Dao động tử điều hòa
Harmonic oscillator

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“Procedure” in QM 1 / Quy trình trong CHLT 1

- Need to determine the physical problem / Xác định bài toán vật lý
- → Determine Hamiltonian H → Schrödinger Eq.
- Calculate wave functions & energy / Tính hàm sóng ψ và năng lượng E

$$\boxed{\Psi(x,t) = \psi(x)\varphi(t) = \psi(x)e^{-iEt/\hbar}}$$

$$\Psi(x,t) = \sum_n \psi_n(x)e^{-\frac{iE_nt}{\hbar}}$$

$$\boxed{\langle Q(x,p)\rangle = \int \Psi(x,t)^* Q(x,p)\Psi(x,t)}$$

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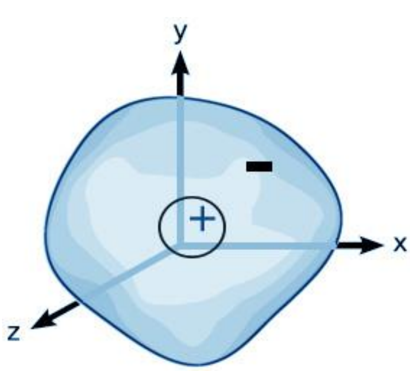
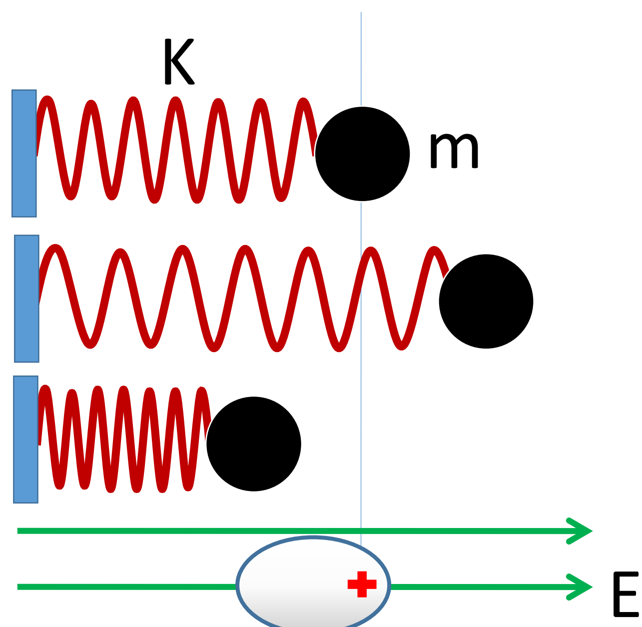
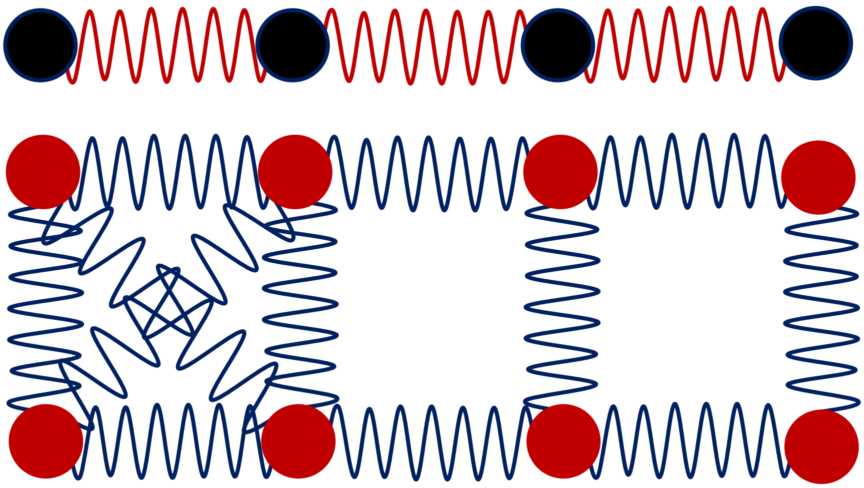
Why oscillator?

