# Lecture 19:
# Quantization of the simple harmonic oscillator

Phy851 Fall 2009

# Systems near equilibrium

- The harmonic oscillator Hamiltonian is:

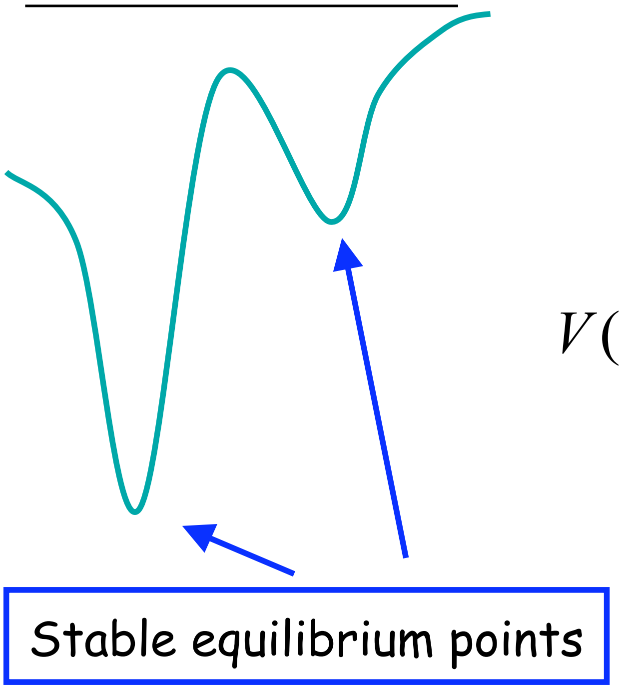
$$H = \frac{P^2}{2m} + \frac{1}{2}kX^2$$

- Or alternatively, using $\omega = \sqrt{\frac{k}{m}}$

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$$

- Why is the SHO so important?
  - Answer: any system near a stable equilibrium is equivalent to an SHO

A Random Potential




Definition of stable equilibrium point:

$$V'(x_0) = 0$$

Expand around $x_0$:

$$V(x) = V(x_0) + V'(x_0)(x - x_0)$$

$$+ \frac{1}{2}V''(x_0)(x - x_0)^2 + \ldots$$

$y = x - x_0$ $\quad V(y) = V_0 + \frac{1}{2}k\,y^2$

# Analysis of energy and length scales

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega_{osc}^2 X^2$$

- The parameters available in the SHO Hamiltonian are: $\hbar, m, \omega_{osc}$

The SHO introduces a single new parameter, which must govern all of the physics

- The frequency defines a quantum energy [J] scale via:

$$E_{osc} = \hbar\omega_{osc}$$

- The frequency also defines a quantum length scale via:

$$E_{osc} = \frac{\hbar^2}{m\lambda_{osc}^2} \quad \hbar\omega_{osc} = \frac{\hbar^2}{m\lambda_{osc}^2} \quad \lambda_{osc} = \sqrt{\frac{\hbar}{m\omega_{osc}}}$$

- This length scale then defines a quantum momentum scale:

$$\mu_{osc} = \frac{\hbar}{\lambda_{osc}} \qquad \mu_{osc} = \sqrt{\hbar m\omega_{osc}}$$

# Dimensionless Variables

- To solve the QM SHO it is very useful to introduce the natural units:
  - Let

$$\overline{X} = \frac{X}{\lambda_{osc}}$$

$$\overline{P} = \frac{P}{\mu_{osc}} = \frac{\lambda_{osc}}{\hbar} P$$

$$\overline{H} = \frac{H}{\hbar\omega_{osc}}$$

$$\hbar\omega_{osc}\overline{H} = \frac{1}{2}\frac{\hbar^2}{m\lambda_{osc}^2}\overline{P}^2 + \frac{1}{2} m\omega_{osc}^2 \lambda_{osc}^2 \overline{X}^2$$

$$\frac{\hbar^2}{m\lambda_{osc}^2} = \frac{\hbar^2}{m}\frac{m\omega_{osc}}{\hbar} = \hbar\omega_{osc}$$

