2. Postulates & Mathematical Structure of Q.M.

Lecture 4:

Coordinate-independent formulation of QM
(Dirac notation)

- State of system: vector in Hilbert space (can be infinite dimensional)

→ ket → $|\psi\rangle$, bra "dual" → $\langle\psi| = |\psi\rangle^{+}$

$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ $\quad (x_1\ x_2\ x_3) = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}^{T}$

cf. classical mechanics: $(\vec{q}, \vec{p})$ vector

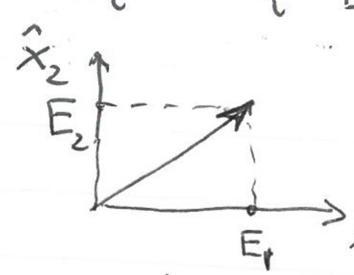
→ $\langle\psi_1|\psi_2\rangle^{*} = \langle\psi_2|\psi_1\rangle$ 6 dimensional phase space.

Note: distinction between vectors (tensors) and their components.

$\vec{E}$

physical object

$E_i = \hat{x}_i \cdot \vec{E}$



coordinate dependent #'s representation of $\vec{E}$ by projection onto orthonormal vector space basis $\hat{x}_i$

+ operators $\hat{O}$

$O|\psi\rangle \equiv |O\psi\rangle$

dual to $|O\psi\rangle$ is $|O\psi\rangle^{+} = \langle O\psi|$

$\langle O\psi| \equiv \langle\psi|O^{+}$ ← defines O^{+}

O^{+} adjoint (Hermitian conjugate) of O

note: $\langle\psi|O\psi\rangle = \langle\psi|O|\psi\rangle = \ldots$

4.2a

- Improper kets/bras → those that are not normalizable to 1, i.e. not integrable.
  e.x. $|x\rangle$, $|p\rangle$
  will normalize these to δ-fnc.
  s.t. $\langle x | x' \rangle = \delta(x-x')$
  $\langle p | p' \rangle = \delta(p-p')$

- representation of $|\psi\rangle$

$$\hat{\Theta}|n\rangle = \theta_n |n\rangle$$

orthonormal set of states
eigenstates of $\hat{\Theta}$

$$|\psi\rangle = \sum_n c_n |n\rangle$$

$$c_n = ?$$

inner-product

$$\langle m|\psi\rangle = \sum_n c_n \underbrace{\langle m|n\rangle}_{\delta_{m,n}}$$

$$\Rightarrow \quad c_m = \langle m|\psi\rangle$$

$$\Rightarrow |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle$$

Note: $\sum_n \underbrace{|n\rangle\langle n|}\psi\rangle$

projection operator
onto state $|n\rangle$

$$\Rightarrow \quad \sum_n \underbrace{|n\rangle\langle n|}_{\text{outer product}} = 1$$

completeness relation

cf. $\hat{x}_i \cdot \vec{E} = c_i$, $\vec{E} = \sum_i c_i \hat{x}_i$

& $\sum_i \hat{x}_i \hat{x}_i = \mathbb{1}$

- **Physical observables:**

matrix elements of Hermitian operators

Ex. $\hat{\vec{x}}$, $V(\hat{\vec{x}})$, $\hat{\vec{p}}$, $\hat{\vec{L}}$, $\hat{H}$

(cf. C.M. fncs of $\vec{q}(t), \vec{p}(t)$: $\mathcal{O}(\vec{q},\vec{p})$)

→ $\hat{\mathcal{O}}$ acts on states in Hilbert space

$$\hat{\mathcal{O}}|\psi\rangle = |\psi'\rangle$$

representation independent, but can be written in specific representation $|n\rangle$

(cf tensors e.g. $\vec{\vec{I}} \rightarrow I_{ij} = \hat{x}_i \cdot \vec{\vec{I}} \cdot \hat{x}_j$ matrix of components)

$\mathcal{O}(x,p) \rightarrow \mathcal{O}(\hat{x},\hat{p}) \equiv \hat{\mathcal{O}}$

$$\hat{\mathcal{O}}|\psi\rangle = |\mathcal{O}\psi\rangle$$

→ $$\langle n'|\hat{\mathcal{O}}|\psi\rangle = \langle n'|\mathcal{O}\psi\rangle \equiv C_{n'}^{\mathcal{O}\psi}$$

$$\sum_n |n\rangle\langle n| = 1$$

$$\sum_n \langle n'|\hat{\mathcal{O}}|n\rangle\langle n|\psi\rangle = \langle n'|\mathcal{O}\psi\rangle$$

$$\Leftrightarrow \sum_n \mathcal{O}_{n'n} C_n^{\psi} = C_{n'}^{\mathcal{O}\psi}$$

$$\hat{\mathcal{O}} \xrightarrow[\text{n-repres.}]{} \langle n'|\hat{\mathcal{O}}|n\rangle \equiv \mathcal{O}_{n'n}$$

