LECTURE 21: The Harmonic Oscillator and The Particle Constrained to a Ring.

What I expect you to learn:

- Properties of the 1D Harmonic Oscillator solutions and how they differ from its classical counterpart

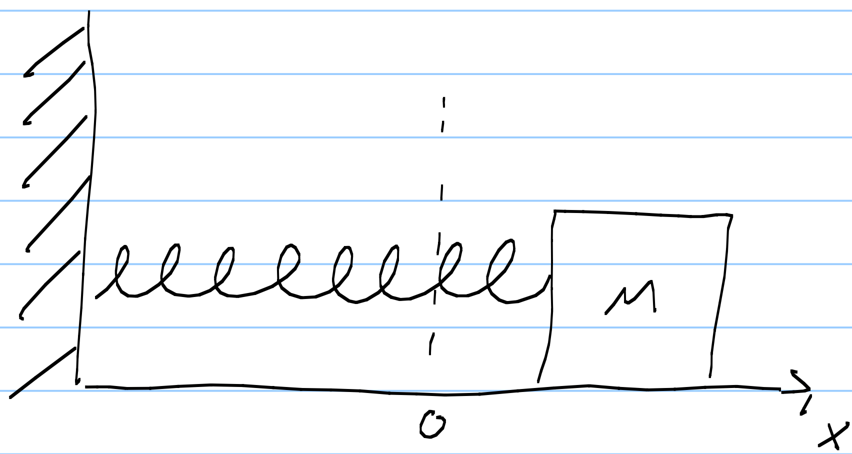
- How to solve the "particle on a ring"

(Corresponds to sections 4.7 of textbook)

(Reminder: Problem set 3 due Nov 10th)

THE HARMONIC OSCILLATOR

Consider the following setup:



mass "m" oscillating about x_0 due to restoring force exerted by a spring.
$F = -Kx$

$$F = ma \rightarrow -Kx = m\frac{d^2x}{dT^2} \rightarrow m\frac{d^2x}{dT^2} + Kx = 0 \quad (1)$$

the solution to (1) is?

$$F = Kx = \frac{dV}{dx} \rightarrow V = \frac{1}{2}Kx^2$$

This parabolic potential is of great importance in both classical and quantum physics

THE HARMONIC OSCILLATOR

Consider the following arbitrary potential

To estimate the motion of a particle at "a" subjected to $V(x)$, I could expand $V(x)$ using a Taylor series:

$$V(x) = V(a) + (x-a)V'(a) + \frac{1}{2!}(x-a)^2 V''(a) + \frac{1}{3!}(x-a)^3 V'''(a) + \dots$$

Since particle is at "a" → minimum, $V'(a) = 0$
We can choose "a" to be at the origin so we'll get

$$\boxed{V(x) = \frac{1}{2} K x^2 + \dots}, \quad \text{with } K = V''(a)$$

THE HARMONIC OSCILLATOR

With $V(x) = \frac{1}{2} K x^2$, the Hamiltonian $= T + V$, will be:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} K x^2$$

the Schrödinger equation: $H\psi = E\psi$, will be:

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

we can rewrite (2) in terms of dimensionless eigenvalues:

$\lambda = \frac{2E}{\hbar\omega}$, $\omega = \sqrt{\frac{K}{m}}$, and the dimensionless variable

$\xi = \alpha x$, $\alpha = \left(\frac{Km}{\hbar^2}\right)^{1/4} = \left(\frac{m\omega}{\hbar}\right)^{1/2}$, (2) becomes:

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0 \qquad (3)$$

THE HARMONIC OSCILLATOR

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0 \qquad (4)$$

The solutions to (4) involve Hermite polynomials. I encourage you to look at how the solutions are obtained in the textbook. You will learn about Hermite Polynomials in later courses. For now we'll just study the solutions. We will derive the solutions to the harmonic oscillator once we are familiar with Dirac notation.

