Intro to QM: 2^{nd} semester

- Web page as usual
- 7 problem sets, 2 in-class midterms
- Last problem set = take-home "final".
- Text: Townsend 2^{nd} ed:
  - Path integral formulation of QM
  - 2-body problems in 3d
  - Central potential bound states (H atom)
  - Time-independent perturbation theory
  - Identical particles & statistics (CM, chemistry, ...)
  - Scattering in 3d
  - Photons (E&M) & interactions w/ charged particles

Review

- $|\psi\rangle \in \mathcal{H}$ w/ $\langle\psi|\psi\rangle = 1$, $|\psi\rangle \simeq e^{i\alpha}|\psi\rangle$, $\alpha \in \mathbb{R}$.
- $|\psi(t)\rangle = \hat{U}(t-t_0)|\psi(t_0)\rangle$, $\hat{U}(t) = \exp\{-\frac{i}{\hbar}\hat{H}t\}$
- Observables $\hat{M} = \hat{M}^\dagger$
  - Possible outcomes = {eigenvalues $\hat{M}$} $\hat{M}|\mu\rangle = \mu|\mu\rangle$
  - $\mu \in \mathbb{R}$, $\langle\mu|\nu\rangle = \delta_{\mu\nu}$ for discrete $\{\mu\}$

    $\langle\mu|\nu\rangle = \delta(\mu-\nu)$ " continuous $\{\mu\}$

    $1 = \sum_\mu |\mu\rangle\langle\mu|$ or $1 = \int d\mu\, |\mu\rangle\langle\mu|$
  - Prob $(\hat{M}=\mu) = \langle\psi|\hat{P}_\mu|\psi\rangle$, $\hat{P}_\mu = \sum_i |\mu,i\rangle\langle\mu,i|$
  - If observe $M=\mu$, $|\psi\rangle \to |\psi\rangle' = \hat{P}_\mu|\psi\rangle / \|\hat{P}_\mu|\psi\rangle\|$.

- Spin systems: finite dim'l $\mathcal{H}_j$

$$\begin{cases} [\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \quad \& \text{ cyclic} \\ \hat{J}^2 \doteq \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \end{cases} ; \quad \hat{J}_\pm \doteq \hat{J}_x \pm i \hat{J}_y$$

- o.n. basis $|j,m\rangle$ $\begin{cases} \hat{J}^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle \\ \hat{J}_z |j,m\rangle = \hbar m |j,m\rangle \end{cases}$

w/ $j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\}$ & $m \in \{-j, -j+1, \dots, j\}$.

$\# = 2j+1 = \dim \mathcal{H}_j$

- Ex: $\hat{H} = \gamma \vec{B} \cdot \vec{J} + \cdots$

- 1d particle: ∞ dim'l $\mathcal{H}_x$
  - $[\hat{X}, \hat{P}] = i\hbar$
  - o.n. basis $|x\rangle$ $\begin{cases} \hat{X}|x\rangle = x|x\rangle & x \in \mathbb{R} \\ \hat{P}|x\rangle = i\hbar \frac{d}{dx}|x\rangle \end{cases}$
  - o.n. basis $|p\rangle$ $\begin{cases} \hat{X}|p\rangle = -i\hbar \frac{d}{dp}|p\rangle \\ \hat{P}|p\rangle = p|p\rangle & p \in \mathbb{R} \end{cases}$
  - $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$
  - Ex: $\hat{H} = \frac{1}{2m}\hat{P}^2 + V(\hat{X})$

Combine spin & motion: <u>1d spin-1/2 particle</u>

$j=\frac{1}{2} \Rightarrow |j=\frac{1}{2}, m=\pm \frac{1}{2}\rangle$ spin states

& also $|x\rangle$ pos'tn states

$\Rightarrow \mathcal{H} = \mathcal{H}_x \otimes \mathcal{H}_{j=1/2}$ w/ o-n basis