$$m\omega_{osc}^2\lambda_{osc}^2 = m\omega_{osc}^2 \frac{\hbar}{m\omega_{osc}} = \hbar\omega_{osc}$$

$$\hbar\omega_{osc}\overline{H} = \frac{1}{2}\hbar\omega_{osc}\overline{P}^2 + \frac{1}{2}\hbar\omega_{osc}\overline{X}^2$$

$$\overline{H} = \frac{1}{2}\overline{P}^2 + \frac{1}{2}\overline{X}^2$$

# Dimensionless Commutation Relations

- Let's compute the commutator for the new variables:

$$\left[\bar{X},\bar{P}\right] = \bar{X}\,\bar{P} - \bar{P}\bar{X}$$

$$X = \lambda\,\bar{X} \quad \rightarrow \quad \bar{X} = \frac{X}{\lambda}$$

$$P = \frac{\hbar}{\lambda}\,\bar{P} \quad \rightarrow \quad \bar{P} = \frac{\lambda}{\hbar}\,P$$

We have stopped writing the subscript 'osc'

$$\left[\bar{X},\bar{P}\right] = \frac{X}{\lambda}\,\frac{\lambda P}{\hbar} - \frac{\lambda P}{\hbar}\,\frac{X}{\lambda}$$

$$= \frac{1}{\hbar}\left(XP - PX\right)$$

$$= \frac{1}{\hbar}\left[X,P\right]$$

$$\left[\bar{X},\bar{P}\right] = i$$

Since the new variables have no units, we lose the $\hbar$

# Switch to `Normal' Variables

- We can make a change of variables:

$$A = \frac{1}{\sqrt{2}}\left(\overline{X} + i\overline{P}\right)$$

$$A^{\dagger} = \frac{1}{\sqrt{2}}\left(\overline{X} - i\overline{P}\right)$$

  - It's more common to use: $a$, $a^{\dagger}$
  - We use $A$, $A^{\dagger}$ to stick with our convention to use capital letters for operators

$$\left[A, A^{\leq}\right] = \left[\frac{1}{\sqrt{2}}\left(\overline{X} + i\overline{P}\right), \frac{1}{\sqrt{2}}\left(\overline{X} - i\overline{P}\right)\right]$$

$$= \frac{1}{2}\left(\left[\overline{X}, -i\overline{P}\right] + \left[i\overline{P}, \overline{X}\right]\right)$$

$$= \frac{1}{2}\left(-i\left[\overline{X}, \overline{P}\right] + i\left[\overline{P}, \overline{X}\right]\right)$$

$$= 1$$

$$\left[A, A^{\dagger}\right] = 1$$

Boson commutation relation

Fermions $\rightarrow AA^{\dagger} + A^{\dagger}A = 1$

# Inverse Transformation

$$A = \frac{1}{\sqrt{2}}\left(\overline{X} + i\overline{P}\right)$$

$$A^{\dagger} = \frac{1}{\sqrt{2}}\left(\overline{X} - i\overline{P}\right)$$

- Inverting the transformation gives:

$$\frac{1}{\sqrt{2}}\left(A + A^{\dagger}\right) = \frac{1}{2}\left(\overline{X} + i\overline{P} + \overline{X} - i\overline{P}\right) = \overline{X}$$

$$\frac{1}{\sqrt{2}}\left(A - A^{\dagger}\right) = \frac{1}{2}\left(\overline{X} + i\overline{P} - \overline{X} + i\overline{P}\right) = i\overline{P}$$

$$\overline{X} = \frac{1}{\sqrt{2}}\left(A + A^{\dagger}\right)$$

$$X = \frac{\lambda}{\sqrt{2}}\left(A + A^{\dagger}\right)$$

$$\overline{P} = \frac{-i}{\sqrt{2}}\left(A - A^{\dagger}\right)$$

$$P = \frac{-i\hbar}{\sqrt{2}\lambda}\left(A - A^{\dagger}\right)$$

# Transforming the Hamiltonian

- The Harmonic Oscillator Hamiltonian was:

