B. Quantum Harmonic Oscillator - 1D case

The problem: $U(x) = \frac{1}{2} K x^2 \equiv \frac{1}{2} m\omega_0^2 x^2$

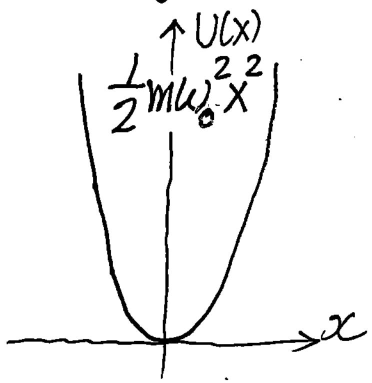
"particle of mass m under the influence of a parabolic ($\sim x^2$) potential energy function"

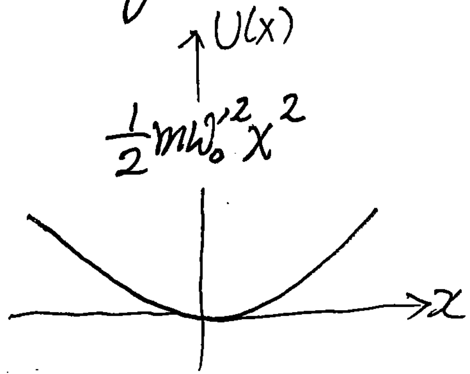
"K" (Spring constant) OR ω_0 (angular freq. $\sqrt{\frac{K}{m}}$) characterizes $U(x)$

Goal: Solve TISE

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2} m\omega_0^2 x^2 \psi(x) = E\psi(x)$$

for $\underbrace{\psi_E(x) \longleftrightarrow E}_{\text{many of them}}$





$\omega_0 > \omega_0'$

different curvatures

Why Harmonic Oscillator?

- Planck (1900), Einstein (1908)