∞-dim'l $\quad$ 2-dim'l

basis: $\left\{ \begin{array}{l} |x,+\rangle = |x\rangle \otimes |j=\frac{1}{2}, m=\frac{1}{2}\rangle \\ |x,-\rangle \equiv |x\rangle \otimes |j=\frac{1}{2}, m=-\frac{1}{2}\rangle \end{array} \right\}$

o-n: $\langle x,\pm|x',\pm\rangle = \delta(x-x') \qquad \langle x,\pm|x',\mp\rangle = 0$

complete: $\int_{-\infty}^{\infty} dx \left(|x+\rangle\langle x+| + |x-\rangle\langle x-| \right) = 1$

$$|\psi\rangle = 1\cdot|\psi\rangle = \int_{-\infty}^{\infty} \Big(|x+\rangle \underbrace{\langle x+|\psi\rangle}_{\equiv \psi_+(x)} + |x-\rangle \underbrace{\langle x-|\psi\rangle}_{\equiv \psi_-(x)} \Big)\, dx$$

so $|\psi\rangle \xleftrightarrow{x, j \text{ basis}} \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}$.

Eg: <u>Spin-1/2 Particle in pot'l & Mag'n field</u>

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x}) + \gamma \vec{B}(\hat{x})\cdot\hat{\vec{J}}$$

Eg, take $\gamma\vec{B}(\hat{x}) = U(\hat{x})\,\hat{z}$ ← (unit vector, not op.)

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x}) + U(\hat{x})\hat{J}_z .$$

Acting on $\begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}$ $\quad \hat{p} \to -i\hbar\frac{d}{dx}, \; \hat{x} \to x, \; \hat{J}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Ch. 8 Path Integral formulation of QM

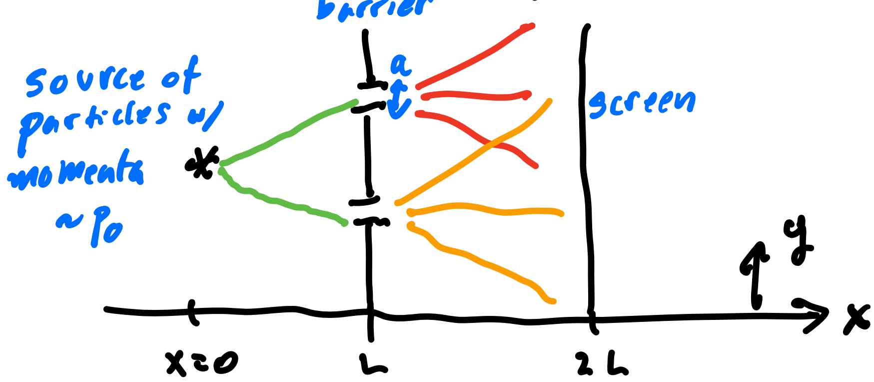
Result: for $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$ (Hamiltonian)

$$\langle x', t' | x_0, t_0 \rangle = \int_{x(t_0)=x_0}^{x(t')=x'} \mathcal{D}[x(t)]\, e^{iS[x(t)]/\hbar}$$

w/ $S[x(t)] = \int_{t_0}^{t'} dt\, L(\dot{x}, x)$ (Action)

w/ $L(\dot{x}, x) = \frac{m}{2}\dot{x}^2 - V(x)$ (Lagrangian)

(1) Ex: double slit experiment

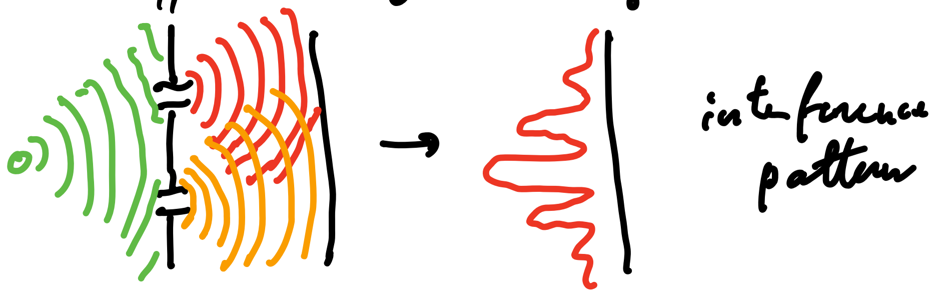


- if $a \lesssim \frac{\hbar}{p_0}$ ← "de Broglie wavelength of particle"

