

ONE OF TWO MOST-FAMOUS PROBLEMS...

THE QUANTUM MECHANICAL HARMONIC OSCILLATOR

aka "Simple Harmonic Oscillator" SHO

A "harmonic oscillator" is basically defined as a system which reacts to a restoring force proportional to displacement.

$$F = -kx$$

That's classically... where "force" has a meaning.

In quantum mechanics POTENTIAL is the thing

But that's easy, since $\vec{F} = -\vec{\nabla}V$

Integrating, we find

$$V(x) = \frac{1}{2} kx^2$$

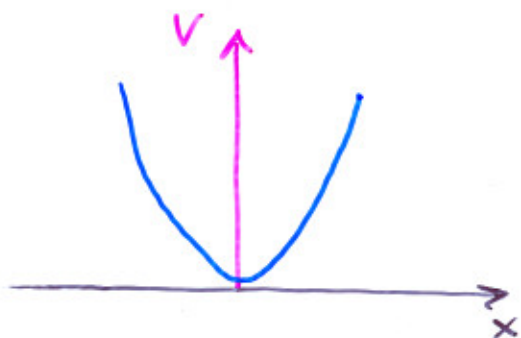
and that defines a quantum oscillator.

This potential just slots into the Schrödinger Equation

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

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

In our standard way of thinking now...



a parabolic potential

The solution to the Sch. Equation involves a power-series.

Instructive if you've not seen it before... comforting

if you have and wondered why you did!

$$\frac{d^2\psi(x)}{dx^2} = \left(\frac{\hbar^2 k^2}{\hbar^2} - \frac{2mE}{\hbar^2} \right) \psi(x)$$

make variable substitutions:

$$y \equiv \sqrt{\frac{mk}{\hbar^2}} x \equiv \kappa x \quad \text{so} \quad \kappa^2 dx^2 = dy^2$$

$$\epsilon \equiv \frac{2E}{\hbar} \sqrt{\frac{m}{k}}$$

$$\frac{d^2\psi}{dy^2} = (y^2 - \epsilon) \psi$$

look at an asymptotic region.. $y^2 \gg \epsilon$

there $\frac{d^2\psi}{dy^2} = y^2 \psi$

which is satisfied by $\psi = e^{\pm y^2/2}$

The wavefunction must vanish at ∞ , so keep only negative sign solution.

So, the whole solution will look like

$$\psi(y) = c e^{-y^2/2} H(y)$$

↑ ↑
a normalization constant.
to be determined

substituting... shows that $H(y)$ satisfies:

$$\frac{d^2 H}{dy^2} - 2y \frac{dH}{dy} + (\epsilon - 1)H = 0 \quad \star$$

A standard way to solve such equations is to assume that the solution can be written as a power series:

$$H(y) = a_0 + a_1 y + a_2 y^2 + \dots = \sum_{n=0}^{\infty} a_n y^n$$

Substitute this into \star and this becomes an equation in the a 's

$$\frac{dH}{dy} = a_1 + 2a_2 y + 3a_3 y^2 + \dots$$

$$\begin{aligned} \frac{d^2 H}{dy^2} &= 2a_2 + 6a_3 y + 12a_4 y^2 + \dots \\ &= \sum_{n=0}^{\infty} (n+1)(n+2) a_{n+2} y^n \end{aligned}$$

$$\begin{aligned} 2y \frac{dH}{dy} &= 2y a_1 + 4a_2 y^2 + \dots \\ &= \sum 2n a_n y^n \end{aligned}$$

putting them together in the form of \star

$$\sum_{n=0}^{\infty} y^n \left[(n+1)(n+2)a_{n+2} - 2na_n + (\epsilon-1)a_n \right] = 0$$

only true for every y if each coefficient is zero.

$$[\dots] = 0$$

$$\Rightarrow a_{n+2} = \frac{2n+1-\epsilon}{(n+1)(n+2)} a_n$$

a RECURSION FORMULA -- no one can write $H(y)$ in terms of a_0 and a_1 -- and generate the rest.

A fine detail... the normalization condition

$$\int_{-\infty}^{\infty} \psi^* \psi dy = 1$$

happens only if $H(y)$ terminates at some value of n .

