

Tues: HW Spm
Read 7.1-7.2

Thurs: Exam II Covers lectures 11-21

2007 Q1-3

2022 All Q

Quantum harmonic oscillator: energy spectrum

The quantum harmonic oscillator is described by a single parameter, ω , the oscillator angular frequency. The Hamiltonian is

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

where \hat{a}^\dagger and \hat{a} are the creation and annihilation operators. These satisfy the crucial algebraic rule:

$$[\hat{a}^\dagger, \hat{a}] = \hat{I}$$

This generates a series of results that provides the oscillator energy spectrum. The spectrum only relies on the structure of the Hamiltonian and the commutation rule.



angular frequency ω

The results are:

Any energy eigenvalue is bounded by

$$E \geq \hbar\omega/2$$

If $|\phi\rangle$ is an energy eigenstate with energy E then

$$\hat{a}|\phi\rangle$$

is an eigenstate with energy $E - \hbar\omega$

$$\hat{a}^+|\phi\rangle$$

is an eigenstate with energy $E + \hbar\omega$ (provided that $E > \hbar\omega$)

There exists a ladder of energy eigenvalues and eigenstates.

state	energy
$ 3\rangle$	$7\hbar\omega/2$
$ 2\rangle$	$5\hbar\omega/2$
$ 1\rangle$	$3\hbar\omega/2$
$ 0\rangle$	$\hbar\omega/2$

$\hat{a}^+ \uparrow$ (green arrows pointing up between levels)
 $\hat{a} \downarrow$ (red arrows pointing down between levels)

The lowest energy is exactly $E = \hbar\omega/2$.

For this state:

$$\hat{a}|\phi\rangle = 0$$

For an oscillator based on position variables we have

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right)$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+)$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right)$$

$$\hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a} - \hat{a}^+)$$

Then we can show that the lowest energy state is unique and thus there is only one state for each energy eigenvalue.

Thus we arrive at :

The possible energy eigenstates and energies for the harmonic oscillator are indexed by

$$n = 0, 1, 2, \dots$$

and the energies and associated states are:

Energies	States
$E_0 = \hbar\omega/2$	$ 0\rangle$ ← ground state ↘ normalized. ↗
$E_1 = 3\hbar\omega/2$	$ 1\rangle$
$E_2 = 5\hbar\omega/2$	$ 2\rangle$
\vdots	\vdots
$E_n = \hbar\omega(n + 1/2)$	$ n\rangle$
\vdots	\vdots

The states so defined are normalized, Thus

$$\langle m|n\rangle = \delta_{mn}$$

They also form a basis and any general state can be expressed as

$$|\Psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$$

where c_n are complex coefficients that satisfy

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

Finally the completeness relation is

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{I}$$

The usual quantum theory framework applies.

1 Harmonic oscillator general states

Consider the following states of a harmonic oscillator

$$|\Psi_A\rangle = \frac{1}{\sqrt{2}} |1\rangle + \frac{i}{\sqrt{2}} |3\rangle$$

$$|\Psi_B\rangle = \frac{1}{\sqrt{2}} |1\rangle - \frac{i}{\sqrt{2}} |3\rangle$$

$$|\Psi_C\rangle = \frac{3}{5} |1\rangle + \frac{4i}{5} |3\rangle$$

- a) Consider single particle in each state. List the *energy measurement* outcomes and probabilities with which they occur.
- b) Given a single particle guaranteed to be in any of the three states, could an energy measurement be used to decide which state with certainty.
- c) Are there any states that can be distinguished via *some* single measurement on a single particle
- d) Determine the expectation value of the measurement outcomes for each state. Given an ensemble of particles, each in the same one of the three states, could an energy measurement decide which state it is?

Answer: a) $\text{Prob}(E_n) = |\langle n | \Psi \rangle|^2$

This gives the following

Possible E_n	Probabilities		
	A	B	C
E_1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{9}{25}$
E_3	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{16}{25}$
no others	possible		

- b) No, in each case either outcome is possible, and none of the possible states is eliminated
- c) Yes $\langle \Psi_A | \Psi_B \rangle = 0$ and since they are orthogonal, there is some measurement that can distinguish.

$$\begin{aligned}
 d) \quad \langle E \rangle &= \sum \text{Prob}(E_n) E_n \\
 &= \sum \text{Prob}(E_n) \hbar \omega (n + 1/2) \\
 &= \hbar \omega \sum \text{Prob}(E_n) (n + 1/2)
 \end{aligned}$$

For A and B

$$\langle E \rangle = \hbar \omega \left[\frac{1}{2} \left(\frac{3}{2} \right) + \frac{1}{2} \left(\frac{7}{2} \right) \right] = \frac{\hbar \omega 10}{4} = \frac{5}{2} \hbar \omega = 2.5 \hbar \omega$$

For C

$$\begin{aligned}
 \langle E \rangle &= \hbar \omega \left[\frac{9}{25} \frac{3}{2} + \frac{16}{25} \frac{7}{2} \right] = \hbar \omega \frac{27 + 112}{50} \\
 &= \frac{139}{50} \hbar \omega = 2.78 \hbar \omega.
 \end{aligned}$$

There is a chance of determining whether C is involved but the statistics mean it is not certain.