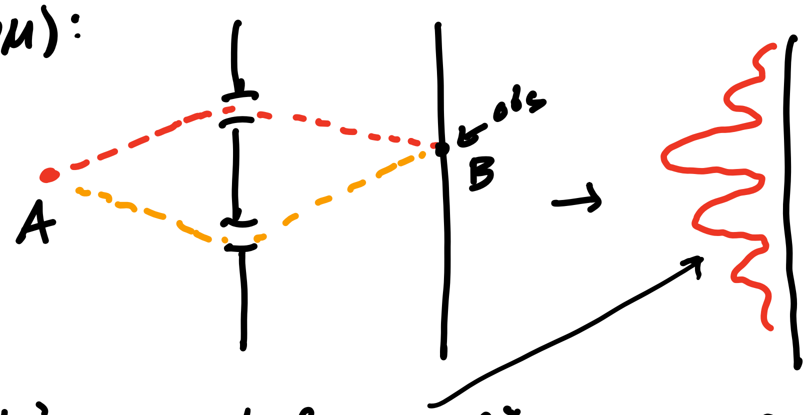
  $\Rightarrow \Delta y\, \Delta p_y \gtrsim \hbar/2$ & $\Delta y \approx a$ (slit) $\Rightarrow \Delta p_y \gtrsim \frac{\hbar}{2a}$

  & if $p_0 \ll \hbar/a \Rightarrow \Delta p_y \gg p_0 \Rightarrow$ particles emerge in "spray".

- Compare to diffraction of waves if $a \ll \lambda$



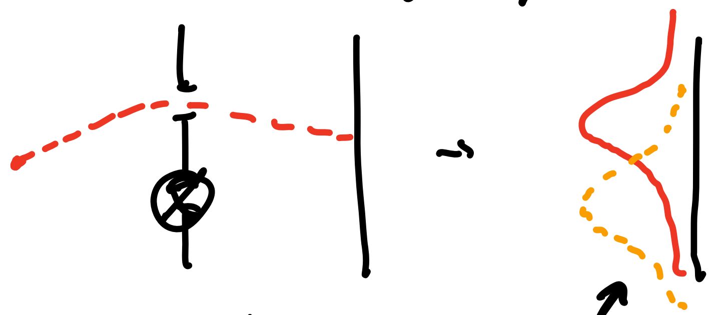
• Find (QM):



~ 2 'paths' → interfere like waves: prob $= |\text{path}_1 + \text{path}_2|^2$

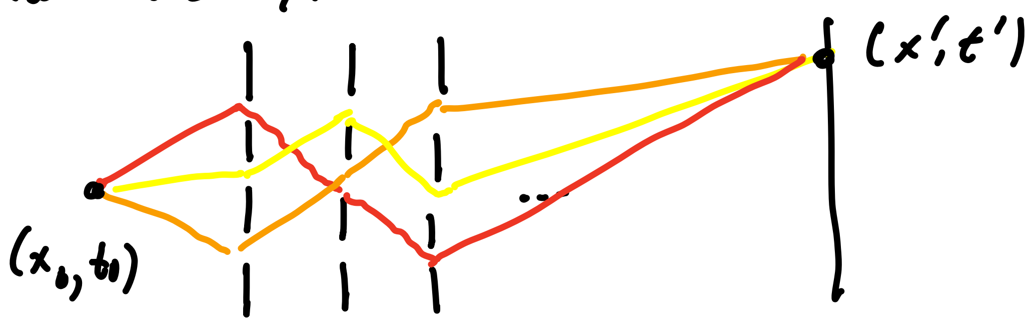
amplitude: $\langle A|B\rangle$

• If close one slit ⇒ only 1 path, no interference



• If observe 1 slit ⇒ know path, same, no interference

(2) Multiscreens/slits ....



add all possibilities ⇒ find prob. $= |\text{sum of all phases}|^2$

• Limit as # screens/slits → ∞ ⇒ continuous sum (integral) over all paths!