- $|\psi\rangle$ has a dual $\langle\psi| = |\psi\rangle^{+}$
- $\Theta|\psi\rangle \equiv |\Theta\psi\rangle \longrightarrow \langle\Theta\psi| \equiv \langle\psi|\Theta^{+}$

  i.e. Θ^{+} acts on $\langle\psi|$ to create dual of $\Theta|\psi\rangle$

  $\Theta \longrightarrow$ Hermitian conjugate of Θ is Θ^{+} (adjoint)

- matrix elements:

$$\langle n|\Theta|m\rangle = \Theta_{nm}$$

$$(\Theta^{+})_{nm} = \langle n|\Theta^{+}|m\rangle = \langle\Theta n|m\rangle = \langle m|\Theta n\rangle^{*}$$

$$= \langle m|\Theta|n\rangle^{*}.$$

$$\Rightarrow (\Theta^{+})_{nm} = \Theta^{*}_{mn}$$

in matrix notation $(\Theta^{+})_{nm} = (\Theta^{*T})_{nm} = \Theta^{*}_{mn}$

Physical observables: $\underline{\Theta = \Theta^{+}}$
are represented by
Hermitian (self-adjoint)
operators

e.x. $x^{+} = x$

$(-i\hbar\nabla)^{+} = -i\hbar\nabla$

→ why only Hermitian operators?

- so that measured observable is a real number

show for hwk that need $O^{+} = O$ so that:

$$\langle \psi | \hat{O} | \psi \rangle = \langle \psi | \hat{O} | \psi \rangle^*$$

representation independent way:

$$= \langle \psi | \hat{O} \psi \rangle^*$$

$$= \langle \hat{O} \psi | \psi \rangle$$

$$= \langle \psi | \hat{O}^{+} | \psi \rangle$$

$$\Rightarrow \hat{O} = \hat{O}^{+}$$

spectre repres. way:

$$\langle \psi | \hat{O} | \psi \rangle = \sum_{n',n} \underbrace{\langle \psi | n' \rangle}_{C_{n'}^*} \underbrace{\langle n' | \hat{O} | n \rangle}_{O_{n'n}} \underbrace{\langle n | \psi \rangle}_{C_n}$$

$$\langle \psi | \hat{O} | \psi \rangle^* = \sum_{n',n} C_{n'} O_{n'n}^* C_n^*$$

$$\overset{\text{require}}{=} \sum_{n,n'} C_n^* O_{nn'} C_{n'}$$

$$\Leftrightarrow \underline{O_{nn'} = O_{n'n}^* \Leftrightarrow O = O^{+}}$$

→ Hermitian ops: (a) real eigenvalues
(b) orthogonal eigenstates

(a) $\hat{O}|n\rangle = O_n|n\rangle$

$$\langle n|\hat{O}|n\rangle = O_n\langle n|n\rangle$$

$$-\quad \langle n|\hat{O}^{+}|m\rangle = O_n^{*}\langle n|n\rangle$$

using $\hat{O} = \hat{O}^{+}$:

$$0 = (O_n - O_n^{*})\langle n|n\rangle$$

$$\Rightarrow \underline{O_n^{*} = O_n}$$

(b)
$$\langle m|\hat{O}|n\rangle = O_n\langle m|n\rangle$$

$$\langle n|\hat{O}|m\rangle = O_m\langle n|m\rangle$$

$$-\quad \langle m|\underbrace{\hat{O}^{+}}_{\hat{O}}|n\rangle = \underbrace{O_m^{*}}_{=O_m}\langle m|n\rangle$$

$$\langle m|\hat{O}|n\rangle$$

$$0 = (O_n - O_m)\langle m|n\rangle$$

$$\Rightarrow \underline{\langle m|n\rangle = 0}$$

cf real symmetric matrix
$\Rightarrow$ λ real
$\hat{e}_\lambda^T \cdot \hat{e}_{\lambda'} = \mathbb{1}_{\lambda\lambda'}$

→ Expectation values:

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{n',n} \langle\psi|n'\rangle\langle n'|O|n\rangle\langle n|\psi\rangle$$

$$= \sum_{n',n} C^{*\psi}_{n'}\, O_{n'n}\, C^{\psi}_{n}$$

$$= \mathrm{Tr}(\hat{\rho}\hat{O}), \quad \text{where } \rho^{\text{pure}}_{n n'} = C^{*\psi}_{n'} C^{\psi}_{n}$$

