NM 03 - quantization and confinement.

the permissible energy levels of matter are quantized.

→ distinguishes materials from one another.

→ think "closed shells" like magic #s

→ gives differences in physical properties (e.g. transparency, conductivity)

→ and size-dependent properties @ nanoscale.

by interactions among energy carriers

idea to intro to MNS later

how was this developed?

19th century: newtonian = particles
electromagnetism = waves.

charges refer to energy of charged particles.

⇒ discrete lines in absorption spectra of hot gases. e.g. (IR characterization)

planck: $E_p = h\nu$ (frequency) $= nh\nu$ (quantum #)

$h = 6.6 \times 10^{-34}$ J/s

"allowable energy" ⇒ later called a photon.

this was used to explain the photoelectricity experiment,

$h\nu_f \geq E_r - E_f$ (put on slide w/ p.e. effect)

work function = "minimum binding energy"

Einstein $E = Mc^2$, photon has a moving mass.

therefore, momentum $p = Mc = \frac{E_f}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} = \frac{\hbar}{k}$ (frequency / wavelength / wavevector)

$k = \frac{h}{2\pi}$

Now we can relate energy + momentum to frequency and wavevector.

wave / particle duality: "double slit" experiment, backstop is perfect absorber.

- "bullet" experiment, $P_1 + P_2 = P_{12}$

- "water pebble" experiment, <u>interference</u>

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos\phi$$

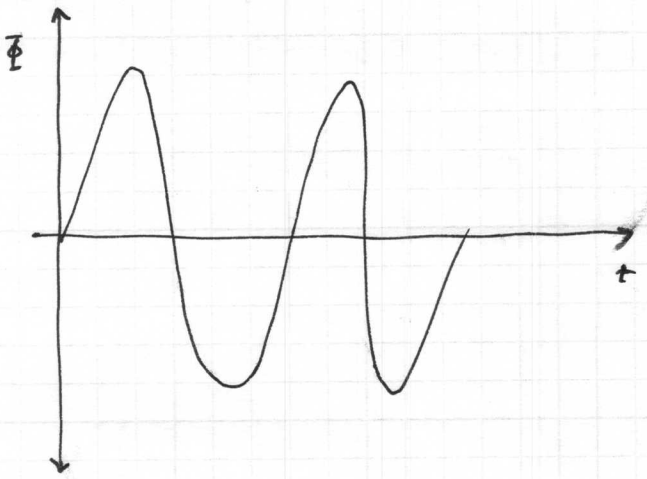
(ϕ: phase based on point on "detector")

- electrons: arrive one at a time, yet interfere like waves.

electron is <u>simultaneously interacting w/ both slits</u>!

uncertainty principle: <u>cannot observe</u> w/o interacting

Now let's consider a simple wave, in 1D:



$$\underline{\Phi} = A \sin\left(2\pi\nu t - 2\pi \dot{x}/\lambda_x\right)\hat{y} = A \sin\left(\omega t - k_x x\right)\hat{y}$$

has periodicity in <u>space and time</u>

this is a <u>travelling wave</u>

→ sit stationary in space, at a point. and we see an oscillation in time

→ sit stationary in time, and see an oscillation in space

$\omega = 2\pi\nu$, ω = angular frequency

wavevector $k = \frac{2\pi}{\lambda_x}\hat{x} = k_x\hat{x}$

(k: magnitude of wavevector)

how fast is the wave moving?

constant phase place = $\omega t - kx$ = constant

$$\frac{dt}{dx} = \frac{\omega}{k} = \nu\lambda = v = \underline{c}$$

(speed of light.)

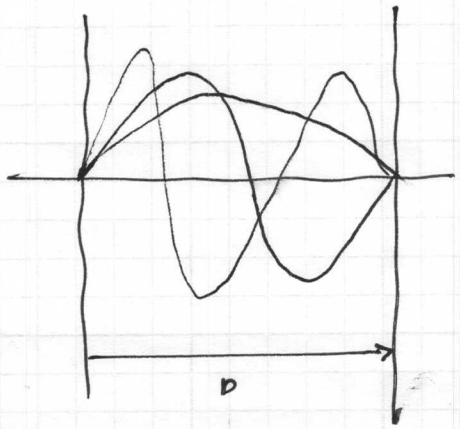
Now consider a wave "pinned" at its ends, a <u>standing wave</u>

add a left-moving wave to a right-moving wave

$$\underline{\Phi} = \left(A\sin(\omega t - kx) + A\sin(\omega t + kx) \right) \hat{y}$$

$k_x = k$ (1D system)

$$= -2A\cos(\omega t)\sin(kx)\,\hat{y}$$



Boundary conditions: $\underline{\Phi}(0) = \underline{\Phi}(D) = 0$

therefore, $\sin(kx) = 0$, because $\cos(\omega t) \neq 0$ unless $t = \frac{n\pi}{2}$