Harmonic Oscillator







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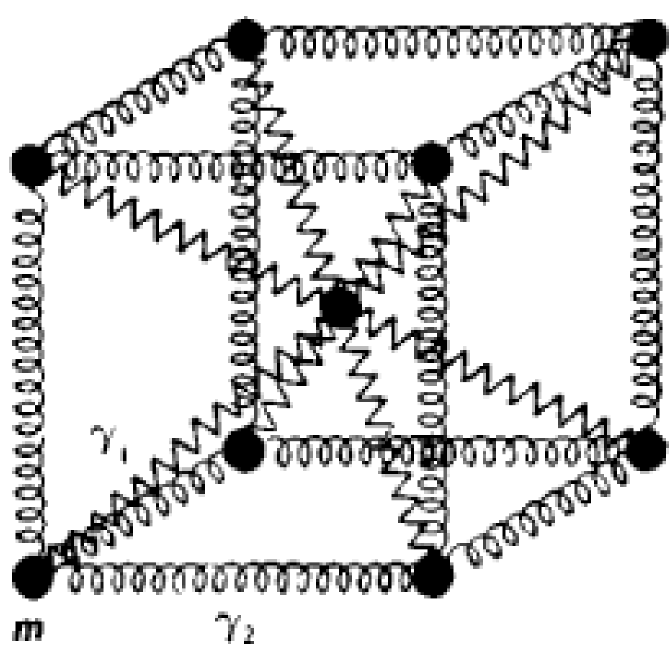

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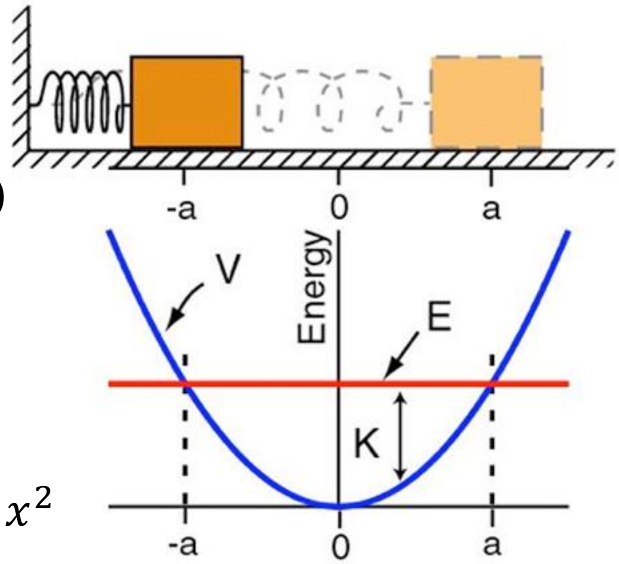
Classical Mechanics / Cơ cổ điển

$$F = -kx = m\frac{d^2x}{dt^2}$$

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

$$\omega \equiv \sqrt{k/m}$$



$$V = \frac{1}{2}kx^2$$

$$V = \frac{1}{2}m\omega^2x^2$$

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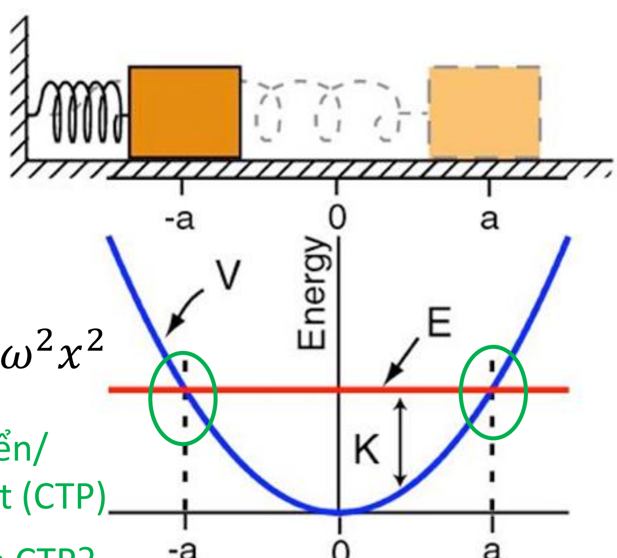
CM



$$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

Điểm quay đầu cổ điển/
classical turning point (CTP)

Determine / Xác định CTP?

