6-2 Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

H can be represented as a product of two complex conjugate linear combinations of coordinate and momentum variables:

$$H = \omega \left(\sqrt{\frac{m\omega}{2}}\, x - i \frac{p}{\sqrt{2m\omega}} \right)\left(\sqrt{\frac{m\omega}{2}}\, x + i \frac{p}{\sqrt{2m\omega}} \right) + \underline{\underline{\frac{1}{2}\hbar\omega}}$$

Why this term? Because x and p do not commute!

$$\left(\sqrt{\frac{m\omega}{2}}\, x - \frac{i p}{\sqrt{2m\omega}} \right)\left(\sqrt{\frac{m\omega}{2}}\, x + \frac{i p}{\sqrt{2m\omega}} \right) =$$

$$= \frac{m\omega x^2}{2} + \frac{p^2}{2m\omega} + \frac{i}{2} \underbrace{(xp - px)}_{\hbar i} =$$

$$= \frac{m\omega x^2}{2} + \frac{p^2}{2m\omega} - \frac{\hbar}{2}$$

We can introduce two mutually hermitian conjugate operators

$$A = \sqrt{\frac{m\omega}{2\hbar}}\, x + i \frac{p}{\sqrt{2m\omega\hbar}}$$

$$A^+ = \sqrt{\frac{m\omega}{2\hbar}}\, x - i \frac{p}{\sqrt{2m\omega\hbar}}$$

- A and A^+ are dimensionless
- we used $x = x^+$ and $p = p^+$

Result:

$$H = \underset{\substack{\nearrow \\ \text{dimension} \\ \text{energy}}}{\hbar\omega} \left(A^+ A + \tfrac{1}{2}\right)$$

$$[A, A^+] = 1$$

Commutation relations:

$$[H, A] = \hbar\omega [A^+ A + \tfrac{1}{2}, A] = \hbar\omega [A^+ A, A] =$$

$$= \hbar\omega (A^+ A A - \underbrace{A A^+}_{1 + A^+ A} A) = \hbar\omega (A^+ A A - A - A^+ A A) = -A\hbar\omega$$

$$[H, A] = -\hbar\omega A, \quad \text{similarly} \quad [H, A^+] = \hbar\omega A^+$$

Proof:

$$(HA - AH)^+ = A^+ H^+ - H^+ A^+ = \underset{H^+ = H}{A^+ H - H A^+} =$$

$$= -[H, A^+]$$

Energy and A cannot be measured simultaneously (uncertainty principle)

$H|E\rangle = E|E\rangle \leftarrow$ eigenvalue problem for the energy

$$HA|E\rangle = AH|E\rangle - \hbar\omega A|E\rangle =$$

$$= (E - \hbar\omega) A|E\rangle$$

$A|E\rangle$ is also an eigenstate of H, but with energy lowered by $\hbar\omega$. Since the energy cannot be negative, there must be a state

$$A|0\rangle = 0$$

If this is true,

$$H|0\rangle = \hbar\omega\,(\underbrace{A^+A}_{\equiv 0}+\tfrac{1}{2})|0\rangle = \underline{\underline{\tfrac{1}{2}\hbar\omega|0\rangle}}$$

zero-point energy

$$HA^+|0\rangle = (\hbar\omega A^+ + A^+H)|0\rangle = \hbar\omega\left(\tfrac{1}{2}+1\right)|0\rangle$$

↑ multiple applications of A^+ result in rising energy by

Normalized ket:

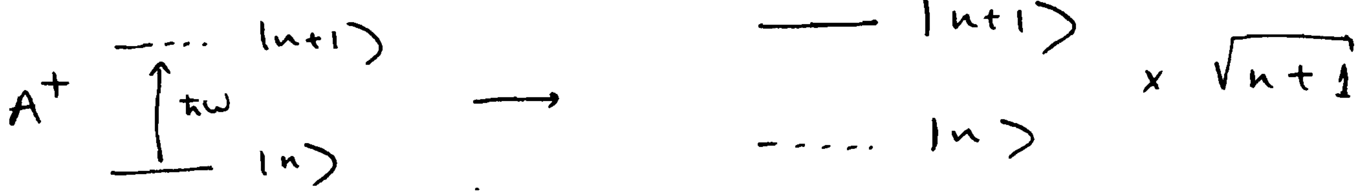
$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}(A^+)^n|0\rangle}$$