(more on this later)

$$= |\psi\rangle\langle\psi|$$

convenient to compute $\langle\psi|\hat{O}|\psi\rangle$ in eigenbasis of $\hat{O}$

$$\hat{O}|n\rangle = O_n|n\rangle$$

$$\Rightarrow \langle\psi|\hat{O}|\psi\rangle = \sum_{n'n} \langle\psi|n'\rangle \underbrace{\langle n'|\hat{O}|n\rangle}_{O_n \underbrace{\langle n'|n\rangle}_{\delta_{n'n}}} \langle n|\psi\rangle$$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_n |\langle n|\psi\rangle|^2 O_n$$

$$= \sum_n |\underbrace{C^{\psi}_n}_{\psi_n}|^2 O_n = \sum_n O_n |\psi_n|^2$$

Density Matrix

1. **Pure states:** only Q.M. uncertainty / probabilistic nature

$\langle \psi_1 | \hat{O} | \psi_1 \rangle$ – average value of $\hat{O}$ found if N identical systems in state $|\psi_1\rangle$ are measured.

$|\psi_1\rangle \qquad , \qquad \langle \psi_1 | \hat{O} | \psi_1 \rangle \equiv \langle \hat{O} \rangle$

equivalently: $\hat{\rho} \equiv |\psi_1\rangle\langle\psi_1| \quad , \quad \langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\hat{O})$

density matrix (operator)

In a basis $|n\rangle \Rightarrow |\psi_1\rangle = \sum C_n |n\rangle$

$$\Rightarrow \hat{\rho} = |\psi\rangle\langle\psi| = \sum_{\substack{m \\ n}} \underbrace{C_n C_m^*}_{\equiv \rho_{mn}} |n\rangle\langle m|$$

$\equiv \rho_{mn}$ – matrix elements of $\hat{\rho}$

$$\underline{\langle \psi | \hat{O} | \psi \rangle} = \sum_{nm} \underbrace{\langle \psi | n \rangle}_{C_n^*} \langle n | \hat{O} | m \rangle \underbrace{\langle m | \psi \rangle}_{C_m}$$

$$= \sum_{nm} \rho_{mn} O_{nm} = \underline{\mathrm{Tr}(\rho O)} \checkmark$$

For pure systems (in single state Q.M.) $\rho_{nm} = C_m^* C_n$

→ product.

$$\mathrm{Tr}\,\rho = \langle \psi | \psi \rangle = \sum_m |C_m|^2 = 1$$

$$\mathrm{Tr}\,\rho^2 = \mathrm{Tr}(|\psi\rangle\langle\psi|\psi\rangle\langle\psi|) = \mathrm{Tr}\,\rho = 1 \checkmark$$

2. Mixed States: uncertainty/prob. nature due to Q.M. AND classical (a mixture of different systems)

Measurement on N systems n_i in state $|\psi_i\rangle$

$\Rightarrow$ classical prob. nature of N systems characterized by prob. $p_i \equiv \frac{n_i}{N}$

$$\Rightarrow \rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$\langle\hat{O}\rangle = \underbrace{\sum_i p_i \underbrace{\langle\psi_i|\hat{O}|\psi_i\rangle}_{\text{Q.M. average}}}_{\text{classical ensemble average}}$$

Q.M. average. if a system in state $|\psi_i\rangle$ then $\langle\hat{O}\rangle = \hat{O}_i$

$$\langle\hat{O}\rangle = \mathrm{Tr}(\rho\hat{O})$$

In $|n\rangle$ representation

$$\rho = \sum_{\substack{i \\ n,m}} \underbrace{p_i c_{ni}^* c_{mi}}_{\equiv \rho_{mn}} |n\rangle\langle m|$$

— matrix elements of $\hat{\rho}$ not a product of c's in general, when mixed state.

props: $\rho^+ = \rho$

$\mathrm{Tr}\hat{\rho}^2 \le \mathrm{Tr}\hat{\rho}$, equality for pure states.

Ex: $$\rho = \frac{e^{-H/k_BT}}{\mathrm{Tr}(e^{-H/k_BT})} \leftarrow$$ density matrix of a syst. at finite T.

$\langle p^2 \rangle = ?$

$$\langle p^2 \rangle = \mathrm{Tr}(\hat{\rho}\, \hat{p}^2) = \mathrm{Tr}(\hat{p}^2 e^{-\beta \hat{H}})/Z$$

$$Z = \mathrm{Tr}(e^{-\beta \hat{H}}) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-\beta \frac{\hbar^2 k^2}{2m}}$$

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

$$\langle \hat{p}^2 \rangle = \frac{1}{Z} \int \frac{dk}{2\pi} \langle p | \hat{p}^2 e^{-\beta \frac{p^2}{2m}} | p \rangle$$

$$= \frac{1}{Z} \int_{-\infty}^{\infty} \frac{d\hbar k}{2\pi\hbar} \hbar^2 k^2 e^{-\beta \frac{\hbar^2 k^2}{2m}}$$

$$= \frac{m}{\beta}$$

$$\boxed{\langle p^2 \rangle = m k_B T}$$ ← equipartition.

$$\left(\langle \frac{p^2}{2m} \rangle = \frac{1}{2} k_B T \right)$$

- Time-evolution of $|\psi\rangle \to$ Schrödinger's Eqn.