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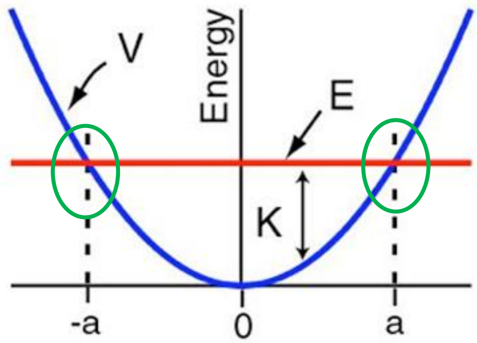
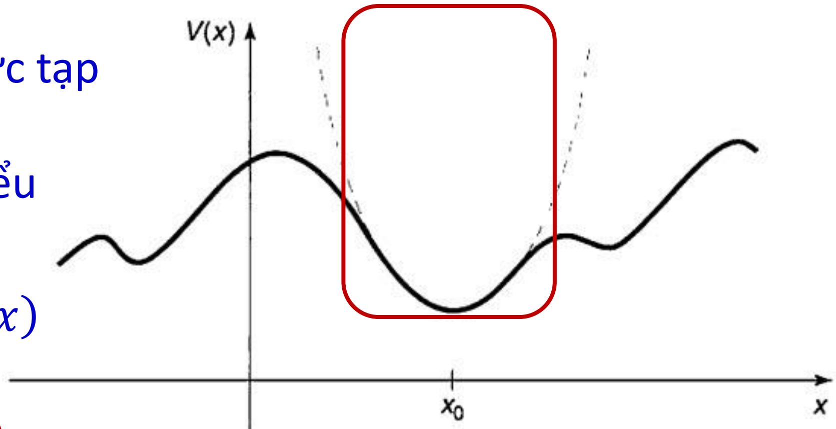
CM



Classical mechanics: Xác suất tìm được hạt trong miền giữa 2 CTP $[-a \to a]$ là 1 (chắc chắn tìm được hạt trong miền này) → Miền này gọi là miền được phép (cổ điển).
Miền ngoài miền được phép, tức là miền $[-\infty \to -a]$ và $[a \to +\infty]$, được gọi là miền cấm (cổ điển) vì xác suất tìm được hạt ở đó bằng 0.
Quantum mechanics: Vẫn có thể tìm được hạt ở miền cấm!!

- Hàm thế có thể phức tạp
- $V(x) \sim$ thế parabol trong lân cận cực tiểu



- Khai triển Taylor $V(x)$ quanh cực tiểu:

$$V(x) = \overset{\text{Const.}}{V(x_0)} + \overset{0}{V'(x_0)}(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \ldots$$

$$V(x) \cong \frac{1}{2}\underbrace{\boxed{V''(x_0)}}_{k}(x - x_0)^2 = \frac{1}{2}kx^2 \quad \boxed{= \frac{1}{2}m\omega^2 x^2}$$

Energy / Năng lượng (toàn phần) (CM / cơ cổ điển)

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

QM/ Cơ lượng tử

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

QM/ Cơ lượng tử

$\hat{p} = -i\hbar\frac{d}{dx}$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

The Schrödinger Eq. / PT Sch. không phụ thuộc thời gian: $\hat{H}\psi = E\psi$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi = E\psi$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + \frac{1}{2}m\omega^2 x^2\psi = E\psi} \qquad [2.44]$$

Giải phương trình Schrödinger cho DĐTĐH

- Cách giải đại số / Algebraic Method
- Cách giải tích / Analytic Method [Read Griffiths book!]

1) Change variables: $(x, p) \to (a_+, a_-)$ (ladder operators/ toán tử bậc thang)
2) Write the Hamiltonian in terms of a_+, a_-: $H(x, p) \to H(a_+, a_-)$
3) → Schrödinger equation $H\psi = E\psi$
4) Solve the Schrödinger equation to find ψ and E

1. $(x, p) \to (a_+, a_-)$

PT Schrödinger KPTTG

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

$$\hat{H}\psi = E\psi \leftrightarrow \frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi \qquad [2.45]$$

$$H = \frac{1}{2m}[\underbrace{p^2}_{u^2} + \underbrace{(m\omega x)^2}_{v^2}] \qquad [2.46]$$

SỐ: $u^2 + v^2 = (iu + v)(-iu + v) = u^2 + v^2 + i(\cancel{uv} - \cancel{vu})$

TTỬ: $u^2 + v^2 \neq (iu + v)(-iu + v) = u^2 + v^2 + i(uv - vu)$

Toán tử thường không giao hoán $\to uv - vu \neq 0$

Ví dụ: xp khác px !