Feynman path integral: Prob $= |a|^2$ w/

$$a \equiv \text{“}\langle x', t' | x_0, t_0\rangle\text{”} \overset{?}{=} \int \underbrace{\mathcal{D}[x(t)]}_{\text{path}} \, \underbrace{e^{i\varphi[x(t)]}}_{\text{some phase which depends on path}}$$

BC's of path → $\begin{cases} x(t_0) = x_0 \\ x(t') = x' \end{cases}$

Usual QM formulation:

- Want to compute "amplitude"

$$\mathcal{A} \doteq \langle x' | \psi(t') \rangle$$

w/ $|\psi(t')\rangle$ = state of particle @ time t'

$$= \hat{U}(t'-t_0)\,|\psi(t_0)\rangle$$

$$= e^{-i\hat{H}(t'-t_0)/\hbar}\,|\psi(t_0)\rangle.$$

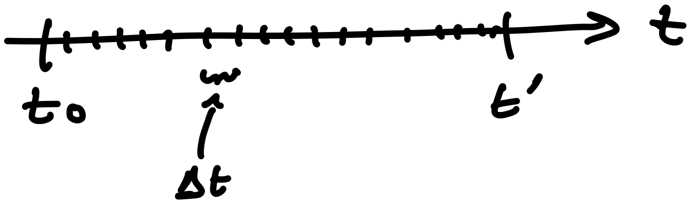
Take $|\psi(t_0)\rangle = |x_0\rangle$ (initial condition).

$$\boxed{\begin{array}{l} \therefore \quad \mathcal{A} = \langle x' | e^{-i\hat{H}(t'-t_0)/\hbar} | x_0 \rangle \\[1em] \text{with} \quad \hat{H} = \frac{1}{2m}\hat{P}^2 + V(\hat{X}) \end{array}}$$

- How to compute $\mathcal{A}$?
  Strategy: sub-divide time interval $t'-t_0$ into many short Δt intervals:

$$\Delta t \doteq \frac{1}{N}(t'-t_0)$$

N



and take $\begin{cases} N \to \infty \\ \Delta t \to 0 \end{cases}$ limit.

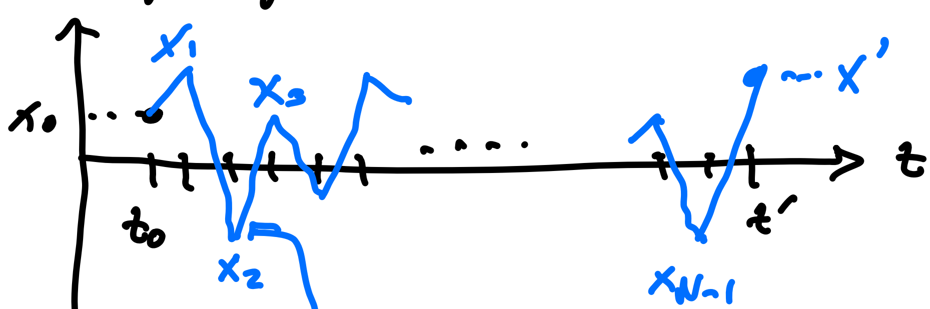
- Then

$$\mathcal{A} = \langle x'| \left(e^{-i\hat{H}\Delta t/\hbar}\right)^N |x_0\rangle$$
$$= \langle x'| \, e^{-i\hat{H}\Delta t/\hbar} \cdot 1 \cdot e^{-i\hat{H}\Delta t/\hbar} \cdot 1 \cdot \quad \cdots \quad |x_0\rangle$$

$$1 = \int_{-\infty}^{\infty} dx \, |x\rangle\langle x|$$

$$\Rightarrow \boxed{\begin{aligned} \mathcal{A} = \int dx_1 \cdots dx_{N-1} \, & \langle x'| e^{-i\hat{H}\Delta t/\hbar} |x_{N-1}\rangle \cdot \\ & \cdot \langle x_{N-1}| e^{-i\hat{H}\Delta t/\hbar} |x_{N-2}\rangle \cdot \\ & \cdot \quad \cdots \quad \cdot \\ & \cdot \langle x_1| e^{-i\hat{H}\Delta t/\hbar} |x_0\rangle \end{aligned}}$$

like putting in $N-1$ "screens" w/ ∞ # holes



approx "$\int$ # paths" as $N \to \infty$, $\Delta t \to 0$.