$\to$ $\hat{H}|\psi\rangle = i\hbar\,\partial_t|\psi\rangle$ $\leftarrow$ repr. independent.

$\to$ in $|n\rangle$ representation:

$$\sum_{n'} \langle n|\hat{H}|n'\rangle\langle n'|\psi\rangle = i\hbar\,\partial_t\langle n|\psi\rangle$$

$$\sum_{n'} H_{nn'}\psi_{n'} = i\hbar\,\partial_t\psi_{n'}$$

$\longrightarrow$ Heisenberg's matrix mechanics.

Note: $\hat{H}|\psi(t)\rangle = i\hbar\,\partial_t|\psi(t)\rangle$

$$\Rightarrow |\psi(t+\varepsilon)\rangle = |\psi(t)\rangle + \varepsilon\frac{1}{i\hbar}\hat{H}|\psi(t)\rangle$$

$\rightarrow$ $-\frac{i}{\hbar}\hat{H}$ is a generator for time translations.

$\to$ formal solution of Schrödinger's Eqn:

$i\hbar\,\partial_t|\psi\rangle = \hat{H}|\psi\rangle$ (cf. $\partial_t f = af$ $\Rightarrow f(t) = e^{at}f(0)$)

$$\Rightarrow |\psi(t)\rangle = \underbrace{e^{-\frac{i}{\hbar}\hat{H}t}}|\psi(0)\rangle$$

time evolution operator: $\hat{U}_t = e^{-i/\hbar\,\hat{H}t}$

(Note: $f(\hat{A}) = f(0) + f'(0)\hat{A} + \frac{1}{2!}f''(0)\hat{A}^2 + \ldots$)

4.8a

- $$\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t} = \overbrace{\sum_{E_n} |E_n\rangle\langle E_n|}^{1} e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\hat{U}_t = \sum_{E_n} |E_n\rangle\langle E_n| e^{-\frac{i}{\hbar}E_n t}$$

- what if $\hat{H}(t)$ - time-dependent?

$$\left(\text{cf. } \partial_t y = h(t) y \rightarrow y(t) = e^{\int_0^t h(t')dt'} y(0)\right)$$

$$\Rightarrow \quad \hat{U}_t \underset{?}{=} e^{-\frac{i}{\hbar}\int_0^t dt' \hat{H}(t')}$$

No! because $[\hat{H}(t), \hat{H}(t')] \neq 0$, for $t \neq t'$

check via Taylor expansion defn of $\hat{U}_t$.

instead evolve $\psi(0) \rightarrow \psi(\varepsilon) \rightarrow \psi(2\varepsilon) \rightarrow \dots \rightarrow \psi(t)$

$$\Rightarrow \quad \hat{U}_{(t,0)} = \hat{U}_{(t,t-\varepsilon)} \hat{U}_{t-\varepsilon, t-2\varepsilon} \cdots \hat{U}_{\varepsilon, 0}$$

$$= e^{-\frac{i}{\hbar}\hat{H}(t)\varepsilon} e^{-\frac{i}{\hbar}\hat{H}(t-\varepsilon)\varepsilon} \dots e^{-\frac{i}{\hbar}\hat{H}(0)\varepsilon}$$

$$\Rightarrow \quad \hat{U}(t,0) = \prod_{t'=0}^{t} e^{-\frac{i}{\hbar}\hat{H}(t')\varepsilon}$$

$$\boxed{\frac{1}{x-i\eta} = P\left(\frac{1}{x}\right) + i\pi\delta(x)}$$

$$\Leftrightarrow \quad \hat{U}(t,0) \equiv T\, e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t')\,dt'}$$

- $$U(r;E) = \frac{\hbar}{\pi} \operatorname{Im} \langle r| \frac{1}{E - H - i\eta} |0\rangle = \sum_n \psi_n^*(r)\psi_n(0) \times \delta(E - E_n)$$

$$= \int_t U(r,t)\, e^{+\frac{iEt}{\hbar}}$$

Note: $U(r, t=0) = \int \frac{dE}{2\pi\hbar} U(r,E) = \sum_n \psi_n^*(r)\psi_n(0) = \langle r|0\rangle = \delta(r)$

$$|\Psi(t)\rangle = \hat{U}_t |\Psi(0)\rangle$$

$$\hat{U}_t^{-1} = \hat{U}_{-t} = e^{\frac{i}{\hbar}\hat{H}t} \underset{\uparrow}{=} \hat{U}^+ = \left(e^{-\frac{i}{\hbar}\hat{H}t}\right)^+$$

using $\hat{H}^+ = \hat{H}$

$\Rightarrow \hat{U}_t^{-1} = \hat{U}_t^+$ - unitary operator.