This leads to 2 conditions

1. For some specific n , $a_{n+2} = 0$ -- which happens $2n+1 = \epsilon = \frac{2E}{\hbar} \sqrt{\frac{\mu}{k}}$
2. If that n is odd, $a_0 = 0$; if that n is even, $a_1 = 0$.

Look at condition 1:

$$2n+1 = \epsilon = \frac{2E}{\hbar} \sqrt{\frac{m}{k}}$$

$$E_n = (n + \frac{1}{2}) \hbar \sqrt{\frac{k}{m}}$$

↑ quantized.

for an oscillator... $f = \sqrt{\frac{k}{m}} \frac{1}{2\pi}$

$$E_n = (n + \frac{1}{2}) \hbar f$$

One of the more famous and important results in quantum mechanics. More in a bit.

Condition 2 leads to a particular set of polynomials

$$H_n(y)$$

the Hermite Polynomials

even functions if n even

odd " n odd

There are many such polynomial sets... most of which have a role in physics problems now where.

They are produced from "generating functions"

Here:

$$S(y, s) = e^{-s^2 + 2sy} = \sum_{n=0}^{\infty} \frac{H_n(y)}{n!} s^n$$

or.

$$H(y) = (-1)^n e^{y^2} \frac{d^n (e^{-y^2})}{dy^n}$$

Put all the constants back in...

$$\Psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{\frac{1}{2}} e^{-\alpha^2 x^2 / 2} H_n(\alpha x)$$

where $\alpha = \sqrt[4]{\frac{m\hbar}{\hbar^2}}$

$H_n(\alpha x)$ are the Hermite polynomials.

Here are the first 5:

