hat{a}^\dagger \hat{a}^\dagger - \hat{a}^\dagger \hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}\hat{a} \right) | n \rangle \\
&= -\frac{\hbar m\omega}{2} \langle n | \left(\hat{a}^\dagger \hat{a}^\dagger | n \rangle - \hat{a}^\dagger \hat{a} | n \rangle - \hat{a}\hat{a}^\dagger | n \rangle + \hat{a}\hat{a} | n \rangle \right) \\
&= -\frac{\hbar m\omega}{2} \langle n | \left(\hat{a}^\dagger \sqrt{n+1} | n+1 \rangle - \hat{a}^\dagger \sqrt{n} | n-1 \rangle - \hat{a}\sqrt{n+1} | n+1 \rangle + \hat{a}\sqrt{n} | n-1 \rangle \right) \\
&= -\frac{\hbar m\omega}{2} \langle n | \left(\sqrt{n+2}\sqrt{n+1} | n+2 \rangle - \sqrt{n}\sqrt{n} | n \rangle - \sqrt{n+1}\sqrt{n+1} | n \rangle + \sqrt{n-1}\sqrt{n} | n-2 \rangle \right) \\
&= -\frac{\hbar m\omega}{2} \left(\sqrt{n+2}\sqrt{n+1} \langle n | n+2 \rangle - n \langle n | n \rangle - (n+1) \langle n | n \rangle + \sqrt{n-1}\sqrt{n} \langle n | n-2 \rangle \right) \\
&= -\frac{\hbar m\omega}{2} \left(\sqrt{n+2}\sqrt{n+1} \cdot 0 - n \cdot 1 - (n+1) \cdot 1 + \sqrt{n-1}\sqrt{n} \cdot 0 \right) \\
&= \frac{\hbar m\omega}{2} (2n+1)
\end{aligned}
$$

Note that one can save themselves a bit of trouble by realizing that only the terms that have an equal amount of creation and annihilation operators (i.e. terms of form $\langle n | \hat{a}^\dagger \hat{a} | n \rangle$ and $\langle n | \hat{a}\hat{a}^\dagger | n \rangle$) yield non-zero average contributions due to orthogonality of different number operator eigenstates.

Now we can get the desired uncertainties (that is, square roots of variance) of position and momentum:

$$
\begin{aligned}
\Delta q &= \sqrt{\Delta q^2} = \sqrt{\langle \hat{q}^2 \rangle - \langle \hat{q} \rangle^2} = \sqrt{\frac{\hbar}{2m\omega} (2n+1) - 0^2} = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)}, \\
\Delta p &= \sqrt{\Delta p^2} = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \sqrt{\frac{\hbar m\omega}{2} (2n+1) - 0^2} = \sqrt{\hbar m\omega \left(n + \frac{1}{2} \right)}.
\end{aligned}
$$

Finally, the Heisenberg uncertainty is obtained by straightforward multiplication:

$$\Delta q \Delta p = \sqrt{\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)}\sqrt{\hbar m\omega\left(n+\frac{1}{2}\right)} = \hbar\left(n+\frac{1}{2}\right)$$

Observe that since $n \in \{0, 1, \dots\}$, we indeed have that $\Delta q \Delta p \geq \hbar/2$, just as Heisenberg postulated!

(d) We obtain the minimal uncertainty $\Delta q \Delta p = \hbar/2$ when $n = 0$, i.e. our system is in its ground state $|\psi\rangle = |0\rangle$. Allow me to take a brief mathematical detour to give a bit of context to this result (feel free to skip it).

Later on you will learn about the position basis for wavefunctions. For the quantum harmonic oscillator, ground state in the position representation is in fact a Gaussian distribution. One of the many fascinating properties of this distribution is that a Fourier transformation of a Gaussian function is itself a Gaussian function! It is in fact the only type of function in Fourier theory that has this property. Generally, the more localized the function is, the less localized its Fourier transform will be and vice versa. More precisely, one can prove an "uncertainty" principle in Fourier theory that states that the width of the signal in time Δt and the corresponding width of its Fourier transform in frequency domain $\Delta\omega$ obey the inequality $\Delta\omega\Delta t \geq 1/2$, where the lower bound is reached for the Gaussian function.