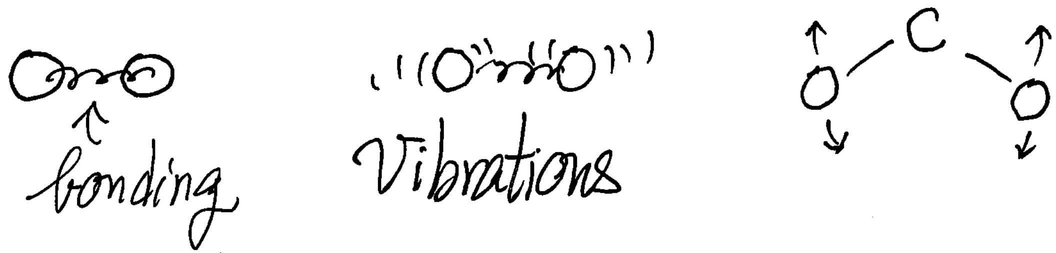
  differ by $h\nu\ (=\hbar\omega)$

  - needed energies of oscillator to be $0,\ h\nu,\ 2h\nu,\ 3h\nu, \ldots$

  to explain thermal radiation and heat capacity $C(T)$ of solids

  differ by $h\nu\ (=\hbar\omega)$

- Molecules



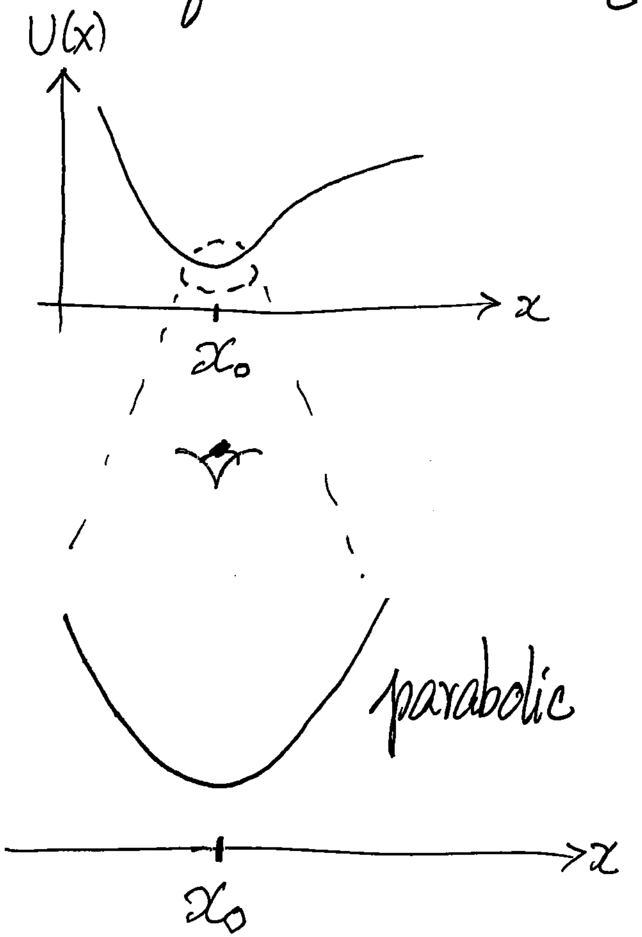
CO_2 vibrations [cause problems in climate change]

- More than 50% of physics is about harmonic Oscillator physics!

- Physics around an equilibrium position is oscillator physics

Equilibrium $\Rightarrow$ $\left.\frac{dU}{dx}\right|_{x_0} = 0$ (x_0 is the equilibrium position)

$U(x_0)$ is a minimum



Sufficiently close to x_0, (ignore higher order terms)

$$U(x) \approx U(x_0) + \cancel{\left.\frac{dU}{dx}\right|_{x=x_0}}^{\,0} \cdot (x-x_0) + \frac{1}{2} \underbrace{\left.\frac{d^2U}{dx^2}\right|_{x=x_0}}_{\text{"Spring Constant K"}} \cdot (x-x_0)^2$$

$$= U(x_0) + \frac{1}{2} K \cdot (x-x_0)^2$$

$$= U(x_0) + \frac{1}{2} m\omega_0^2 (x-x_0)^2$$

[a harmonic Oscillator!]

$\therefore$ <u>Oscillator physics is everywhere!</u>

Higher-order $\Rightarrow$ <u>Anharmonic terms</u>

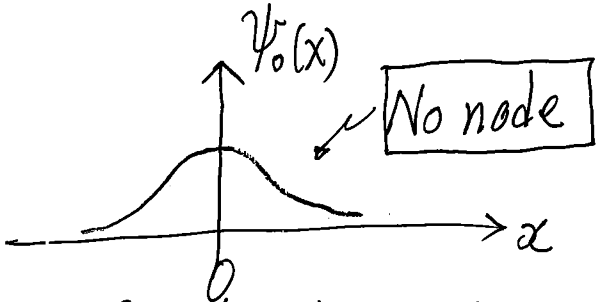
Strategy "0": Educated Guess on behavior of TISE Solutions

Think like a physicist!

- $U(x)$ is symmetric about $x=0$

[alternating even/odd $\psi_n(x)$'s]

- $U(x)$ keeps on increasing $\Rightarrow$ infinitely many bound states

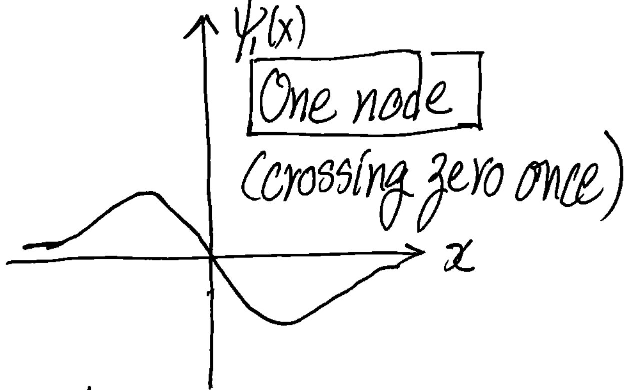


Ground state (G.S.)