$$1.\ (x, p) \rightarrow (a_+, a_-)$$

$$H = \frac{1}{2m}[p^2 + (m\omega x)^2]$$

$$\underbrace{(iu + v)}_{A_-}\underbrace{(-iu + v)}_{A_+} = u^2 + v^2 + i(uv - vu)$$

$$\boxed{a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)} \qquad [2.47]$$

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \qquad a_- = \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x)$$

$$1.\ (x, p) \rightarrow (a_+, a_-)$$

$$\boxed{a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)}$$

$$a_- a_+ = \frac{1}{2\hbar m\omega}(+ip + m\omega x)(-ip + m\omega x)$$

$$a_- a_+ = \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2 - im\omega(xp - px)]$$

Commutator / Giao hoán tử

Giao hoán tử của hai toán tử A và B là

$$[A, B] \equiv AB - BA \qquad [2.48]$$

Giao hoán tử bằng 0 → hai toán tử này được gọi là giao hoán với nhau (có thể đổi chỗ cho nhau):

$$[A, B] = AB - BA = 0 \ \rightarrow AB = BA$$

$$a_- a_+ = \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2 - im\omega\underbrace{(xp - px)}_{[x,p]}]$$

$$a_- a_+ = \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2] - \frac{i}{2\hbar}[x, p] \qquad [2.49]$$

Find the commutator / Xác định giao hoán tử

$$[A, B] = ?$$

- Let $[A, B]$ act on a test function / Tác động giao hoán tử lên 1 hàm thử:
- $[A, B]f(x)$
- $[A, B]f(x) = (AB - BA)f(x) = ABf(x) - BAf(x)$
- $= A\big(Bf(x)\big) - B\big(Af(x)\big) = Xf(x)$
- $\rightarrow [A, B] = X$

Find the commutator $[x, p]$

$$[x,p]f(x) = \left[x\frac{\hbar}{i}\left(\frac{d}{dx}f(x)\right) - \frac{\hbar}{i}\frac{d}{dx}\left(xf(x)\right)\right] \qquad p = \frac{\hbar}{i}\frac{d}{dx}$$

$$= \left[\cancel{x\frac{\hbar}{i}\left(\frac{d}{dx}f(x)\right)} - \frac{\hbar}{i}\left(\frac{d}{dx}x\right)f(x) - \cancel{\frac{\hbar}{i}x\left(\frac{d}{dx}f(x)\right)}\right] \qquad [2.50]$$

$$= -\frac{\hbar}{i}f(x) = i\hbar f(x)$$

$$\boxed{[x,p] = i\hbar} \qquad [2.51]$$

2. Write the Hamiltonian in terms of a_-, a_+

$$a_- a_+ = \frac{1}{2\hbar m\omega}\left[p^2 + (m\omega x)^2\right] - \frac{i}{2\hbar}[x,p]$$

$$a_- a_+ = \frac{1}{\hbar\omega}\underbrace{\frac{1}{2m}\left[p^2 + (m\omega x)^2\right]}_{H} - \frac{i}{2\hbar}i\hbar \qquad H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$$

$$a_- a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2} \qquad [2.52]$$

$$H = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right) \qquad [2.53]$$

$a_+ a_- = ?$ $\quad$ $a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)$

$$a_+ a_- = \frac{1}{\hbar\omega} H - \frac{1}{2} \quad [2.54]$$

$$[a_-, a_+] = 1 \quad [2.55]$$

$$H = \hbar\omega\left(a_+ a_- + \frac{1}{2}\right) \quad [2.56]$$

3. The Schrödinger Equation

$$H\psi = \hbar\omega\left(a_+ a_- + \frac{1}{2}\right)\psi = E\psi$$

$$H\psi = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)\psi = E\psi$$

$$\boxed{\hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi} \quad [2.57]$$

4. Calculate wave functions and energy

"Theorem":
If ψ satisfies the Schrödinger equation with energy E, $H\psi = E\psi$,
then $a_+\psi$ satisfies the Schrödinger equation with energy $(E + \hbar\omega)$,
$H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$,
and $a_-\psi$ satisfies the Schrödinger equation with energy $(E - \hbar\omega)$,
$H(a_-\psi) = (E - \hbar\omega)(a_-\psi)$.