$$H_0(\alpha x) = 1$$

$$H_1(\alpha x) = 2\alpha x$$

$$H_2(\alpha x) = 4\alpha^2 x^2 - 2$$

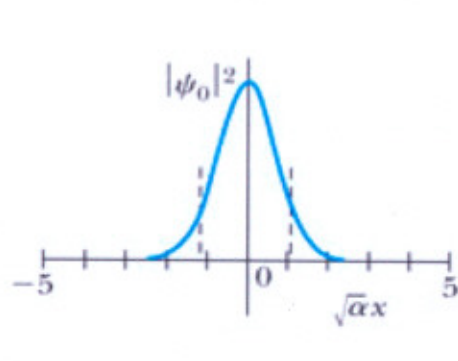
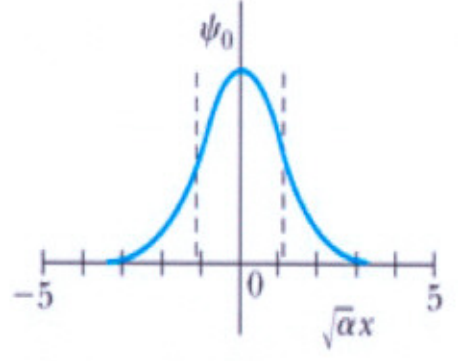
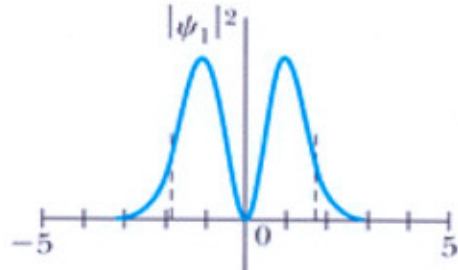
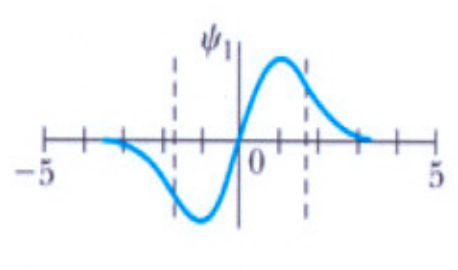
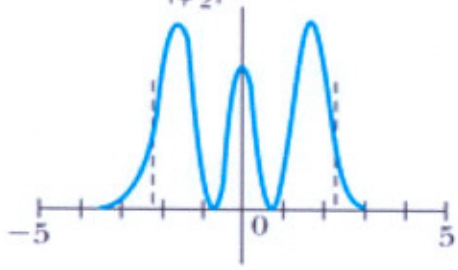
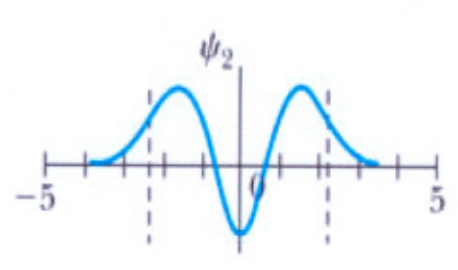
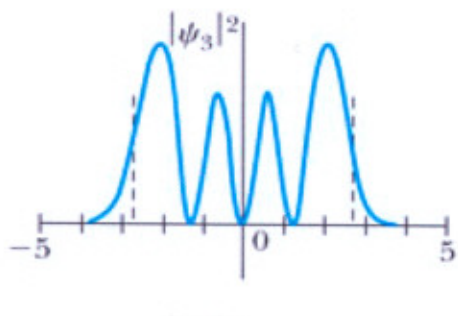
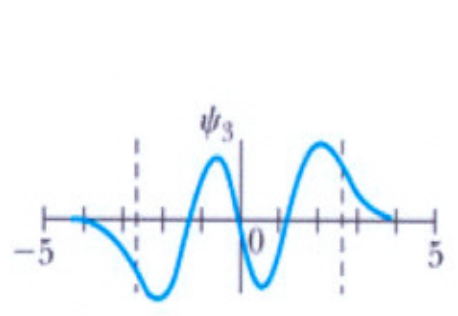
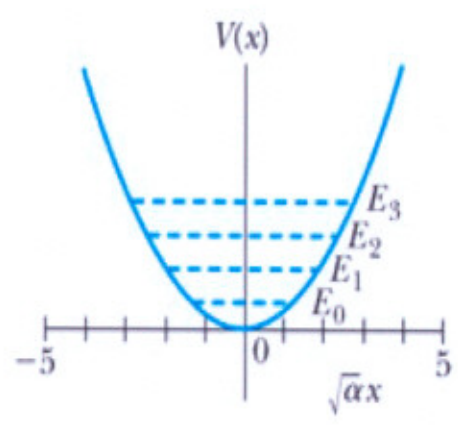
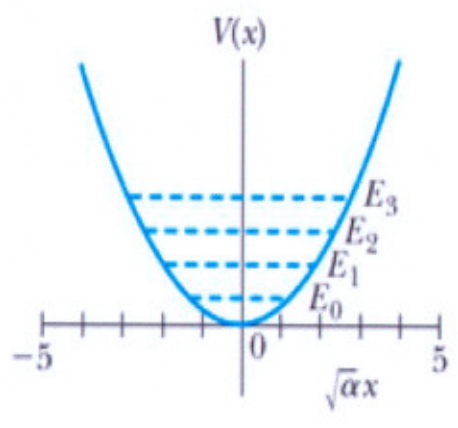
$$H_3(\alpha x) = 8\alpha^3 x^3 - 12\alpha x$$