Useful properties

$$A^+|n\rangle = \frac{1}{\sqrt{n!}}(A^+)^{n+1}|0\rangle = \frac{\sqrt{n+1}}{\sqrt{(n+1)!}}(A^+)^{n+1}|0\rangle =$$

$$= \sqrt{n+1}\;|n+1\rangle$$

A^+, raising operator, moves the harmonic oscillator to the next energy level separated from $|n\rangle$ by the energy $\hbar\omega$



$$A|n\rangle = \frac{1}{\sqrt{n!}}(AA^+)(A^+)^{n-1}|0\rangle = \frac{1}{\sqrt{n!}}(1 + A^+A)(A^+)^{n-1}|0\rangle$$

if you keep moving A down the chain of A^+, you get a factor n:

$$A\underbrace{A^+ \cdots\cdots A^+}_{n} = n\underbrace{A^+ \cdots\cdots A^+}_{n-1} + (A^+)^n A$$

$$A|n\rangle = \frac{n}{\sqrt{n!}}(A^+)^{n-1}|0\rangle = \sqrt{n}\,\frac{1}{\sqrt{(n-1)!}}(A^+)^{n-1}|0\rangle = \sqrt{n}\,|n-1\rangle$$

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

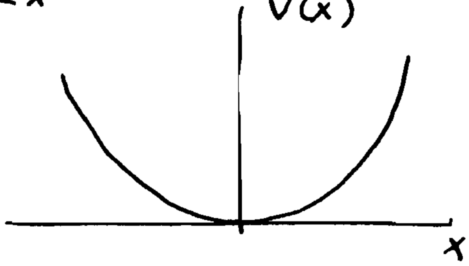
Therefore, $A^+A|n\rangle = A^+\sqrt{n}\,|n-1\rangle = n|n\rangle$

and

$$H|n\rangle = \hbar\omega\left(A^+A + \tfrac{1}{2}\right)|n\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right)|n\rangle$$

4-7 The harmonic oscillator

$$H = \frac{p^2}{2m} + V(x), \qquad V(x) = \frac{1}{2} k x^2$$



SE:

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dx^2} + \frac{1}{2} k x^2 u(x) = E\, u(x)$$

$$y = \sqrt{\frac{m\omega}{\hbar}}\, x, \qquad \varepsilon = \frac{2E}{\hbar\omega}$$

$$\boxed{\frac{d^2 u}{dy^2} + (\varepsilon - y^2)\, u = 0}$$

solution:

solution exists only for discrete values of n

$$\boxed{\begin{aligned} &\varepsilon = 2n+1 \\ &u(y) = c\, H_n(y)\, e^{-y^2/2} \end{aligned}}$$