Generating energy eigenstates

We can generate energy eigenstates via

Given a single state $|n\rangle$

→

Repeatedly use raising and lowering operators to generate all states

There are two important facts from the energy spectrum calculation that give the remaining results:

$$\begin{aligned}\hat{a}|0\rangle &= 0 \\ \hat{a}^+\hat{a}|n\rangle &= n|n\rangle\end{aligned}$$

Then the creation and annihilation operators act as:

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

for some β . Now we can fix β via

$$\begin{aligned}(\hat{a}|n\rangle)^\dagger &= \langle n|\hat{a}^\dagger \\ &\parallel \\ &\beta^*\langle n-1|\end{aligned}$$

$$\text{Thus } \langle n|\hat{a}^+\hat{a}|n\rangle = \beta^*\langle n-1|\beta|n-1\rangle = |\beta|^2$$

$$\Rightarrow \langle n|n|n\rangle = |\beta|^2$$

$$\Rightarrow n\langle n|n\rangle = |\beta|^2$$

$$\Rightarrow |\beta| = \sqrt{n}$$

The convenient rule is that β is positive. Thus

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

Similarly consider

$$\hat{a}^+ |n\rangle = \alpha |n+1\rangle$$

Then the same derivation gives

$$\langle n | \hat{a} \hat{a}^+ |n\rangle = |\alpha|^2$$

$$\text{But } [\hat{a}, \hat{a}^+] = \hat{I} \Rightarrow \hat{a} \hat{a}^+ - \hat{a}^+ \hat{a} = \hat{I}$$

$$\Rightarrow \hat{a} \hat{a}^+ = \hat{I} + \hat{a}^+ \hat{a}$$

and $\langle n | \hat{a} \hat{a}^+ |n\rangle = 1 + n$. Thus $\alpha = \sqrt{n+1}$. Combining these gives

$$\boxed{\begin{aligned} \hat{a} |n\rangle &= \sqrt{n} |n-1\rangle \\ \hat{a}^+ |n\rangle &= \sqrt{n+1} |n+1\rangle \end{aligned}}$$

Generating wavefunctions

The creation operator can be used to generate wavefunctions. Here

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

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right) |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i}{m\omega} \left(-i\hbar \frac{\partial}{\partial x} \right) \right) \phi_n(x) = \sqrt{n+1} \phi_{n+1}(x)$$

$$\Rightarrow \phi_{n+1}(x) = \sqrt{\frac{m\omega}{2(n+1)\hbar}} \left(x - \frac{\hbar}{m\omega} \frac{\partial}{\partial x} \right) \phi_n(x)$$

So if we can find $\phi_0(x)$ then the remaining states can be generated by repeated multiplication and differentiation.

The ground state can be generated by

$$\hat{a} |0\rangle = 0$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{X} + \frac{i}{m\omega} \hat{P} \right) |0\rangle = 0$$

$$\Rightarrow \left(\hat{X} + \frac{i}{m\omega} \hat{P} \right) |0\rangle = 0$$

$$\Rightarrow \left(X + \frac{i}{m\omega} \left(-i\hbar \frac{\partial}{\partial x} \right) \right) \phi_0(x) = 0$$

$$\Rightarrow \frac{\hbar}{m\omega} \frac{\partial \phi_0}{\partial x} + X \phi_0(x) = 0$$

$$\Rightarrow \frac{d\phi_0}{dx} + \frac{m\omega}{\hbar} X \phi_0(x) = 0$$

$$\Rightarrow \frac{d\phi_0}{\phi_0} = -\frac{m\omega}{\hbar} X dx$$

$$\Rightarrow d(\ln \phi_0) = -\frac{m\omega}{2\hbar} d(x^2)$$

$$\Rightarrow \ln \phi_0 = -\frac{m\omega}{2\hbar} X^2 + \text{const}$$

$$\Rightarrow \phi_0(x) = A e^{-m\omega x^2/2\hbar}$$

Normalization gives:

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar}$$

2 Wavefunction for the $n = 1$ harmonic oscillator state

The ground state harmonic oscillator wavefunction is

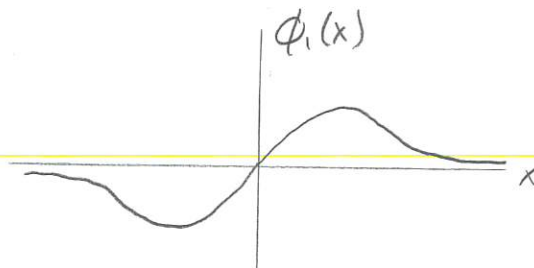
$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}.$$

This is normalized. Determine the wavefunction for the $n = 1$ energy eigenstate.