To be physically valid, solutions to (4) require:

$$\boxed{\lambda = 2n+1, \quad n = 0, 1, 2}$$

They are given by:

$$\psi_n(\xi) = e^{-\xi^2/2} H_n(\xi)$$

$H_n(\xi) \longrightarrow$ Hermite polynomials

$$H_n(\xi) = e^{\xi^2/2}\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2}$$

$$H_0(\xi) = 1, \quad H_1(\xi) = 2\xi, \quad H_2(\xi) = 4\xi^2 - 2$$

THE HARMONIC OSCILLATOR

$\boxed{\lambda = 2n+1, \ n = 0, 1, 2}$, with $\lambda = \frac{2E}{\hbar\omega}$

$\Rightarrow 2E = \hbar\omega\lambda = \hbar\omega(2n+1)$

$$\boxed{\Rightarrow E_n = \hbar\omega(n + 1/2) \qquad n = 0, 1, 2, 3}$$

Note: - that lowest energy $\neq 0$ $= E_0 = \frac{\hbar\omega}{2}$
(zero-point energy)

- the wave function associated with E_0 peaks at $x = 0$. Classically, what is the most probable location of the particle?

Let's look at the solutions (www.falstad.com/qm1d/)

THE HARMONIC OSCILLATOR

Example problem: Using Heisenberg's Uncertainty principle, find the minimum of the energy of a particle in a potential well: $V(x) = \frac{1}{2}Kx^2$, by minimizing E with respect to x.

$$E = T + V = \frac{1}{2}mv^2 + \frac{1}{2}Kx^2$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \qquad \left(\omega^2 = \frac{K}{m} \right)$$

$$\Delta x \Delta p > \hbar \quad , \quad \Delta x \simeq \frac{\hbar}{\Delta p} \quad , \quad \Delta p \simeq \frac{\hbar}{\Delta x}$$

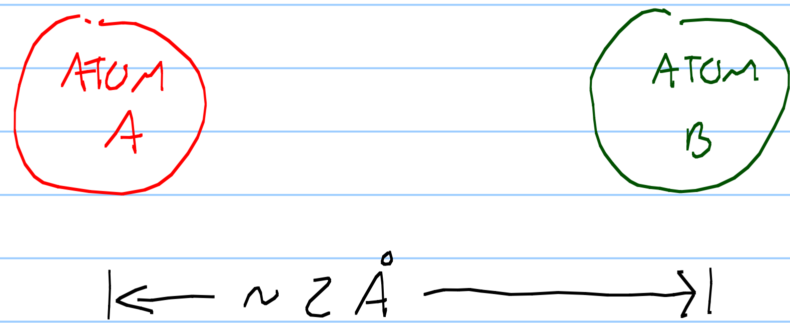
$$\frac{dE}{dx} = \frac{d}{dx}\left(\frac{\hbar^2}{2mx^2} + \frac{1}{2}m\omega^2x^2 \right) = 0$$

$$= \frac{-2\hbar^2}{2mx^3} + \frac{2m\omega^2x}{2} = 0 \Rightarrow x^4 = \frac{\hbar^2}{m^2\omega^2} \, , \quad x = \sqrt{\frac{\hbar}{m\omega}}$$

$$E = \frac{\hbar^2}{\hbar} \cdot \frac{m\omega}{2m} + \frac{1}{2}m\omega^2 \frac{\hbar}{m\omega} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{2} = \hbar\omega$$

THE HARMONIC OSCILLATOR

Example: the diatomic molecule



RESTORING FORCE FOR SMALL DISPLACEMENTS FROM EQUILIBRIUM IS WELL DESCRIBED BY THE FORCE OBTAINED FROM HARMONIC OSCILLATOR POTENTIAL.