$$\overline{H} = \frac{1}{2}\left(\overline{P}^2 + \overline{X}^2\right)$$

$$\overline{X} = \frac{1}{\sqrt{2}}\left(A + A^\dagger\right) \qquad \overline{P} = \frac{-i}{\sqrt{2}}\left(A - A^\dagger\right)$$

$$\overline{X}^2 = \frac{1}{2}\left(A + A^\dagger\right)\left(A + A^\dagger\right)$$

$$\overline{X}^2 = \frac{1}{2}\left(AA + AA^\dagger + A^\dagger A + A^\dagger A^\dagger\right)$$

$$\overline{P}^2 = -\frac{1}{2}\left(AA - AA^\dagger - A^\dagger A + A^\dagger A^\dagger\right)$$

$$= \frac{1}{2}\left(-AA + AA^\dagger + A^\dagger A - A^\dagger A^\dagger\right)$$

$$\overline{H} = \frac{1}{2}\left(\overline{P}^2 + \overline{X}^2\right)$$

$$= \frac{1}{2}\left(AA^\dagger + A^\dagger A\right)$$

$$AA^\dagger - A^\dagger A = 1$$

$$\therefore AA^\dagger = A^\dagger A + 1$$

$$\overline{H} = A^\dagger A + \frac{1}{2}$$

# Energy Eigenvalues

- In original units we have:

$$\lambda = \sqrt{\frac{\hbar}{m\omega}}$$

$$H = \frac{\hbar^2}{m\lambda^2}\overline{H}$$

$$= \frac{\hbar^2}{m}\frac{m\omega}{\hbar}\left(A^\dagger A + \frac{1}{2}\right)$$

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

- Let's define the energy eigenstates via

$$\overline{H}\left|\varepsilon\right\rangle = \varepsilon\left|\varepsilon\right\rangle$$

$$\left(A^\dagger A + \frac{1}{2}\right)\left|\varepsilon\right\rangle = \varepsilon\left|\varepsilon\right\rangle$$

$$\left\langle\varepsilon\middle|\varepsilon'\right\rangle = \delta_{\varepsilon,\varepsilon'}$$

We expect a discrete spectrum as the classical motion is bounded

# Proof that there is a ground state

- For any energy eigenstate we have:

$$\left\langle \varepsilon \left| \overline{H} \right| \varepsilon \right\rangle = \varepsilon \left\langle \varepsilon | \varepsilon \right\rangle = \varepsilon$$

$$\left\langle \varepsilon \left| A^{\dagger} A + \frac{1}{2} \right| \varepsilon \right\rangle = \left\langle \varepsilon \left| A^{\dagger} A \right| \varepsilon \right\rangle + \frac{1}{2} \left\langle \varepsilon | \varepsilon \right\rangle$$

$$= \left| A \left| \varepsilon \right\rangle \right|^{2} + \frac{1}{2}$$

- The norm of a vector is always a real positive number

$$\left\| \psi \right\rangle \right|^{2} \geq 0$$

- Thus we see that:

$$\varepsilon \geq \frac{1}{2}$$

- So the energy eigenvalues are bounded from below by _.

# Setting up for The Big Trick

- Lets look at the commutator:

$$\left[A, \overline{H}\right] = \left[A, A^\dagger A + \frac{1}{2}\right] = \left[A, A^\dagger A\right]$$

$$= AA^\dagger A - A^\dagger AA$$

$$= \left(1 + A^\dagger A\right)A - A^\dagger AA$$

$$= A$$

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$$A\overline{H} - \overline{H}A = A$$

$$\overline{H}A = A\overline{H} - A$$

$$\overline{H}A = A\left(\overline{H} - 1\right)$$

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$$\overline{H}A^\dagger - A^\dagger \overline{H} = A^\dagger$$

$$\overline{H}A^\dagger = A^\dagger \overline{H} + A^\dagger$$

$$\overline{H}A^\dagger = A^\dagger\left(\overline{H} + 1\right)$$

# The Big Trick Begins

- Combine these relations with the eigenvalue equation:

$$\overline{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$$

$$\overline{H}A = A\left(\overline{H} - 1\right) \qquad \overline{H}A^{\dagger} = A^{\dagger}\left(\overline{H} + 1\right)$$