Answer:

$$\begin{aligned}\phi_1(x) &= \sqrt{\frac{m\omega}{2(0+1)\hbar}} \left(x - \frac{\hbar}{m\omega} \frac{\partial}{\partial x}\right) \phi_0(x) \\ &= \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{\hbar}{m\omega} \frac{d}{dx}\right) \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \\ &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left[x - \frac{\hbar}{m\omega} \frac{m\omega}{2\hbar} (2x)\right] e^{-m\omega x^2/2\hbar} \\ &= \left(\frac{m\omega}{2\hbar}\right)^{1/2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2x e^{-m\omega x^2/2\hbar} \\ &= \sqrt{\frac{2m\omega}{\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} x e^{-m\omega x^2/2\hbar}.\end{aligned}$$

The wavefunction has the illustrated form



Demo: QuVis Harmonic Oscillator

Position and momentum expectation values

The position and momentum expectation values can be calculated via the observables \hat{x} and \hat{p} . Then for a system in state $|\Psi\rangle$

$$\langle x \rangle = \langle \Psi | \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger) | \Psi \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \Psi | (\hat{a} + \hat{a}^\dagger) | \Psi \rangle$$

$$\langle p \rangle = \langle \Psi | -i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a} - \hat{a}^\dagger) | \Psi \rangle = -i\sqrt{\frac{\hbar m\omega}{2}} \langle \Psi | (\hat{a} - \hat{a}^\dagger) | \Psi \rangle$$

This allows one to calculate expectation values purely by operations on the raising and lowering operators

Harmonic oscillator time evolution

In general as the oscillator evolves

$$\begin{aligned} |n\rangle &\rightarrow e^{-i\hat{H}t/\hbar} |n\rangle \\ &= e^{-iE_n t/\hbar} |n\rangle \\ &= e^{-i\hbar\omega(n+1/2)t/\hbar} |n\rangle \\ &= e^{-i\omega t(n+1/2)} |n\rangle \end{aligned}$$

This can be applied to superposition states

4 Harmonic oscillator superposition temporal behavior

A harmonic oscillator is initially in the state

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle.$$

- a) Determine the state at a later time.
 b) Determine $\langle x \rangle$ at any later time.

Answer: a)
$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} |0\rangle + \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} |1\rangle.$$

$$= \frac{1}{\sqrt{2}} e^{-i\hbar\omega t/2\hbar} |0\rangle + \frac{1}{\sqrt{2}} e^{-i3\hbar\omega t/2\hbar} |1\rangle$$

$$= \frac{1}{\sqrt{2}} e^{-i\omega t/2} |0\rangle + \frac{1}{\sqrt{2}} e^{-i3\omega t/2} |1\rangle$$

b)
$$\langle x \rangle = \langle \Psi(t) | \hat{x} | \Psi(t) \rangle = \frac{1}{2} \left[e^{i\omega t/2} \langle 0 | + e^{i3\omega t/2} \langle 1 | \right] \hat{x} \left[e^{-i\omega t/2} |0\rangle + e^{-i3\omega t/2} |1\rangle \right]$$

$$= \frac{1}{2} \left\{ \langle 0 | \hat{x} | 0 \rangle + e^{-i\omega t} \langle 0 | \hat{x} | 1 \rangle + e^{i\omega t} \langle 1 | \hat{x} | 0 \rangle + \langle 1 | \hat{x} | 1 \rangle \right\}$$

Now
$$\langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle m | (\hat{a} + \hat{a}^\dagger) | n \rangle.$$

Thus
$$\langle 0 | \hat{x} | 0 \rangle = \sqrt{\hbar} \langle 0 | (1) \rangle = 0$$

$$\langle 1 | \hat{x} | 1 \rangle = \sqrt{\hbar} \langle 1 | (|0\rangle + \sqrt{2}|2\rangle) \rangle = 0$$

$$\langle 0 | \hat{x} | 1 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle 0 | [\hat{a}^\dagger | 0 \rangle + \hat{a} | 1 \rangle] \rangle = \sqrt{\frac{\hbar}{2m\omega}} [\langle 0 | 1 \rangle + \sqrt{2} \langle 0 | 2 \rangle]$$

Similarly
$$\langle 1 | \hat{x} | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}}$$

Thus

$$\langle x \rangle = \frac{1}{2} \sqrt{\frac{\hbar}{2m\omega}} (e^{-i\omega t} + e^{i\omega t}) = \sqrt{\frac{\hbar}{2m\omega}} \cos(\omega t)$$

The position expectation value oscillates with frequency ω .