Significance of this particular property comes into play in the physical context when coupled with the fact that one can convert from position representation to momentum representation by means of a Fourier transform! That is to say, for a quantum harmonic oscillator, the ground state has the same functional form both in position and in momentum space, and the lower bound of the Heisenberg uncertainty is reached as a consequence of the result from Fourier theory. Yet the most fascinating of all is the fact that the uncertainty principle emerges regardless of whether we work in discrete or in continuous basis, which in turn can be traced down to the fact that L^2–space of square integrable functions is isometrically isomorphic to the l^2–space of sequences with a finite norm induced by the inner product.

4. Consider the pendulum discussed on Lecture 3, where the potential energy is given by $V(\theta) = mgl(1 - \cos\theta)$.

   (a) Following the steps in the lecture notes, derive the classical Hamiltonian of the pendulum *without* making the approximation $1 - \cos\theta \approx \theta^2/2$. Use $q = \theta$ as the generalized coordinate.

   (b) Expand the cosine in the Hamiltonian up to fourth order in θ and replace the canonical coordinates with operators: $\theta \to \hat{\theta}$, $p \to \hat{p}$ to obtain a quantized Hamiltonian. Note that this is now an *an*harmonic oscillator, since there are terms that are higher than second order. Write the Hamiltonian using the harmonic ladder operators

$$\hat{a} = \sqrt{\frac{ml^2\omega}{2\hbar}}\left(\hat{\theta} + \frac{\mathrm{i}}{ml^2\omega}\hat{p}\right),$$
$$\hat{a}^\dagger = \sqrt{\frac{ml^2\omega}{2\hbar}}\left(\hat{\theta} - \frac{\mathrm{i}}{ml^2\omega}\hat{p}\right),$$

where $\omega = \sqrt{g/l}$ as in the lecture notes.

(c) Calculate the expectation values $\langle 0|\hat{H}|0\rangle$, $\langle 1|\hat{H}|1\rangle$ and $\langle 2|\hat{H}|2\rangle$ using the relations

$$\begin{aligned}\hat{a}^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle\\ \hat{a}|n\rangle &= \sqrt{n}\,|n-1\rangle,\\ \hat{a}|0\rangle &= 0,\\ \langle n|m\rangle &= \delta_{nm}.\end{aligned}$$

The interesting observation from the above result is that the energy differences $\Delta E_{12} = \langle 2|\hat{H}|2\rangle - \langle 1|\hat{H}|1\rangle$ and $\Delta E_{01} = \langle 1|\hat{H}|1\rangle - \langle 0|\hat{H}|0\rangle$ are equal in the case of the harmonic oscillator, but different for the anharmonic oscillator.

Solution:

(a) The potential energy is as given, and the kinetic energy is the same as in the lecture notes, so the Lagrangian is

$$L = T - V = \frac{1}{2}ml^2\dot{\theta}^2 - mgl(1-\cos\theta).$$

From this, we find the generalized momentum, and use it to express $\dot{\theta}$:

$$p = \frac{\partial L}{\partial\dot{\theta}} = ml^2\dot{\theta} \Rightarrow \dot{\theta} = \frac{p}{ml^2}.$$

The classical Hamiltonian is then

$$\begin{aligned}H = \dot{\theta}p - L &= \dot{\theta}\cdot ml^2\dot{\theta} - \left(\frac{1}{2}ml^2\dot{\theta}^2 - mgl(1-\cos\theta)\right)\\ &= \frac{1}{2}ml^2\dot{\theta}^2 + mgl(1-\cos\theta)\\ &= \frac{p^2}{2ml^2} + mgl(1-\cos\theta),\end{aligned}$$

where in the last step, we have used Eq. (1).

(b) Expanding the cosine using

$$\cos x \approx 1 - \frac{x^2}{2} + \frac{x^4}{24} + \cdots \Rightarrow 1 - \cos x \approx \frac{x^2}{2} - \frac{x^4}{24} + \cdots,$$

we find

$$H \approx \frac{p^2}{2ml^2} + \frac{1}{2}mgl\theta^2 - \frac{1}{24}mgl\theta^4.$$

The quantized Hamiltonian is thus

$$\hat{H} = \frac{\hat{p}^2}{2ml^2} + \frac{1}{2}mgl\hat{\theta}^2 - \frac{1}{24}mgl\hat{\theta}^4.$$