<u>Unitary</u> ops play same role as <u>canonical</u> tranformation in C.M.

→ preserve norm of $|\Psi\rangle$ & commutators of operators.

$$\underline{\langle\Psi_1|\Psi_2\rangle} = \langle\Psi_1|U^+U|\Psi_2\rangle = \underline{\langle U\Psi_1|U\Psi_2\rangle}$$

⟹ "rotation" in Hilbert space.

→ Schrödinger's picture:

- $\hat{O}$'s are time independent
- $|\Psi(t)\rangle$ evolve in time $= U_t|\Psi(0)\rangle$

$$O_{observe}(t) = \langle\Psi(t)|\hat{O}|\Psi(t)\rangle$$

→ Heisenberg picture:

- $\hat{O}$'s evolve in time
- $|\Psi(0)\rangle$ are time independent.

$$O_{\text{observe}}(t) = {}_S\langle \Psi(t)|\hat{O}_S|\Psi(t)\rangle_S$$

$$= {}_H\langle \Psi(0)|\underbrace{U_t^{+}\hat{O}_S U_t}_{\hat{O}_H(t)}|\Psi(0)\rangle_H$$

$$\hat{O}_H(t) = U_t^{+}\hat{O}U_t = e^{i/\hbar \hat{H}t}\hat{O}e^{-i/\hbar \hat{H}t}$$

$$\frac{d}{dt}\hat{O}_H(t) = e^{i/\hbar \hat{H}t}\frac{i}{\hbar}\hat{H}\hat{O}e^{-i/\hbar \hat{H}t} + e^{i/\hbar \hat{H}t}\hat{O}\left(-\frac{i}{\hbar}\hat{H}\right)e^{-i/\hbar \hat{H}t}$$

$$= \frac{i}{\hbar}\left[\hat{H}, \hat{O}_H(t)\right] \quad (\text{note: } \hat{H}_H = \hat{H}_S)$$

$$\boxed{\frac{d}{dt}\hat{O}_H = \frac{1}{i\hbar}\left[\hat{O}_H, \hat{H}\right]} \leftarrow \text{equivalent to Schrödinger's picture.} \quad \left(+\partial_t\hat{O}\right)$$

if also explicit t dependence.

cf C.M.: $\frac{d}{dt}O = \{O, H\} \Rightarrow \frac{1}{i\hbar}[\,,\,] = \{\,,\,\}$

- Connection to coordinate representation:

$\hat{r}|r\rangle = r|r\rangle$

$\Rightarrow |\psi\rangle \rightarrow \langle r|\psi\rangle = \psi(r)$

$\langle r|r'\rangle = \delta(r-r')$
improper kets/bras

$$|\psi\rangle = \sum_n c_n |n\rangle$$

$$\langle r|\psi\rangle = \sum_n c_n \langle r|n\rangle$$

$$\psi(r) = \sum_n c_n \psi_n(r)$$

Note:

$\psi(r,0) = \int dr_0\, \psi(r_0,0)\, \delta(r-r_0)$

cf

$\psi(r,0) = \sum_n c_n\, \varphi_n(r)$

$$\Rightarrow \hat{\Theta}|\psi\rangle = |\Theta\psi\rangle$$

$$\int_{r'} \underbrace{\langle r|\hat{\Theta}|r'\rangle}_{\Theta(r,r')} \underbrace{\langle r'|\psi\rangle}_{\psi(r')} = \psi_\Theta(r)$$

$$\int_{r'} \Theta(r,r')\,\psi(r') = \psi_\Theta(r)$$

- Ex.1. $V(\hat{r}) \rightarrow \langle r|V(\hat{r})|r'\rangle = V(r)\underbrace{\langle r|r'\rangle}_{\delta(r-r')}$

$$\Rightarrow \hat{V}(r,r') = V(r)\,\delta(r-r')$$

- Ex.2. $\hat{p} \rightarrow \langle r|\hat{p}|r'\rangle = \sum_{p,p'} \underbrace{\langle r|p\rangle}_{\psi_p(r)} \underbrace{\langle p|\hat{p}|p'\rangle}_{p\,\delta_{p,p'}} \underbrace{\langle p'|r'\rangle}_{\psi^*_{p'}(r')}$

$$\hat{P}_{r,r'} = \langle r|\hat{p}|r'\rangle = \sum_p \psi_p^*(r')\,\psi_p(r)\, p$$