→ WE LIMIT OURSELVES TO VIBRATIONS ALONG THE LINE JOINING THE NUCLEI (WE'LL SEE ROTATIONS LATER)

$$E = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 + \frac{1}{2} C x^2 \qquad (5)$$

$x = 0$ is equilibrium position

THE HARMONIC OSCILLATOR

WE'LL USE THE REDUCED MASS AGAIN:

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \quad , \quad \mu = \frac{m_1 m_2}{m_1 + m_2} \qquad (6)$$

With respect to the center of mass, the momenta will be equal and opposite so we have:

$$E = \frac{p^2}{2m_1} + \frac{p^2}{2m_2} + \frac{1}{2} C x^2 \quad , \text{ with } (6) \text{ we have:}$$

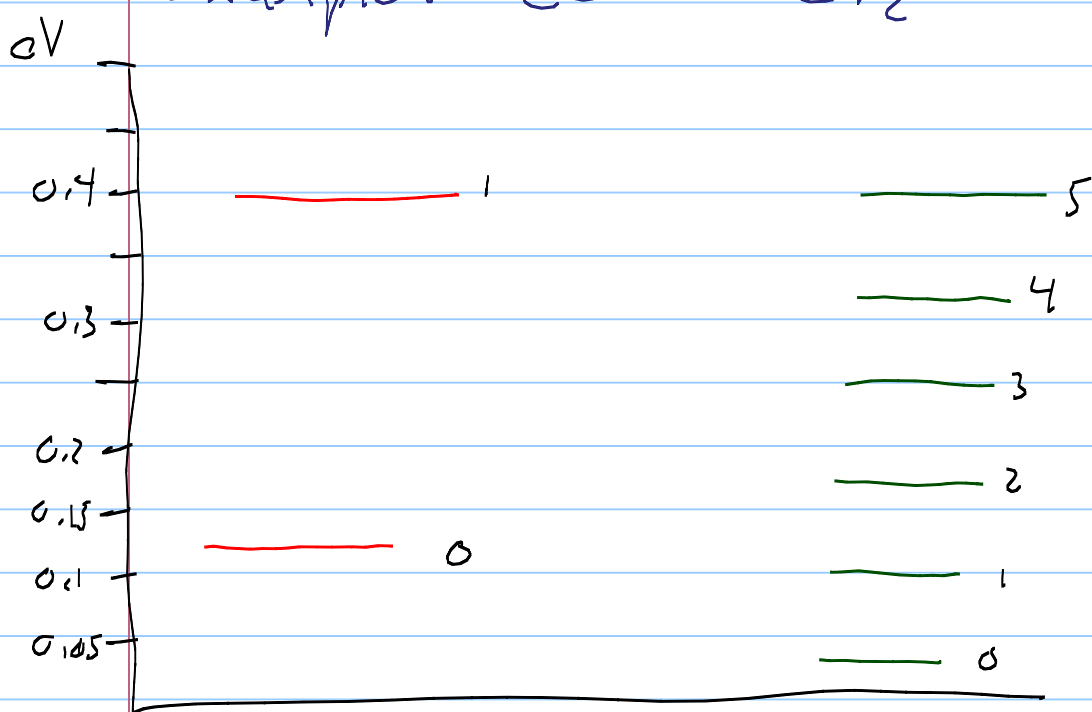
$$E = \frac{p^2}{2\mu} + \frac{1}{2} C x^2$$

→ equivalent to a single particle of mass μ in a 1-D harmonic oscillator potential.

The Schrodinger equation is: $\frac{-\hbar^2}{2\mu} \frac{d^2\psi}{dx^2} + \frac{1}{2} C x^2 \psi = E\psi$

THE HARMONIC OSCILLATOR

Example: CO Cl_2



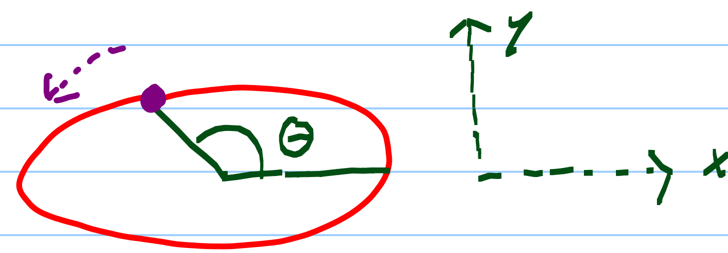
	CO	Cl_2
μ :	6.9	17.5
C :	18.6	3.2

$\sqrt{\frac{C}{\mu}}$ for CO : 1.64

$\sqrt{\frac{C}{\mu}}$ for Cl_2 : 0.42

1-D problems : exercise

Consider a particle confined to 1-D ring :