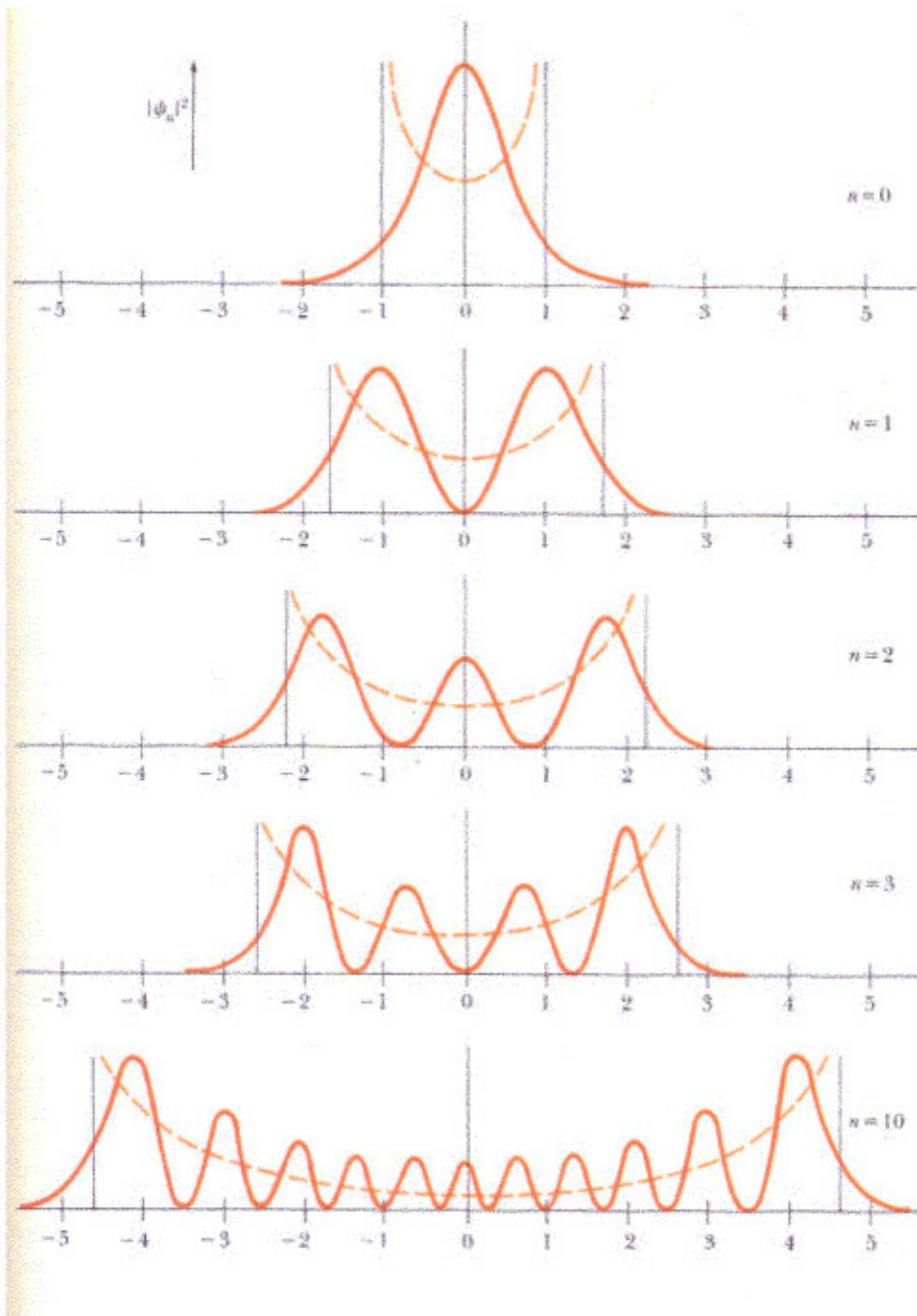
$$H_4(\alpha x) = 16\alpha^4 x^4 - 48\alpha^2 x^2 + 12$$

So, the first 2 "eigenfunctions" - wave functions are:

$$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha^2 x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x e^{-\alpha^2 x^2/2}$$





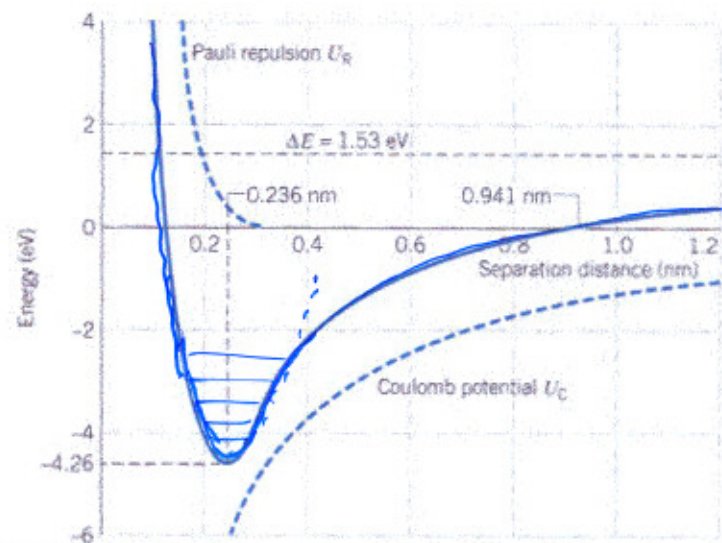
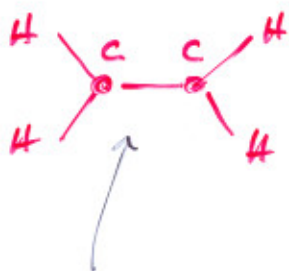


FIGURE 9.19 Molecular energy in NaCl. The “zero” of the energy scale represents neutral Na and Cl atoms. The solid curve is the sum of the three contributions to the molecular energy.