$$-i\hbar\vec{\nabla}\psi_p(r) = \vec{p}\,\psi_p(r) \Rightarrow \psi_p(r) \sim e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

$$\rightarrow \sum_p \frac{1}{L^3\hbar^3} e^{+\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}')}\, p = -i\hbar\vec{\nabla}_r\,\delta(r-r')$$

$$\Rightarrow \int_{r'} p(r,r')\,f(r') = \int_{r'} -i\hbar\vec{\nabla}_r\,\delta(r-r')\,f(r')$$

$$\int_r p(r,r')\, f(r') = \int_{r'} i\hbar \vec{\nabla}_{r'} \delta(r-r')\, f(r')$$

$$= -i\hbar \vec{\nabla}_r f(r)$$

- Ex. 3. $\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle$

$$\langle r|\hat{H}|r'\rangle\langle r'|\psi\rangle = i\hbar\,\partial_t\langle r|\psi\rangle$$

$$\int_{r'} H(r,r')\,\psi(r') = i\hbar\,\partial_t\,\psi(r)$$

$$H(r,r') = \langle r|\frac{\hat{p}^2}{2m} + V(\hat{r})|r'\rangle$$

$$H(r,r') = \left(-\frac{\hbar^2}{2m}\nabla_r^2 + V(r)\right)\delta(r-r')$$

$$\Rightarrow \int_{r'} H(r,r')\,\psi(r') = i\hbar\,\partial_t\,\psi(r)$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m}\nabla_r^2 + V(r)\right)\psi(r) = i\hbar\,\partial_t\,\psi(r)$$

- Ex. 4. evolution operator $\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t}$

$$\langle r|\hat{U}_t|r'\rangle = U(r,r';t) = \langle r|e^{-\frac{i}{\hbar}\hat{H}t}|r'\rangle$$

Look at free particle $\hat{H}^0 = \frac{\hat{p}^2}{2m} \rightarrow H^0_{r,r'} = -\frac{\hbar^2}{2m}\nabla^2\delta(r-r')$

$$\Rightarrow U_0(r,r';t) = e^{+\frac{i}{\hbar}\frac{\hbar^2}{2m}\nabla_r^2 t}\,\delta(r-r')$$

$$= \sum_{p,p'}\langle r|p\rangle\langle p|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t}|p'\rangle\langle p'|r'\rangle$$

$$= \frac{1}{V}\sum_p e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}\, e^{i\frac{\vec{p}\cdot}{\hbar}(\vec{r}-\vec{r}')}$$

(4.12)

$$U^{\circ}(\vec{r},\vec{r}\,';t) = \int \frac{d^3p}{(2\pi)^3\hbar^3} e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} \; e^{i(\vec{r}-\vec{r}\,')\cdot\frac{\vec{p}}{\hbar}} = ?$$

Digression on Gaussian integrals:

- $$I_0 = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2} = \left(\frac{2\pi}{a}\right)^{1/2} = 2\left(\frac{2}{a}\right)^{1/2}\int_0^\infty dy\,\tfrac{1}{2}y^{-1/2}e^{-y} = \left(\frac{2}{a}\right)^{1/2}\underbrace{\Gamma(1/2)}_{\sqrt{\pi}}$$

$$I_1 = \int_{-\infty}^{\infty} dx\, x\, e^{-\frac{1}{2}ax^2} = 0 = I_{2n+1} = 0$$

$$I_2 = \int_{-\infty}^{\infty} dx\, x^2 e^{-\frac{1}{2}ax^2} = -2\frac{\partial}{\partial a} I_0 = \left(\frac{2\pi}{a}\right)^{1/2}\frac{1}{a}$$

$$I_2 = \left(\frac{2\pi}{a}\right)^{1/2}\frac{1}{a} = I_0\,\frac{1}{a}$$

$$I_4 = (-2)^2\frac{\partial^2}{\partial a^2} I_0 = (-2)\frac{\partial}{\partial a} I_2 = \left(\frac{2\pi}{a}\right)^{1/2}\frac{3}{a^2}$$

$$\boxed{I_{2n} = (-2)^n\frac{\partial^n}{\partial a^n} I_0 = \left(\frac{2\pi}{a}\right)^{1/2}\frac{(2n-1)!!}{a^n}}$$

also from general scaling of I_p integral.