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$$\overline{H}A|\varepsilon\rangle = A\left(\overline{H} - 1\right)|\varepsilon\rangle$$

$$= A(\varepsilon - 1)|\varepsilon\rangle$$

$$\overline{H}\left(A|\varepsilon\rangle\right) = (\varepsilon - 1)\left(A|\varepsilon\rangle\right)$$

Definition of $|\varepsilon-1\rangle$

- This means that $A|\varepsilon\rangle$ is proportional to the eigenstate $|\varepsilon\text{-}1\rangle$: $\overline{H}|\varepsilon - 1\rangle = (\varepsilon - 1)|\varepsilon - 1\rangle$

by comparison we see →

$$A|\varepsilon\rangle = c_{\varepsilon}|\varepsilon - 1\rangle$$

$c_{\varepsilon}$ is an unknown coefficient

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$$\overline{H}A^{\dagger}|\varepsilon\rangle = A^{\dagger}\left(\overline{H} + 1\right)|\varepsilon\rangle$$

$$\overline{H}A^{\dagger}|\varepsilon\rangle = A^{\dagger}(\varepsilon + 1)|\varepsilon\rangle$$

$d_{\varepsilon}$ is an unknown coefficient

$$A^{\dagger}|\varepsilon\rangle = d_{\varepsilon}|\varepsilon + 1\rangle$$

# Raising and lowering operators

$$A|\varepsilon\rangle = c_\varepsilon|\varepsilon - 1\rangle \qquad A^\dagger|\varepsilon\rangle = d_\varepsilon|\varepsilon + 1\rangle$$

$$|\varepsilon - 1\rangle = \frac{A}{c_\varepsilon}|\varepsilon\rangle \qquad |\varepsilon + 1\rangle = \frac{A^\dagger}{d_\varepsilon}|\varepsilon\rangle$$

THEOREM:

- If state $|\varepsilon\rangle$ exists then either state $|\varepsilon\text{-}1\rangle$ exists or $c_\varepsilon$=0
- If state $|\varepsilon\rangle$ exists then either state $|\varepsilon+1\rangle$ exists or $d_\varepsilon$=0

$AA^\dagger - A^\dagger A = 1$

$A^\dagger A = AA^\dagger - 1$

$A^\dagger A + \frac{1}{2} = AA^\dagger - 1 + \frac{1}{2} = AA^\dagger - \frac{1}{2}$

- Now consider: $\langle\varepsilon|\overline{H}|\varepsilon\rangle = \varepsilon$ $=$

$$\langle\varepsilon|A^\dagger A + \frac{1}{2}|\varepsilon\rangle = |c_\varepsilon|^2 + \frac{1}{2} \qquad \langle\varepsilon|AA^\dagger - \frac{1}{2}|\varepsilon\rangle = |d_\varepsilon|^2 - \frac{1}{2}$$

(↑ $\overline{H}$) (↑ $\overline{H}$)

- So clearly we must have:

$$\varepsilon = |c_\varepsilon|^2 + \frac{1}{2} \qquad \varepsilon = |d_\varepsilon|^2 - \frac{1}{2}$$

- So $c_\varepsilon$ is only zero for $\varepsilon=1/2$ and $d_\varepsilon$ is only zero for $\varepsilon$=-1/2

This means that actually $d_e$ is never zero

$$\varepsilon \geq \frac{1}{2} \qquad |c_\varepsilon|^2 = \varepsilon - \frac{1}{2} \qquad |d_\varepsilon|^2 = \varepsilon + \frac{1}{2}$$