normalization constant

Hermitian polynomial

$H_0(y) = 1$

$H_1(y) = 2y$

$H_2(y) = 4y^2 - 2$

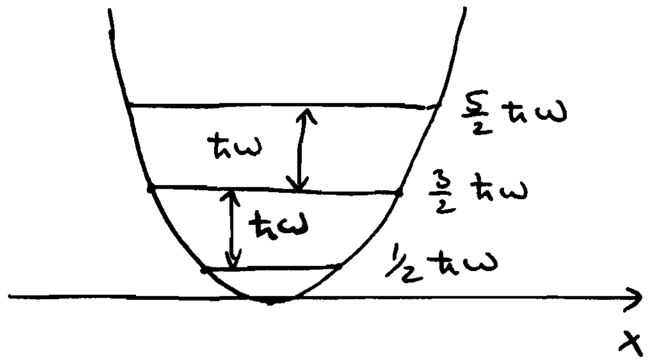
$$\varepsilon_n = 2n + 1$$

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)}$$

Spectrum of energies of the harmonic oscillator

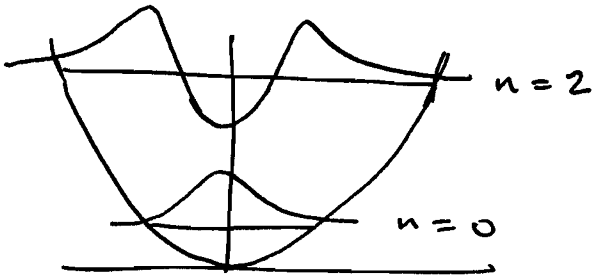
Harmonic oscillator: properties

① Energies are separated by $\hbar\omega$



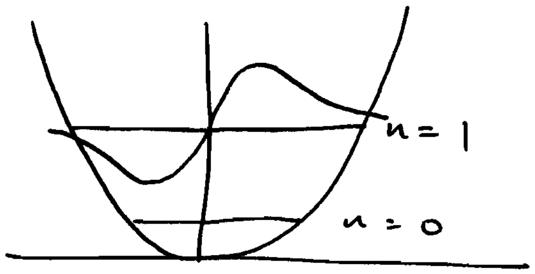
$n = 0 \leftarrow$ zero-point energy, nonzero because of the uncertainty principle

② Wave functions are even for $n = 0, 2, 4, \ldots$



$$\boxed{u_{2m}(-x) = u_{2m}(x)}$$

③ Wave functions are odd at $n = 1, 3, 5, 7, \ldots$



$$\boxed{u_{2m+1}(-x) = -u_{2m}(x)}$$

④ Operators algebra:

$$A^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

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

$$A^+A\,|n\rangle = n\,|n\rangle$$

$$\langle x|n\rangle = u_n(x)$$

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

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

$$\hat{H}\,|n\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right)|n\rangle$$

Example: 6-9

Prove that $\langle n|\hat{x}|n\rangle$ and $\langle n|\hat{p}|n\rangle$ both vanish

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

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

$$\langle n|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\hat{A} + \hat{A}^{+}\right)|n\rangle =$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\Big(\underbrace{\langle n|\sqrt{n}\,|n-1\rangle}_{=0} + \underbrace{\langle n|\sqrt{n+1}\,|n+1\rangle}_{=0}\Big) = 0$$

$$\langle n|\hat{p}|n\rangle = \sqrt{\frac{\hbar\omega m}{2}}\,\langle n|\hat{A} - \hat{A}^{+}|n\rangle$$

$$= \sqrt{\frac{\hbar\omega m}{2}}\Big(\underbrace{\langle n|\sqrt{n}\,|n-1\rangle}_{=0} - \underbrace{\langle n|\sqrt{n+1}\,|n+1\rangle}_{=0}\Big) = 0$$

Example: Calculate $\langle n|x^2|n\rangle$

$$\langle n|x^2|n\rangle = \frac{\hbar}{2m\omega}\langle n|\hat{A}\hat{A} + \hat{A}^{+}\hat{A}^{+} + \hat{A}\hat{A}^{+} + \hat{A}^{+}\hat{A}|n\rangle$$

$$= \frac{\hbar}{2m\omega}\langle n|\hat{A}^{+}\hat{A} + \hat{A}\hat{A}^{+}|n\rangle = \frac{\hbar}{2m\omega}\langle n|2A^{+}A + 1|n\rangle =$$

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

$\langle n|V|n\rangle = \langle n|\frac{p^2}{2m}|n\rangle$

$$\langle n|V(x)|n\rangle = \langle n|\frac{m\omega^2 x^2}{2}|n\rangle = \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right)$$

$$\langle n|\frac{p^2}{2m}|n\rangle = \langle n|H - V(x)|n\rangle = \frac{\hbar\omega}{2}\left(n + \frac{1}{2}\right)$$

6-3. Operators algebra and the Schrödinger equation

How do we get SE from the operator algebra?

By using the x-representation of the quantum states!