- solve the Schrodinger equation for this configuration using polar coordinates
- what are the allowed momenta and energies?
- compare the results to those of the infinite well potential

Exercise continued

Note:

- we will treat this as a time-independent problem

- There is no potential so we have

$$-\frac{\hbar}{2m}\nabla^2\psi(x,y) = E\psi(x,y) \qquad (1)$$

- This is really a 1-D problem since ψ only depends on θ

∇^2 : $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

$\hookrightarrow$ will give 0

Exercise continued

$$x = r\cos\theta \qquad\qquad r^2 = x^2 + y^2$$
$$y = r\sin\theta$$

$$dx = \frac{dx}{d\theta}\, d\theta = -r\sin\theta\, d\theta$$

$$dx^2 = r^2 \sin^2\theta\, d\theta^2$$
$$dy^2 = r^2 \cos^2\theta\, d\theta^2$$

$$(dx^2 + dy^2) = r^2\, d\theta^2$$

$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \rightarrow \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$$

If you are not familiar with the methodology associated with changing coordinate systems, see: Arfken, section on "coordinate systems"

Exercise continued

$$\frac{1}{r^2}\,\frac{-\hbar^2}{2m}\,\frac{\partial^2}{\partial\theta^2}\psi = E\psi, \quad \text{or:} \quad \frac{\partial^2}{\partial\theta^2}\psi = \left[\frac{-2mr^2E}{\hbar^2}\right]\psi \quad (2)$$

Normalisation:

$$\int_0^{2\pi} |\psi(\theta)|^2 \, d\theta = 1$$

Continuity condition:

$$\psi(\theta) = \psi(\theta + 2\pi)$$

A solution to (2) is

$$A e^{-iK\theta} + B e^{iK\theta}, \quad K = \frac{r}{\hbar}\sqrt{2mE}$$

Normalise:

$$\int_0^{2\pi} \left(A^* e^{+iK\theta} + B^* e^{-iK\theta}\right)\left(A e^{-iK\theta} + B e^{iK\theta}\right) d\theta$$

Exercise continued

$$\int_0^{2\pi} \left[|A^2| + |B|^2 + A^*B\, e^{2iK\theta} + B^*A\, e^{-2iK\theta} \right] d\theta$$

$$= \int_0^{2\pi} \left[|A^2| + |B|^2 + \underbrace{(A^*B + B^*A) \cdot 2 \cdot \cos 2K\theta}_{=0} \right] d\theta$$

$$\Rightarrow \quad 2\pi\left(|A|^2 + |B|^2\right) = 1$$

$$|A|^2 + |B|^2 = \frac{1}{2\pi}$$

Let's set $B = 0$ for now (particle going clockwise)

$$\Rightarrow \quad A = \frac{1}{\sqrt{2\pi}}$$

Exercise continued

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}} e^{-ik\theta}$$

we need to have

$$\psi(\theta) = \psi(\theta + 2\pi) \Rightarrow$$

$$\frac{1}{\sqrt{2\pi}} e^{-ik\theta} = \frac{1}{\sqrt{2\pi}} e^{-ik(\theta+2\pi)} = \frac{1}{\sqrt{2\pi}} e^{-ik\theta} e^{-ik2\pi}$$

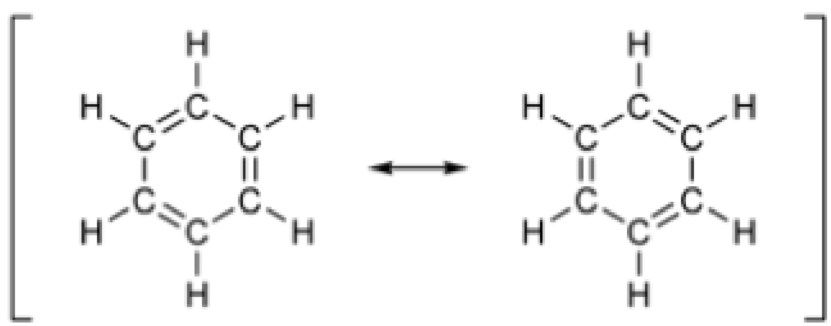
$$\Rightarrow e^{-ik2\pi} = 1 = e^{-i2\pi n}$$