Even

Lowest energy

$\Rightarrow$ Spread not too wide

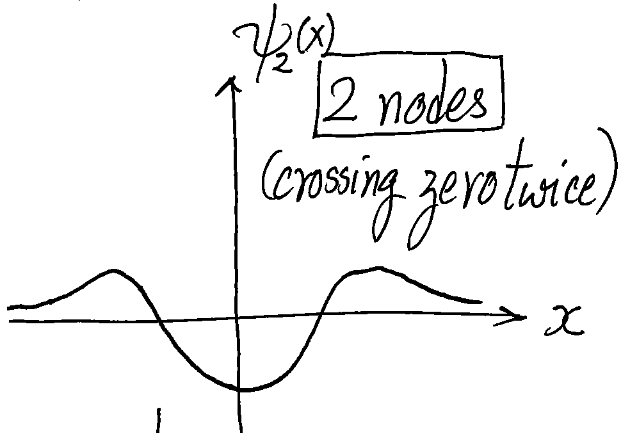


1st excited state

Odd

Energy higher than G.S.

$\Rightarrow$ go farther in $\pm x$



2nd excited state

Even

Even higher energy

$\Rightarrow$ farther into $\pm x$

Approach 1: Solving TISE by the "Series Solutions" Method

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m\omega_0^2 x^2 \psi(x) = E\psi(x) \quad \text{Plus well-behaved } \psi(x)$$

Key Steps[+] in Solving

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega_0^2 x^2\right)\psi = 0} \quad (1)$$

Step 1: Always useful to change to dimensionless variables

Meaning: The problem provides $(m, \omega_0, \hbar)$

"x" is a length: Any length set by $(m, \omega_0, \hbar)$? $\sqrt{\frac{\hbar}{m\omega_0}}$ is a length

"E" is an energy: Any energy set by $(m, \omega_0, \hbar)$? $\hbar\omega_0$ or $\frac{\hbar\omega_0}{2}$ is an energy

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[+] Details will be filled in later (see Appendix).

Define $\underset{\text{no unit}}{y} \equiv \sqrt{\dfrac{m\omega_0}{\hbar}}\, x$; $\underset{\text{no unit}}{\alpha} \equiv \dfrac{E}{\left(\frac{1}{2}\hbar\omega_0\right)}$

[measure length in $\sqrt{\dfrac{\hbar}{m\omega_0}}$] [measure energy in units of $\left(\frac{1}{2}\hbar\omega_0\right)$]

TISE (Eq.(1)) becomes: $$\boxed{\frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0} \quad (2)$$ look Simpler!

Step 2: Solving Eq.(2) by method of series solution plus boundary conditions

Results: Any α will not give well-behaved ψ

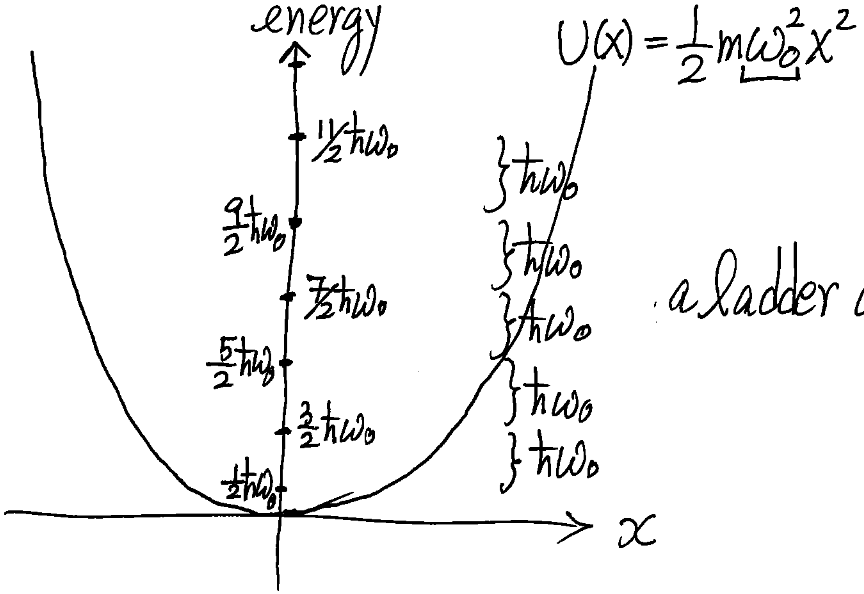
> Only when $\alpha = 2n+1$ ($n = 0, 1, 2, \cdots$), ψ is $\underbrace{\text{well-behaved}}_{\text{does not blow up}}$ as $y \to \pm\infty$