For harmonic oscillator:

$$\langle x | A | 0 \rangle = 0$$

$$\langle x | \hat{x} + \frac{\hat{p}}{m\omega} | 0 \rangle = 0$$

$$\langle x | \hat{x} | 0 \rangle \underset{\uparrow}{=} \langle \hat{x} x | 0 \rangle = x \langle x | 0 \rangle = x\, u_0(x)$$

$\hat{x}$ is a Hermitian operator

wave function of the ground state in x-representation

$$\langle x | \hat{p} | 0 \rangle = \int_{-\infty}^{\infty} dp \, \langle x | \hat{p} | p \rangle \langle p | 0 \rangle =$$

$$= \int_{-\infty}^{\infty} dp \; p \langle x | p \rangle \langle p | 0 \rangle = \int_{-\infty}^{\infty} dp \; p \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \langle p | 0 \rangle =$$

$$= \frac{\hbar}{i} \frac{d}{dx} \int_{-\infty}^{\infty} dp \langle x | p \rangle \langle p | 0 \rangle = \frac{\hbar}{i} \frac{d}{dx} \langle x | 0 \rangle$$

$$\left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) u_0(x) = 0 \rightarrow \boxed{u_0(x) = C e^{-m\omega x^2/2\hbar}}$$

Normalization:

$$c^2 \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{m\omega x^2}{\hbar}\right) = c^2 \sqrt{\frac{\pi\hbar}{m\omega}} \rightarrow c = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

Finally:

$$\boxed{u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)}$$

<u>Deriving the Schrödinger equation</u>:

$$\langle x | \frac{\hat{p}^2}{2m} + V(\hat{x}) | E \rangle = \langle x | \hat{H} | E \rangle = E \langle x | E \rangle$$

$$\langle x | V(\hat{x}) | E \rangle = \langle V(\hat{x}) x | E \rangle = V(x) \langle x | E \rangle$$

$$\langle x | \hat{p} | E \rangle = \int_{-\infty}^{\infty} dp \, \langle x | \hat{p} | p \rangle \langle p | E \rangle =$$

completeness relation

$$= \int_{-\infty}^{\infty} dp \, p \, \langle x | p \rangle \langle p | E \rangle = \frac{\hbar}{i} \frac{d}{dx} \langle x | E \rangle$$

$$\langle x | \hat{p}^2 | E \rangle = \left(\frac{\hbar}{i} \frac{d}{dx}\right)^2 \langle x | E \rangle$$

$$\langle x | \hat{H} | E \rangle = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \langle x | E \rangle + V(x) \langle x | E \rangle =$$

$$= E \langle x | E \rangle$$

SE is a particular x, E - representation of a more general operators algebra

6-4. Time-dependent operators

We have shown that operators algebra can replace the wave function $\psi(x)$ in solving quantum problems. How about time evolution?

SE: $$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle$$

Solution: $$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

quantum state at $t=0$

What is $e^{-iHt/\hbar}$?

This is an operator defined through the Taylor expansion of the exponent:

$$e^{-iHt/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!} (-iHt/\hbar)^n$$

Expectation value:

$$\langle B\rangle_t = \langle \psi(t)|B|\psi(t)\rangle =$$

$$= \langle e^{-iHt/\hbar}\psi(0)|\, B \,|e^{-iHt/\hbar}\psi(0)\rangle$$

$$= \langle\psi(0)| \left(e^{-iHt/\hbar}\right)^{\dagger} B\, e^{-iHt/\hbar} |\psi(0)\rangle =$$

$$\left(e^{-iHt/\hbar}\right)^{\dagger} = e^{iH^{\dagger}t/\hbar} = e^{iHt/\hbar}$$

H is a hermitian operator

$$= \langle \psi(0) | B(t) | \psi(0) \rangle$$

where $$B(t) = e^{iHt/\hbar} \, B \, e^{-iHt/\hbar}$$

This is the essence of the Heisenberg picture: operators evolve in time instead of wave functions

$$\frac{dB(t)}{dt} = \frac{i}{\hbar} H e^{iHt/\hbar} B e^{-iHt/\hbar} +$$

$$+ e^{iHt/\hbar} B e^{-iHt/\hbar} \left(-\frac{i}{\hbar} H\right) =$$

$$= \frac{i}{\hbar}\left(H B(t) - B(t) H\right) = \frac{i}{\hbar} [H, B(t)]$$

Evolution equation for operators:

$$\boxed{\frac{dB(t)}{dt} = \frac{i}{\hbar} [H, B(t)]}$$