- From generating fnc:

$$J(h) = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2 + hx}$$

$$= \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}a(x - h/a)^2}\; e^{\frac{1}{2}a^{-1}h^2}$$

$$J(h) = \left(\frac{2\pi}{a}\right)^{1/2} e^{\frac{1}{2}a^{-1}h^2}$$

$$I_m = \frac{\partial^m}{\partial h^m} J(h)\Big|_{h=0} = \left(\frac{2\pi}{a}\right)^{1/2}\frac{(2n-1)!!}{a^{m/2}} \qquad m = 2n$$

- Many variables:

$$J(\vec{h}) = \int_{-\infty}^{\infty} d^dx\, e^{-\frac{1}{2}\vec{x}\cdot\vec{\vec{A}}\cdot\vec{x} + \vec{h}\cdot\vec{x}} = \left(\frac{(2\pi)^d}{\det A}\right)^{1/2} e^{\frac{1}{2}\vec{h}\cdot\vec{\vec{A}}^{-1}\cdot\vec{h}}$$

$$\psi(x,t) = \int_{x'} U(x,t;x',0)\,\psi(x';0)$$

take $\psi(x';0) = \delta(x'-x_0) = \langle x|x_0\rangle$

$$\Rightarrow \underline{\psi(x,t) = U(x,t;x_0,0)}$$

$$U_0(\vec r, \vec r\,'; t) = \int \frac{d^3p}{(2\pi)^3\hbar^3} e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} e^{i(\vec r - \vec r\,')\cdot\vec p/\hbar} \left(\Theta(t) \text{ causality}\right)$$

- product of d (= 3) Gaussian integrals, one for each dimension.

$$U(x, x'; t) = \int \frac{dp_x}{2\pi\hbar} e^{-\frac{i}{\hbar}\frac{p_x^2}{2m}t} e^{\frac{i}{\hbar}(x-x')p}$$

with $a = \dfrac{it}{\hbar m}$, $h = \dfrac{i}{\hbar}(x - x')$

$$\Rightarrow \boxed{U_0(x, x'; t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{+i\frac{m}{2t}(x-x')^2/\hbar}\,\Theta(t)}$$

Note: for $x \simeq x' \Leftrightarrow x = x(t)$, $x' = x(0)$ & $t \to 0$

$$\frac{1}{2}\frac{m}{t}(x-x')^2 \simeq t\frac{1}{2}m\left(\frac{x(t)-x(0)}{t}\right)^2$$

$$\simeq \Delta t \underbrace{\frac{1}{2}m\dot x^2}_{L(x(t))} \simeq S$$

$$= \Delta t L$$

$$U(x, x'; t) \sim e^{iS/\hbar}, \quad S = \frac{1}{2}\int_0^t m\dot x^2$$

... much more on this later

- $\hat U$ in $|p\rangle$ representation:

$$\langle p|\hat U^0|p\rangle = \langle p| e^{-\frac{i}{\hbar}\hat H_0 t}|p'\rangle$$

$$= \delta_{p,p'}\, e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}$$

Note: $\langle r|\hat U^0|r'\rangle \underset{FT}{=} \sum_{p,p'} U_{p,p'}\, e^{\frac{ip\cdot r}{\hbar}} e^{-\frac{ip'r'}{\hbar}}$

Note

$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$ is not time ordered

$\Rightarrow U_{n,n'}(t) = e^{-\frac{i}{\hbar}E_n t}\,\delta_{n,n'} = \langle c(t)\,c^\dagger(0)\rangle$

$U_{n,n'}(E) = \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n t}\, e^{\frac{i}{\hbar}Et}\,dt\;\delta_{n,n'}$

$= \hbar\,\delta(E-E_n)\,\delta_{n,n'}$

clear since S. Eqn in $t\to E$: $(E-E_n)U(E)=0$

$\Rightarrow U(E) \propto \delta(E-E_n)$

But for soln of interacting probs, or even just prob. with a potential in terms of free particles

e.g. $\left(\frac{\hat{p}^2}{2m}+\hat{V}\right)\Psi = E\Psi \Rightarrow (E-E_n^\circ)\Psi = V\Psi$

solve by Green's fnc $(E-E_n^\circ)G^\circ = 1$

which in t-domain is $(i\hbar\partial_t - E_n^\circ)G^\circ(t) = \delta(t)$

$\Rightarrow G^\circ = \frac{1}{E-E_n^\circ} \Rightarrow \hat{G}^\circ \equiv \hat{U}_{R/A} = \frac{1}{E-\hat{H}^\circ}$ $\Rightarrow G^\circ(t)$ has $\theta(t)$ or $-\theta(-t)$

Note: in Keldysh $G_{A,R} = \langle \hat{\bar{\phi}}\,\phi\rangle$ response field