Repeated theme: B.C.'s (physics) selects specific allowed energies

$\therefore$ Energy Eigenvalues (or physically allowed energies) are

$$\alpha \equiv \frac{E}{(\frac{1}{2}\hbar\omega_0)} = 2n+1 \Rightarrow \boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega_0\,, \quad n = 0,1,2,\cdots}$$

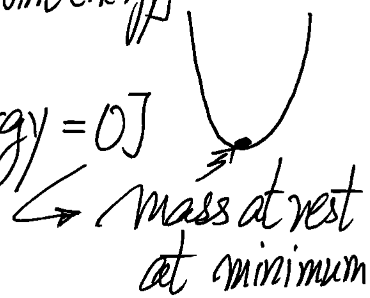
- Infinity many E_n
- Allowed energies are <u>evenly spaced</u> by $\hbar\omega_0$



a ladder of $\hbar\omega_0$

- $E_0 = \underbrace{\text{Ground state energy}}_{\text{lowest possible (QM)}} = \frac{1}{2}\hbar\omega_0$ [zero-point energy]

[classical physics: lowest energy $= 0$]



This is exactly what Planck and Einstein asked for!

Energy Eigenfunctions:

$$\boxed{\psi_n(y) = \underset{\substack{\uparrow \\ \text{normalization} \\ \text{constant}}}{A_n}\ \underbrace{H_n(y)}_{\substack{\text{Hermite} \\ \text{Polynomials}}}\ e^{-\frac{1}{2}y^2}}$$

$e^{-\frac{1}{2}y^2}$ ← gives tails so that $\psi_n \to 0$ as $y \to \pm\infty$

- Polynomial (多項式): <u>Finite number of terms</u> [e.g. $a_0 + a_1 y + a_2 y^2 + \cdots + a_{13} y^{13}$] ← y^{13}: stopped!
- Hermit Polynomials: $H_0, H_2, H_4, \cdots$ only carry $y^{(\text{even power})}$ terms

  $\therefore H_{\text{even}\#}(y)$ is even function

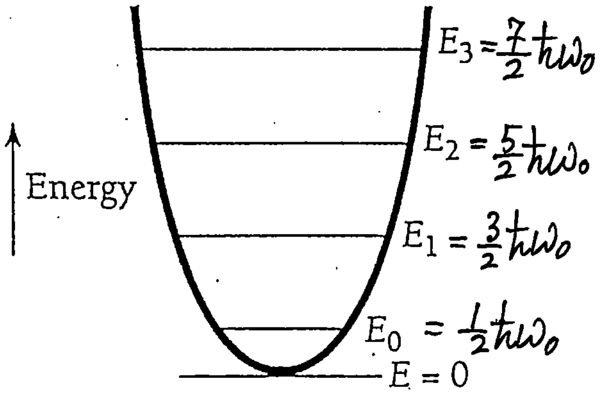
  $H_1, H_3, H_5, \cdots$ only carry $y^{(\text{odd power})}$ terms

  $\therefore H_{\text{odd}\#}(y)$ is odd function
- There are tables to look up $H_n(y)$ ["Google" Hermite Polynomials]