4. Calculate wave functions and energy

Proof: $H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$

$H = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)$ [2.56]

$$Ha_+\psi = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)a_+\psi = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi$$

$$= \hbar\omega a_+\left(a_-a_+ + \frac{1}{2}\right)\psi = \hbar\omega a_+\left(\underbrace{a_-a_+}_{a_+a_-+1} + \frac{1}{2}\right)\psi$$

$$= a_+\hbar\omega\left[\left(a_+a_- + \frac{1}{2} + 1\right)\right]\psi$$

$[a_-, a_+] = a_-a_+ - a_+a_- = 1$

$$= a_+\left[\underbrace{\hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi}_{H\psi = E\psi} + \hbar\omega\psi\right] = a_+(E + \hbar\omega)\psi$$

$$= (E + \hbar\omega)(a_+\psi)$$

4. Calculate wave functions and energy

$$\boxed{H(a_-\psi) = (E - \hbar\omega)(a_-\psi)}$$

$$H a_-\psi = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)a_-\psi = \hbar\omega\left(a_-a_+a_- - \frac{1}{2}a_-\right)\psi$$

$$= \hbar\omega a_-\left(\underbrace{a_+a_-}_{a_-a_+-1} - \frac{1}{2}\right)\psi = a_-\hbar\omega\left(a_-a_+ - \frac{1}{2} - 1\right)\psi$$

$$= a_-\left[\underbrace{\hbar\omega\left(a_-a_+ - \frac{1}{2}\right)\psi}_{H\psi=E\psi} - \hbar\omega\psi\right] = a_-(E - \hbar\omega)\psi$$

$$= (E - \hbar\omega)(a_-\psi)$$

4. Calculate wave functions and energy

$$\boxed{H(a_+\psi) = (E + \hbar\omega)(a_+\psi)}$$

a_+ help to climb up in energy ($\hbar\omega$): $\rightarrow$ a_+: raising operator

$$H(a_+(a_+\psi))$$
$$= (E + \hbar\omega + \hbar\omega)(a_+(a_+\psi))$$
$$H(a_+^2\psi) = (E + 2\hbar\omega)(a_+^2\psi)$$

$$\boxed{H(a_+^n\psi) = (E + n\hbar\omega)(a_+^n\psi)}$$

4. Calculate wave functions and energy

$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$$

$$H(a_-\psi) = (E - \hbar\omega)(a_-\psi)$$

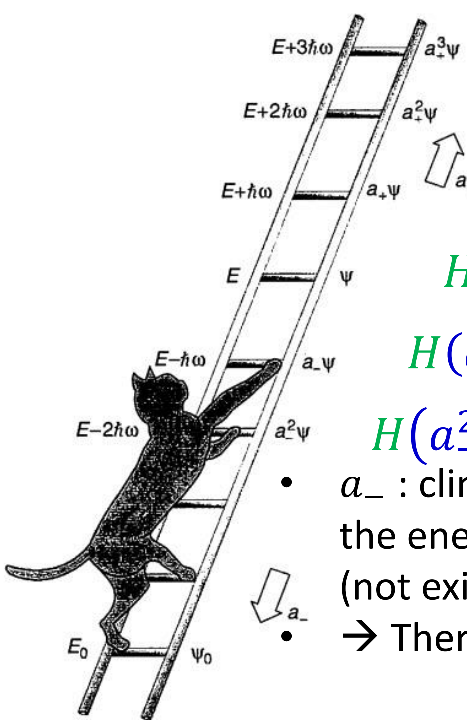
$$H(a_+(a_+\psi)) = (E + \hbar\omega + \hbar\omega)(a_+(a_+\psi))$$
$$H(a_+^2\psi) = (E + 2\hbar\omega)(a_+^2\psi)$$
$$H(a_+^n\psi) = (E + n\hbar\omega)(a_+^n\psi)$$

$$H(a_-^2\psi) = (E - 2\hbar\omega)(a_-^2\psi)$$
$$\ldots$$
$$H(a_-^n\psi) = (E - n\hbar\omega)(a_+^n\psi)$$

a_+ help to climb up in energy ($\hbar\omega$): $\rightarrow a_+$: raising operator

a_- help to climb down in energy ($\hbar\omega$): $\rightarrow a_+$: lowering operator

a_+, a_- are called ladder operators (or creation/annihilation operators)



$$H(a_+^n\psi) = (E + n\hbar\omega)(a_+^n\psi)$$
$$H(a_+^2\psi) = (E + 2\hbar\omega)(a_+^2\psi)$$
$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$$
$$H\psi = E\psi$$
$$H(a_-\psi) = (E - \hbar\omega)(a_-\psi)$$
$$H(a_-^2\psi) = (E - 2\hbar\omega)(a_-^2\psi) \ldots$$