- Next,

$$\lim_{\Delta t\to 0} \langle x'| e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x\rangle = \langle x'|\, \underset{\hookrightarrow\, 1 = \int dp\, |p\rangle\langle p|}{1} \cdot e^{-i\frac{\Delta t}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} |x\rangle$$

$$= \int dp \langle x'|p\rangle \langle p| \exp\left\{ -\frac{i\Delta t}{\hbar} \underbrace{\left(\frac{\cancel{\hat{p}^2}\to p^2}{2m} + V(\cancel{\hat{x}}\to x)\right)}_{E(p,x)} \right\} |x\rangle$$

$$= \int dp\, \underbrace{\langle x'|p\rangle\langle p|x\rangle}_{\frac{1}{2\pi\hbar} e^{ip(x'-x)/\hbar}} e^{-\frac{i\Delta t}{\hbar}E(p,x)}$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left\{ \frac{i\Delta t}{\hbar}\left[p\cdot\frac{x'-x}{\Delta t} - E(p,x)\right]\right\}$$

$\int dp$ is Gaussian $\cdots\!>$

$$= \left(\frac{m}{2\pi\hbar\, i\Delta t}\right)^{1/2} \exp\left\{ \frac{i\Delta t}{\hbar}\left[\frac{m}{2}\left(\frac{x'-x}{\Delta t}\right)^2 - V(x)\right]\right\}$$

$$\bullet \Rightarrow \mathcal{A} = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \int dx_1 \cdots dx_{N-1} \left(\frac{m}{2\pi\hbar i \Delta t}\right)^{N/2} \cdot$$

} " $\int \mathcal{D}[x(t)]$ " integral over $\forall$ paths

" $e^{i\varphi[x(t)]}$ " path-dependent phase }

$$\cdot \exp\left\{ \frac{i}{\hbar} \underbrace{\Delta t \sum_{i=1}^{N}}_{\int_{t_0}^{t'} dt} \left[\frac{m}{2} \underbrace{\left(\frac{x_i - x_{i-1}}{\Delta t}\right)}_{\frac{dx(t)}{dt}}^2 - V(x_{i-1}) \right] \right\}$$

$$\Rightarrow \mathcal{A} = \int \mathcal{D}[x(t)] \cdot \exp\left\{ \frac{i}{\hbar} \int_{t_0}^{t'} dt \underbrace{\left[\frac{m}{2} \dot{x}^2 - V(x) \right]}_{L(\dot{x}, x)} \right\}$$

$L(\dot{x}, x)$ Lagrangian

$$\Rightarrow \mathcal{A} = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} \underbrace{\int_{t_0}^{t'} dt \cdot L(\dot{x}, x)}_{S[x(t)]}}$$

$S[x(t)]$ "Action"

$$\Rightarrow \boxed{\mathcal{A} = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}}$$

Path Integral (Feynman)

• Uses:

- Relativistic QM = QFT
  & many-body QM = $\left\{ \begin{array}{l} \text{Cond. Matt. physics} \\ \text{statistical physics} \end{array} \right.$

- Gives different & helpful view on classical limit "$\hbar \to 0$":

  $\Rightarrow$ $S \gg \hbar$ $\Rightarrow$ "stationary phase approx."
  Path integral is dominated by paths that extremize S:

  $$\frac{\delta S[x(t)]}{\delta x(t)} = 0 \quad \Leftrightarrow$$ Euler-Lagrange equations of motion
  = classical mechanics

- Certain approximate methods in non-relativistic QM ("WKB approx.", "semi-classical methods") are most easily understood using the P.I.

- Best formulation for numerically simulating QM systems.