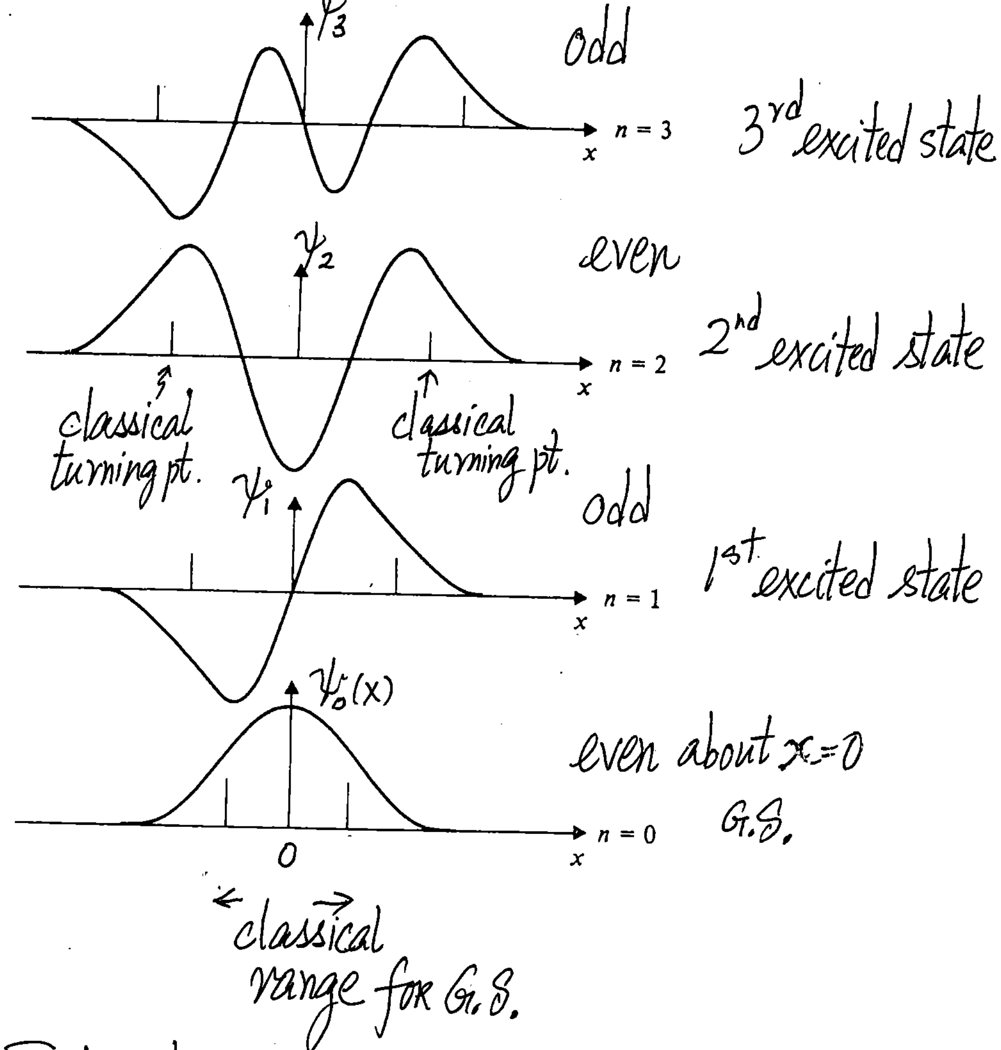
Lowest four E_n and $\psi_n(x)$

$$E_n = (n+\tfrac{1}{2})\hbar\omega_0 \ ; \ n = 0, 1, 2, \ldots$$

$$\psi_n \sim H_n(y)\, e^{-\frac{1}{2}y^2} \ ; \ y = \sqrt{\frac{m\omega_0}{\hbar}}\, x$$



Classically, higher energy has farther turning points



Tails into classically forbidden regions

[This is what we guessed from experience!]