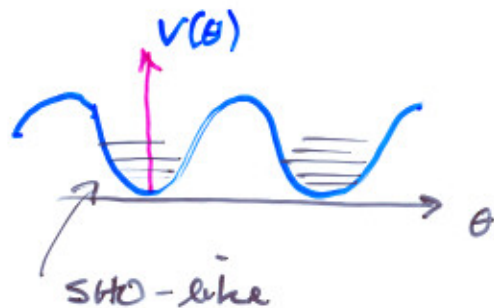
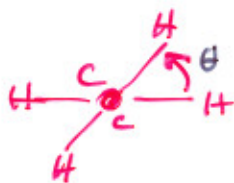
C_2H_4 example



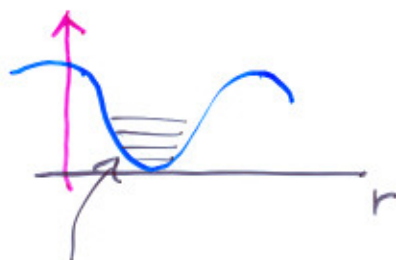
planar is most stable

but there can be torsional excitations.

from the end:



crystal lattice



vibrational excitations

lead to the "emission"

of quantized "quasi-particle"

states called phonons

the quanta of crystal vibrations

Look at the energies.

$$E_n = (n + \frac{1}{2})hf$$

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

They are evenly spaced.

They have a finite, non-zero value in the lowest state, $n=0$ --- the **Ground State**

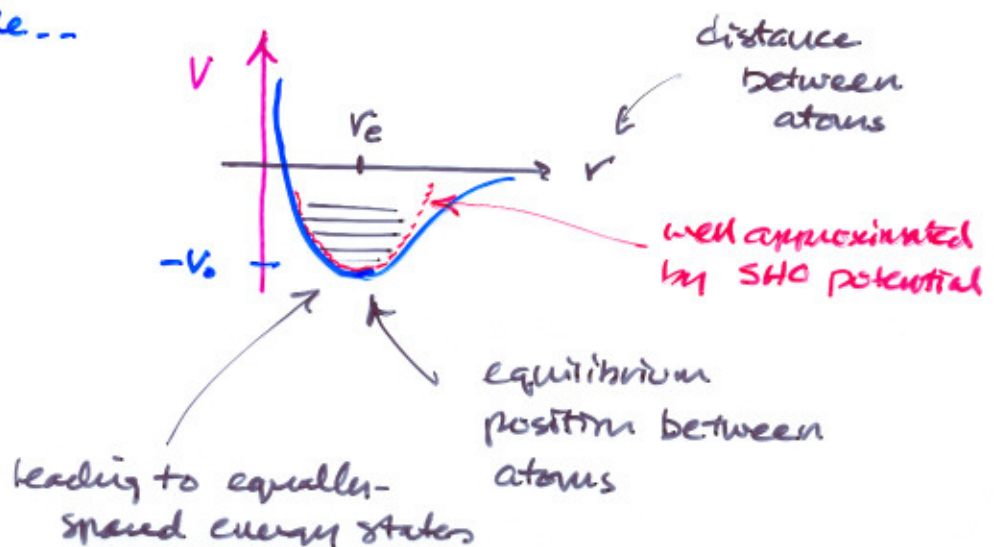
$$E_0 = \frac{1}{2}hf$$

called the Zero Point Energy

→ no classical analog

EXAMPLES AROUND---

Diatom molecule--



→ which we interpret as $\text{O} \text{---} \text{O} \text{---} \text{O}$ vibrational-like quantized states.