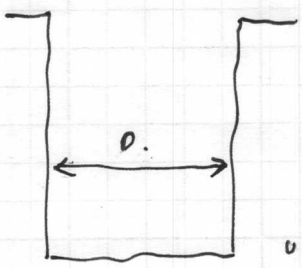
$$\sin\left(\frac{2\pi}{\lambda} x\right) = 0$$

solved if $\frac{D \cdot 2\pi}{\lambda} = n\pi$

$$\Rightarrow D = \frac{n\lambda}{2}$$

1D constraint for a standing wave "pinned" at its ends.

if this is a "particle in a box" (infinite potential well)



we know $E = Mc^2$

$\Rightarrow$ sketch later w/ schrodinger eqn.

relating momentum and energy, as before,

$$p = \frac{h}{\lambda} = \frac{hn}{2D}$$

$$E = mc^2 = \frac{p^2}{2m} = \frac{1}{2m}\left(\frac{h^2n^2}{4D^2}\right) = \frac{1}{2m}\left(\frac{hn}{2D}\right)^2$$

we formalize this in QM using schrodinger's eqn, which applies to the wavefunction of any matter (ψ)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{d\psi}{dt}, \quad \hbar = \frac{h}{2\pi}, \quad V = \text{potential energy}$$

function of position and time

wavefunction: probability that matter is at position r at time t

↑ density function

so $\int_{-\infty}^{\infty} \psi\psi^* \, dx = 1$

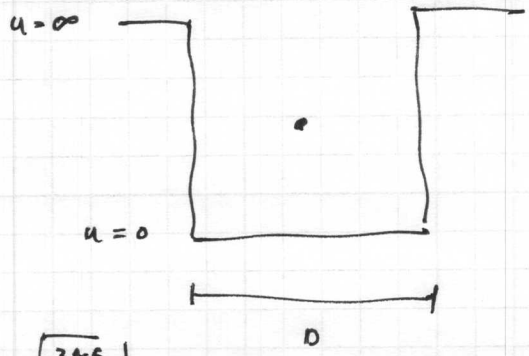
steady-state schrodinger eqn, when $V(r,t) = V(r)$, varies with position only

seperate variables to give

$$-\frac{\hbar^2}{2m}\nabla^2\psi + (V - E)\psi = 0$$

↑ eigenvalues = allowed energy states.

now consider particle in a 1D well, width D.



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (u-E)\psi = 0$$

general solution

$$\psi = A\exp\left\{-ix\sqrt{\frac{2mE}{\hbar^2}}\right\} + B\exp\left\{ix\sqrt{\frac{2mE}{\hbar^2}}\right\}$$

for $0 < x < D$

$\psi = 0$ elsewhere.

BC's.

at $x = 0$: $A + B = 0$

at $x = D$: $A\exp\left\{-iD\sqrt{\frac{2mE}{\hbar^2}}\right\} + B\exp\left\{-iD\sqrt{\frac{2mE}{\hbar^2}}\right\} = 0$

solve this system: $\sin\left(D\sqrt{\frac{2mE}{\hbar^2}}\right)_n = 0 \qquad \sin(n\pi) = 0$

$$\Rightarrow \quad n\pi = D\sqrt{\frac{2mE}{\hbar^2}}$$

$$\Rightarrow \quad E_n = \frac{1}{2m}\left(\frac{\hbar n}{2D}\right)^2$$

if we solve for a 2D case, we have two quantum numbers.

$$E_{ln} = \frac{(l^2 + n^2)\,\pi^2 \hbar^2}{2M D^2}$$

Harmonic oscillator : model for a single bond.

general shape of interatomic potential. ⟵ see slide. graphic (ether)

$$U(x') = U(x_0) + \frac{1}{2}\left[\frac{d^2U}{dx'^2}\right]_{x'=x_0} (x'-x_0)^2 + O(x'-x_0)^3 + \cdots,$$

$$F = -\frac{dU}{dx'} = -k(x'-x_0)$$

↖ spring constant, so $U = \frac{kx'^2}{2}$

$$\frac{-\hbar^2}{2M}\left(\frac{d^2\psi}{dx^2}\right) + \left(\frac{kx^2}{2} - E\right)\psi = 0$$

$\psi(0)$ = finite

$\psi(x \to \infty,\ x \to -\infty) = 0$

solve to get $E_n = \left(n + \frac{1}{2}\right)\hbar\nu$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{M}}$$

(natural frequency!)

(Mass $= \frac{M_1 M_2}{M_1 + M_2}$)

⟹ energy is distributed in different modes

⟹ connection to optical spectroscopy which measures bond resonances.