- For those not interested in the mathematics involved here, what was discussed up to here is the bare minimum on quantum oscillator physics.
  (i) Knowing the key features of $(E_n \leftrightarrow \psi_n(x))$ and form of TISE
  (ii) $E_n = (n + \frac{1}{2})\hbar\omega_0$ [an important result in all of physics]
- You should also know how to check if a function is a solution to TISE or not.

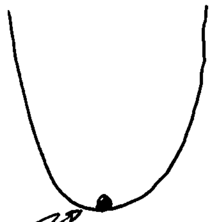
Go To Appendix here

Think like a physicist: Advanced level

Why couldn't we have an allowed energy $< \frac{1}{2}\hbar\omega_0$?

Classical Physics

lowest energy $= 0$

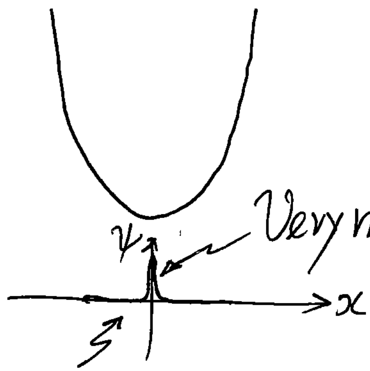


mass at bottom at rest

(k.e. $= 0$, $U = 0$)

Quantum Physics

This would be



Very narrow

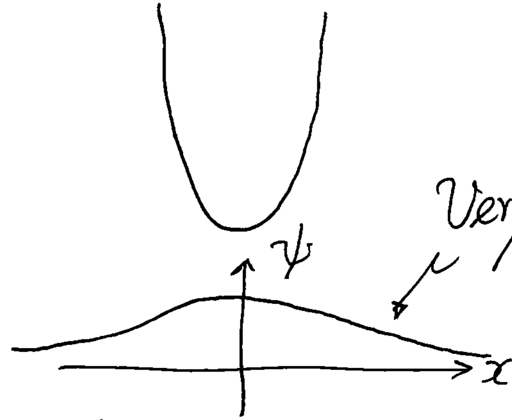
this has high k.e. part

$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi\right)$ high

Although p.e. [e.g. $\langle U \rangle$] is low

[total energy may not be low.]

How about ?



Very broad

$\langle KE \rangle$ is low

But $\langle PE \rangle$ is high

[total energy may not be low]

True $\psi_0(x)$ is a compromise!

Features about G.S. $\psi_0(x)$

- Gaussian function
- Fourier transform $F(k)$ is also Gaussian
- $\Delta x \cdot \Delta p = \frac{\hbar}{2}$ (an optimal situation, only for G.S. ψ_0)

Exercises

- Δx for $\psi_n(x)$ [any n]
- Δp for $\psi_n(x)$ [any n]
- $\Delta x \cdot \Delta p$ for $\psi_n(x)$ [any n]
- $|\psi_n(x)|^2$ vs x $\left\{\begin{array}{l}\text{small } n \\ \text{large } n\end{array}\right\}$ compare with classical physics

Remarks

- Treated in detail because not so many problems can be solved analytically

Physics

- Oscillator QM is useful in
  - Molecular physics [vibrational]
  - Solid state physics
  - EM fields $\rightarrow$ photons

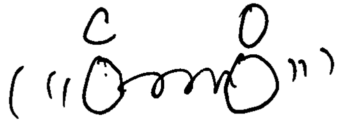
[$\frac{1}{2}\varepsilon_0 E^2 + \frac{1}{2\mu_0}B^2$ not so different from]

$$\frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2$$

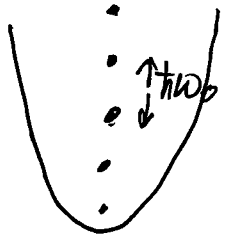
Techniques

- Useful in
  - obtaining other special functions [e.g. Bessel functions, Legendre polynomials, spherical harmonics (EM, QM)]
- Solving Hydrogen atom