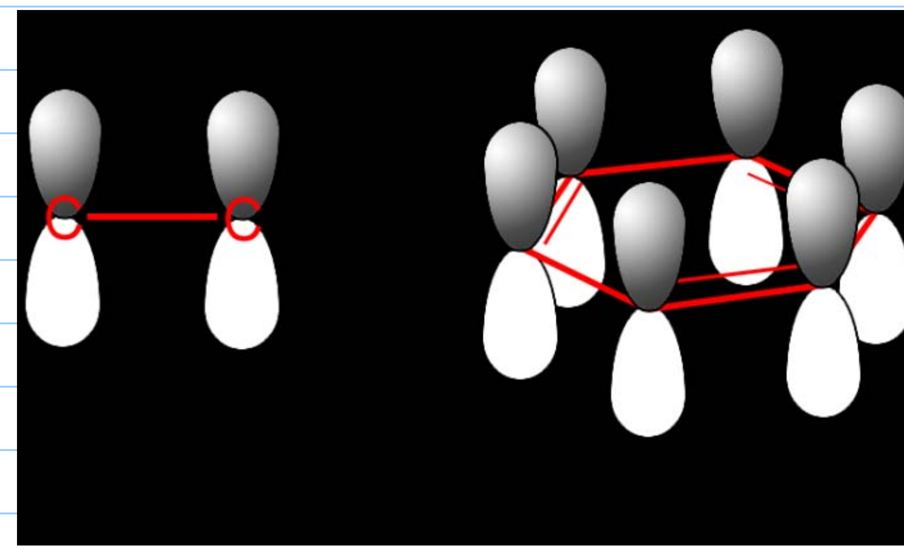
$$n = k = \sqrt{2mE} \cdot \frac{r}{\hbar}$$

$$\Rightarrow \boxed{E_n = \frac{n^2\hbar^2}{2mr^2}}$$, for ∞ well we got: $\boxed{E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}}$

Comments on 1-D ring problem

→ This simple model can be used To get approximate energy levels of Benzene rings





Some electrons are in delocalized orbitals and their wave function is spread aroud The ring

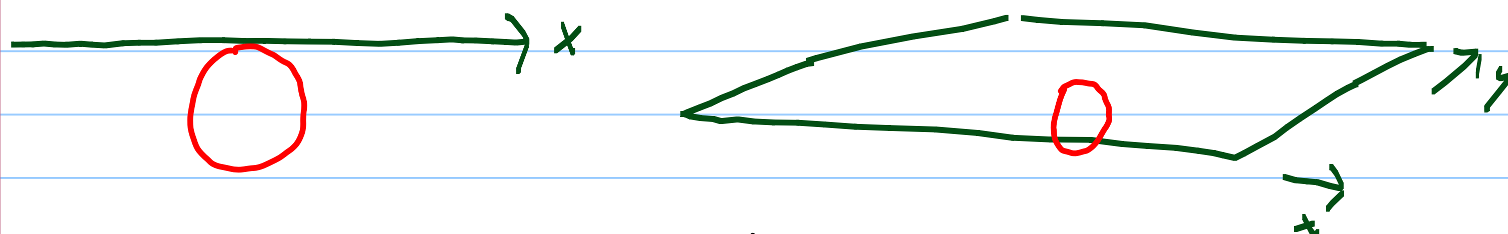
Comments on 1-D ring problem

More exotic analogy (we'll skip the field theory):

- imagine that there are extra dimensions of space

  → since we do not see them, they would have to be small and curled up on themselves e.g.

on a circle



How would a particle whose wavefunction goes around the circle behave from our point of view?

→ let's take a look at some slides on "LED"