From the given definitions of $\hat{a}$ and $\hat{a}^\dagger$, we find

$$\begin{aligned}
\hat{a} + \hat{a}^\dagger &= 2\sqrt{\frac{ml^2\omega}{2\hbar}}\hat{\theta} \Rightarrow \hat{\theta} = \sqrt{\frac{\hbar}{2ml^2\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \Rightarrow \hat{\theta}^2 = \frac{\hbar}{2ml^2\omega}\left(\hat{a} + \hat{a}^\dagger\right)^2 \\
&\Rightarrow \frac{1}{2}mgl\hat{\theta}^2 = \frac{\hbar g}{4l\omega}\left(\hat{a} + \hat{a}^\dagger\right)^2 = \frac{\hbar\omega}{4}\left(\hat{a} + \hat{a}^\dagger\right)^2, \\
\hat{a} - \hat{a}^\dagger &= \frac{2i}{ml^2\omega}\sqrt{\frac{ml^2\omega}{2\hbar}}\hat{p} \Rightarrow \hat{p} = -i\sqrt{\frac{\hbar ml^2\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right) \Rightarrow \hat{p}^2 = -\frac{\hbar ml^2\omega}{2}\left(\hat{a} - \hat{a}^\dagger\right)^2 \\
&\Rightarrow \frac{\hat{p}^2}{2ml^2} = -\frac{\hbar\omega}{4}(\hat{a} - \hat{a}^\dagger)^2,
\end{aligned}$$

and

$$\hat{\theta}^4 = \frac{\hbar^2}{4m^2l^4\omega^2}\left(\hat{a} + \hat{a}^\dagger\right)^4 \Rightarrow \frac{1}{24}mgl\hat{\theta}^4 = \frac{\hbar^2 g}{96ml^3\omega^2}\left(\hat{a} + \hat{a}^\dagger\right)^4 = \frac{\hbar^2}{96ml^2}\left(\hat{a} + \hat{a}^\dagger\right)^4.$$

With these, we have

$$\hat{H} = -\frac{\hbar\omega}{4}(\hat{a} - \hat{a}^\dagger)^2 + \frac{\hbar\omega}{4}\left(\hat{a} + \hat{a}^\dagger\right)^2 - \frac{\hbar^2}{96ml^2}\left(\hat{a} + \hat{a}^\dagger\right)^4.$$

Now, we note that

$$\begin{aligned}
\left(\hat{a} + \hat{a}^\dagger\right)^2 - \left(\hat{a} - \hat{a}^\dagger\right)^2 &= \hat{a}^2 + (\hat{a}^\dagger)^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} - \left(\hat{a}^2 + (\hat{a}^\dagger)^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\right) \\
&= 2\hat{a}^\dagger\hat{a} + 2\hat{a}\hat{a}^\dagger = 2\hat{a}^\dagger\hat{a} + 2(1 + \hat{a}^\dagger\hat{a}) \\
&= 4\hat{a}^\dagger\hat{a} + 2,
\end{aligned}$$

so that

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) - \frac{\hbar^2}{96ml^2}(\hat{a} + \hat{a}^\dagger)^4.$$

(c) You don't actually have to do the following proof as long as you understand the point; it's enough to state the underlined result. It's also possible to do the exercise by brute force and not use this result at all. The actual solution to the problem begins after the last italicized sentence.

Consider an inner product of the general form

$$\langle m|\hat{a}^{i_1}(\hat{a}^\dagger)^{j_1}\hat{a}^{i_2}(\hat{a}^\dagger)^{j_2}...\hat{a}^{i_n}(\hat{a}^\dagger)^{j_n}|m\rangle,$$

i.e. $\langle m|\hat{A}|m\rangle$, where *$\hat{A}$ is some arbitrary product of $\hat{a}$'s and $\hat{a}^\dagger$'s*. Using the definitions of $\hat{a}$ and $\hat{a}^\dagger$ given in the problem statement, we can easily determine $\hat{A}|m\rangle$

up to a constant:

$$\begin{aligned}
&\hat{a}^{i_1}(\hat{a}^\dagger)^{j_i}\hat{a}^{i_2}(\hat{a}^\dagger)^{j_2}...\hat{a}^{i_n}(\hat{a}^\dagger)^{j_n}|m\rangle \\
&\propto \hat{a}^{i_1}(\hat{a}^\dagger)^{j_i}\hat{a}^{i_2}(\hat{a}^\dagger)^{j_2}...\hat{a}^{i_n}|m+j_n\rangle \\
&\propto \hat{a}^{i_1}(\hat{a}^\dagger)^{j_i}\hat{a}^{i_2}(\hat{a}^\dagger)^{j_2}...(\hat{a}^\dagger)^{j_{n-1}}|m+j_n-i_n\rangle \\
&\cdots \\
&\propto |m+j_1+j_2+...+j_n-i_1-i_2-...-i_n\rangle
\end{aligned}$$