Practical Appendix : Selection Rule in transitions between vibrational states



CO : Vibrational states



$\omega_0 = \sqrt{\dfrac{K}{\mu}}$ $\quad \mu$ = reduced mass

In determining if light could induce a transition between a state n and a state m, the integral involved is

$$x_{mn} \equiv \int_{-\infty}^{\infty} \psi_m^*(x) \; x \; \psi_n(x)\, dx \qquad \text{OR} \qquad \langle m | \hat{x} | n \rangle \text{ short hand}$$

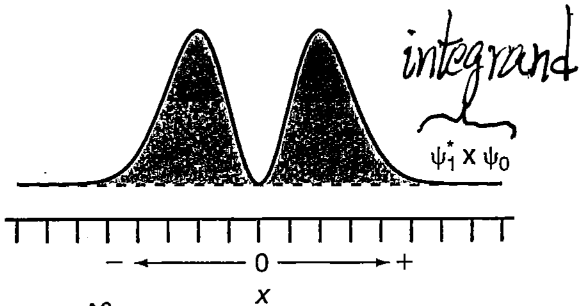
different

- If it is zero, then no transition between m and n states
- If it is not zero, then brightness of spectral line $\propto |x_{mn}|^2$

For oscillator states, $x_{mn} \neq 0$ only if m & n differ by ± 1

If $m = n$ or m & n differ more than ± 1, $x_{mn} = 0$

- Check by doing integrals
- Check by inspection



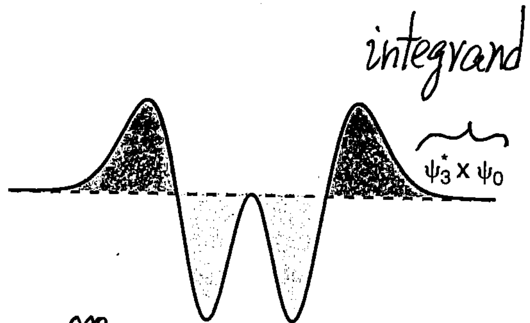
$$\int_{-\infty}^{\infty} \psi_1^*(x) \times \psi_0(x)dx$$

= Area under curve

$\neq 0$

$n=0 \leftrightarrow n=1$ <u>allowed</u>

$\Delta n = \pm 1$

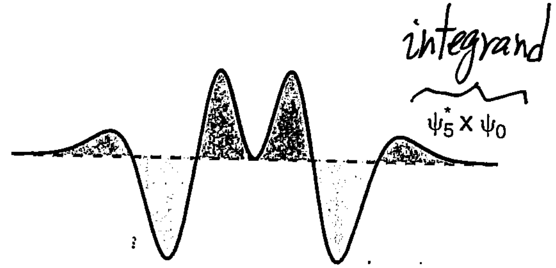


$$\int_{-\infty}^{\infty} \psi_3^*(x) \times \psi_0(x)dx$$

= Area "under" curve

= 0

$n=0 \leftrightarrow n=3$ <u>forbidden</u>



$$\int_{-\infty}^{\infty} \psi_5^*(x) \times \psi_0(x)dx$$

= Area "Under" Curve

= 0

$n=0 \leftrightarrow n=5$ <u>forbidden</u>

$$\int_{-\infty}^{\infty} \underbrace{\psi_m^*(x)}_{\substack{\text{even} \\ (m=\text{even})}} \underbrace{x}_{\text{odd}} \underbrace{\psi_n(x)}_{\substack{\text{even} \\ (n=\text{even})}} dx = 0 \qquad \because \text{ integrand is odd}$$

$$\int_{-\infty}^{\infty} \underbrace{\psi_m^*(x)}_{\substack{\text{odd} \\ (m=\text{odd})}} \underbrace{x}_{\text{odd}} \underbrace{\psi_n(x)}_{\substack{\text{odd} \\ (n=\text{odd})}} dx = 0 \qquad \because \text{ integrand is odd}$$

$\therefore$ $\Delta n = \pm 1$ is the condition for $x_{mn} \neq 0$ (allowed transition) between oscillator (vibrational) states.

This "rule" is used in molecular spectrum ($\sim$IR region)