- a_- : climb down ($\hbar\omega$): The further down, the lower the energy → reach a state with energy less than 0! (not exist!)
- → There must exist a "lowest rung", ψ_0 , such that

$$a_-\psi_0 = 0$$

4. Calculate wave functions and energy

$$a_-\psi_0 = 0 \qquad [2.58]$$

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \qquad a_- = \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x)$$

$$\psi_0 = ? \qquad a_-\psi_0 = \underbrace{\frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)}_{a_-}\psi_0 \qquad p = \frac{\hbar}{i}\frac{d}{dx}$$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0$$

4. Calculate wave functions and energy

$$\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0 \iff \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0$$

$$\int\frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}\int x dx \implies ln\,\psi_0 = -\frac{m\omega}{2\hbar}x^2 + const.$$

$$\implies \psi_0 = Ae^{-\frac{m\omega}{2\hbar}x^2}$$

4. Calculate wave functions and energy

Find A (normalize the wave function)

$$1 = |A|^2 \int_{-\infty}^{+\infty} e^{-\frac{m\omega}{\hbar}x^2} dx = |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}}$$

$$\boxed{\Longrightarrow \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}} \qquad [2.59]$$

4. Calculate wave functions and energy

The energy E_0 corresponds to the state $\psi_0(x)$

$$H\,\psi_0 = E_0\,\psi_0$$

$$\hbar\omega\left(a_+a_- + \frac{1}{2}\right)\psi_0 = E_0\,\psi_0$$

$$a_-\,\psi_0 = 0 \Longrightarrow \frac{1}{2}\hbar\omega\,\psi_0 = E_0\,\psi_0$$

$$E_0 = \frac{1}{2}\hbar\omega \qquad [2.60]$$

$\psi_0(x)$: the ground state of the quantum oscillator

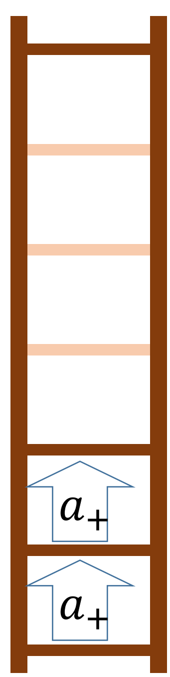
4. Calculate wave functions and energy

Determine the n^{th} state and energy: $\psi_n(x)$, E_n

$$E_0 + n\hbar\omega = E_n \qquad \psi_n = A_n a_+^n \psi_0$$

$$E_n = \frac{1}{2}\hbar\omega + n\hbar\omega$$

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



$$E_0 + 2\hbar\omega = E_2 \qquad \psi_2 = A_2 a_+^2 \psi_0$$

$$E_0 + \hbar\omega = E_1 \qquad \psi_1 = A_1 a_+ \psi_0$$

$$\frac{1}{2}\hbar\omega = E_0 \qquad \psi_0$$

4. Calculate wave functions and energy

$$\boxed{\psi_n(x) = A_n a_+^n \, \psi_0(x) \ \ \text{với} \ \ E_n = \left(n + \frac{1}{2}\right)\hbar\omega} \qquad [2.61]$$

A_n is the normalization constant

Find the first excited state

$\psi_1(x) = ?$

$\psi_1(x) = A_1 a_+ \ \psi_0(x)$

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x)$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\psi_1(x) = A_1 a_+ \ \psi_0(x) = A_1 \frac{1}{\sqrt{2\hbar m\omega}} (-ip + m\omega x)\ \psi_0(x)$$

$$\psi_1(x) = A_1 \frac{1}{\sqrt{2\hbar m\omega}} \left(-\hbar \frac{d}{dx} + m\omega x\right) \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= A_1 \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\, x e^{-\frac{m\omega}{2\hbar}x^2} \qquad [2.62]$$

Normalize: $\int |\ \psi_1(x)|^2 dx = 1 \ \rightarrow A_1 = 1$