So,

$$\begin{aligned}
\langle m|\hat{a}^{i_1}(\hat{a}^\dagger)^{j_i}\hat{a}^{i_2}(\hat{a}^\dagger)^{j_2}...\hat{a}^{i_n}(\hat{a}^\dagger)^{j_n}|m\rangle &\propto \langle m|m+j_1+j_2+...+j_n-i_1-i_2-...-i_n\rangle \\
&= \delta_{m,(m+j_1+j_2+..+j_n-i_1-i_2-...-i_n)} \\
&= \delta_{(j_1+j_2+...+j_n),(i_1+i_2+...+i_n)},
\end{aligned}$$

which is to say *the inner product $\langle m|\hat{A}|m\rangle$ is nonzero if and only if $\hat{A}$ has the same number of $\hat{a}$'s and $\hat{a}^\dagger$'s.*

We can then compute the expectation values as

$$\begin{aligned}
\langle n|\hat{H}|n\rangle &= \langle n|\left[\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)-\frac{\hbar^2}{96ml^2}(\hat{a}+\hat{a}^\dagger)^4\right]|n\rangle \\
&= \langle n|\,\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)|n\rangle - \langle n|\,\frac{\hbar^2}{96ml^2}(\hat{a}+\hat{a}^\dagger)^4\,|n\rangle \\
&= \hbar\omega\left(n+\frac{1}{2}\right)-\frac{\hbar^2}{96ml^2}\langle n|\,(\hat{a}+\hat{a}^\dagger)^4\,|n\rangle\,.
\end{aligned}$$

The expression $(\hat{a}+\hat{a}^\dagger)^4 = (\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger)$ contains a sum of different operators made up of different numbers of $\hat{a}$'s and $\hat{a}^\dagger$'s. As shown in the beginning, only the operators with the same number of $\hat{a}$'s and $\hat{a}^\dagger$'s have nonzero expectation values in the number states $|n\rangle$, so we have

$$\langle n|\,(\hat{a}+\hat{a}^\dagger)^4\,|n\rangle = \langle n|\,\hat{a}^2(\hat{a}^\dagger)^2+\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger+\hat{a}(\hat{a}^\dagger)^2\hat{a}+(\hat{a}^\dagger)^2\hat{a}^2+\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}+\hat{a}^\dagger\hat{a}^2\hat{a}^\dagger\,|n\rangle\,,$$

where we have only kept the terms with equal numbers of $\hat{a}$'s and $\hat{a}^\dagger$'s. This form could still be simplified considerably using the commutation relation $[\hat{a},\hat{a}^\dagger]=1$. We can also just compute the expectation value from here:

$$\begin{aligned}
&\frac{\hbar^2}{96ml^2}\langle n|\,\hat{a}^2(\hat{a}^\dagger)^2+\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger+\hat{a}(\hat{a}^\dagger)^2\hat{a}+(\hat{a}^\dagger)^2\hat{a}^2+\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}+\hat{a}^\dagger\hat{a}^2\hat{a}^\dagger\,|n\rangle \\
&= \frac{\hbar^2}{96ml^2}\left[(n+1)(n+2)+(n+1)^2+n(n+1)+n(n-1)+n^2+n(n+1)\right. \\
&= \frac{\hbar^2}{96ml^2}\left(n^2+3n+2+n^2+2n+1+n^2+n+n^2-n+n^2+n^2+n\right) \\
&= \frac{\hbar^2}{96ml^2}\left(6n^2+6n+3\right).
\end{aligned}$$

All in all,

$$\langle n|\hat{H}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{\hbar^2}{96ml^2}\left(6n^2+6n+3\right),$$

from which we get

$$\begin{aligned}\langle 0|\hat{H}|0\rangle &= \frac{1}{2}\hbar\omega - \frac{\hbar^2}{32ml^2},\\ \langle 1|\hat{H}|1\rangle &= \frac{3}{2}\hbar\omega - \frac{5\hbar^2}{32ml^2},\\ \langle 2|\hat{H}|2\rangle &= \frac{5}{2}\hbar\omega - \frac{13\hbar^2}{32ml^2}.\end{aligned}$$

As noted in the exercise, for the harmonic oscillator, the energy spacings are equal: $\Delta E_{12} = \Delta E_{01} = \Delta E_{n,n+1} = \hbar\omega$ for any $n \geq 0$, while for the anharmonic oscillator, they depend on n:

$$\Delta E_{n,n+1} = \hbar\omega - \frac{\hbar^2}{8ml^2}(n+1).$$