# Ground State energy

- Let the ground state $|\varepsilon_0\rangle$ have energy:

$$\varepsilon_0 = \frac{1}{2} + \delta$$

$\delta < 1$

$$\varepsilon_0 = \left|c_{\varepsilon_0}\right|^2 + \frac{1}{2}$$

$$\left|c_{\varepsilon_0}\right|^2 = \delta$$

- Remember our statement:
  - If state $|\varepsilon\rangle$ exists then either state $|\varepsilon\text{-}1\rangle$ exists or $c_\varepsilon$=0
  - Conclusion: either $\delta = 0$, or there is a state lower than the ground state

    The second option is obviously a contradiction

  - For $|\varepsilon_0\rangle$ to be the ground state requires $\delta = 0$

$$\varepsilon_0 = \frac{1}{2}$$

# Excited states

- If the ground state $|\varepsilon_0\rangle$ exists, then the state $|\varepsilon_0+1\rangle$ exists

$$|\varepsilon+1\rangle = \frac{A^\dagger}{d_\varepsilon}|\varepsilon\rangle$$

$$|d_\varepsilon|^2 = \varepsilon + \frac{1}{2}$$

This is just a result we proved on slide 13

The point is just that we aren't dividing by zero

- Following this chain of reasoning, we can establish the existence of states at energies:

$$\varepsilon = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \ldots$$

# Are there more states?

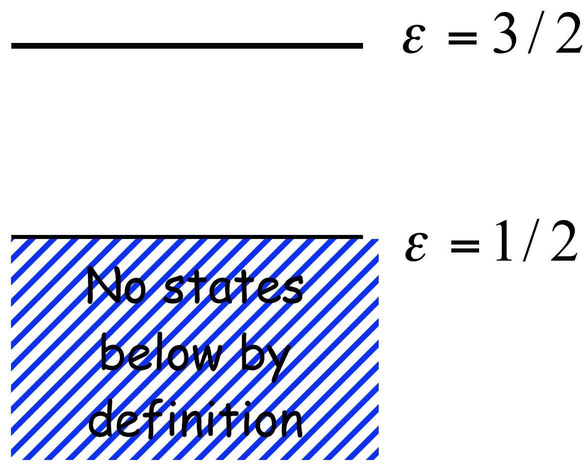
- So far we see that a ladder of states ***must*** exist:

$$|\varepsilon = 1/2\rangle$$

$$|\varepsilon = 3/2\rangle = A^\dagger|\varepsilon = 1/2\rangle$$

$$|\varepsilon = 5/2\rangle = \frac{A^\dagger}{\sqrt{2}}|\varepsilon = 3/2\rangle$$

$$\vdots \qquad\qquad \vdots$$




- Are there any states in between?
  - Assume a state exists with

$$\varepsilon = 1/2 + x$$

$$0 < x < 1$$

This state lies between $\varepsilon$=1/2 and $\varepsilon$=3/2

  - We have $|c_\varepsilon|^2 = \varepsilon - \frac{1}{2} = x$

$$\frac{A}{\sqrt{x}}|1/2 + x\rangle = |x - 1/2\rangle$$

x-1/2 < 1/2

  - So either $x$=0 or there is a state below the ground state! Conclusion: $x$=0

- If there is a state between 5/2 and 3/2, then a state must exist between 3/2 and 1/2 and then a state must exist below 1/2, etc…

- So no states between the half integers!

# Spectrum of the SHO

- We now see that the energy eigenstates can be labeled by the integers so that:

$$\overline{H}\left|n\right\rangle = \left(n + \frac{1}{2}\right)\left|n\right\rangle; \quad n = 0,1,2,3,\ldots$$

- We can always go back to our original units by putting in the energy scale factor:

$$H\left|n\right\rangle = \hbar\omega\left(n + \frac{1}{2}\right)\left|n\right\rangle; \quad n = 0,1,2,3,\ldots$$

$$\left|\varepsilon = \tfrac{1}{2}\right\rangle = \left|n = 0\right\rangle$$

$$\left|\varepsilon = \tfrac{3}{2}\right\rangle = \left|n = 1\right\rangle$$