$= \langle \bar{\phi}_{quantum}\,\phi_{class}\rangle$

$= \langle(\bar{\phi}_+ - \bar{\phi}_-)(\phi_+ + \phi_-)\rangle$

positive/negative branches

$= \ldots = \langle\phi(t)\,\phi^\dagger(0)\rangle\,\theta(\pm t)$

- $\hat{U}$ in $|E_n\rangle$ representation:

$$U_{n,n';t} = \langle E_n | \hat{U} | E_{n'} \rangle \quad , \quad \hat{H}|E_n\rangle = E_n |E_n\rangle$$

$$\Rightarrow U_{nn'}(t) = e^{-\frac{i}{\hbar} E_n t} \delta_{n,n'}$$

also: $$U^R_{n,n'}(\omega) = \int_{-\infty}^{\infty} dt \, U_{n,n'}(t) \, e^{i\omega t} \, \Theta(t)$$

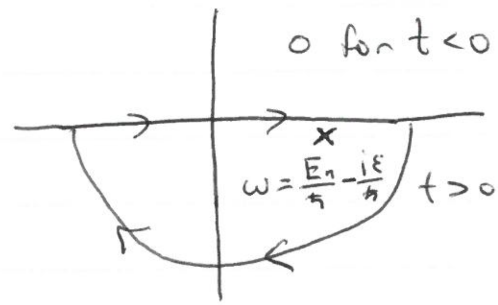
$$= \delta_{n,n'} \int_0^{\infty} dt \; e^{-\frac{i}{\hbar}(E_n - \hbar\omega - i\varepsilon)t}$$

convergence factor so that ok for $t > 0$

$$\underset{R/A}{U_{nn'}(\omega)} = \frac{+i\hbar \, \delta_{n,n'}}{\hbar\omega - E_n \pm i\varepsilon}$$

$$= \langle E_n | \frac{+i\hbar}{\hbar\omega - \hat{H} + i\varepsilon} | E_{n'} \rangle$$

$$\rightarrow \hat{U}_{R/A}(\omega) = \frac{+i\hbar}{\hbar\omega - \hat{H} \pm i\varepsilon}$$



Equivalently solve:

$$(-\hat{H} + i\hbar\partial_t)|\psi(t)\rangle = \underbrace{i\hbar|\psi(0)\rangle\,\delta(t)}_{\text{encodes initial condition discontinuity}}$$

$$|\psi(t)\rangle = \underbrace{(-\hat{H} + i\hbar\partial_t)^{-1}_{tt'}}_{\equiv \hat{U}_t} i\hbar\,\delta(t')\,|\psi(0)\rangle$$

$$i\hbar\partial_t|\psi(t)\rangle =$$
$$= i\hbar|\psi(0)\rangle\,\partial_t\Theta(t)$$
$$= i\hbar|\psi(0)\rangle\,\delta(t)$$

<u>note:</u> not unique: $\Longrightarrow$

$$\hat{U}(\omega) = \int \hat{U}(t')\, e^{i\omega t'} dt'$$

- Any representation can be used, but some more convenient than others.

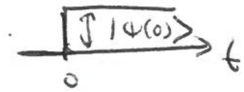
e.g. $\frac{\hat{p}^2}{2m} = \hat{H}$, simplest in $|p\rangle$

$V(\hat{x})$, simplest in $|x\rangle$

$$(-\hat{H} + i\hbar\partial_t)|\psi(t)\rangle = \underbrace{i\hbar|\psi(0)\rangle\,\delta(t)}$$

"retarded"
$t > 0$

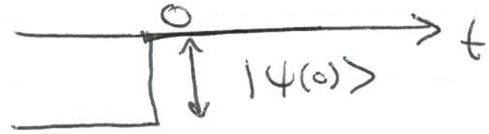
$$= i\hbar\,\partial_t\,\Theta(t)|\psi(0)\rangle$$



or

$$= -i\hbar\,\partial_t\,\Theta(-t)|\psi(0)\rangle$$

$$\hat{U}_{R/A}(\omega) = \frac{i\hbar}{\hbar\omega - \hat{H} \pm i\varepsilon}$$



only encodes discontinuity
can always add a t-indep. fnc.

i.e. $i\hbar|\psi(0)\,\delta(t)$

$$= i\hbar\,\partial_t(\Theta(t) + \underset{\text{fixed by b.c.}}{\underbrace{C}})|\psi(0)\rangle$$

e.g. $|\psi(t<0)\rangle = 0$

"retarded", causal

$\Rightarrow$ $\boxed{\text{Canonical quantization}}$:

classical:		quantum:	
$H(p,q)$	$\rightarrow$	$H(\hat{p},\hat{q})$	; $H(\hat{p},\hat{q})|\psi\rangle = i\hbar\partial_t|\psi\rangle$
$O(p,q)$	$\rightarrow$	$O(\hat{p},\hat{q})$	; $[\hat{q},\hat{p}] = i\hbar$
			$\Leftrightarrow \dot{\hat{O}} = \frac{1}{i\hbar}[\hat{O},\hat{H}]$.

Note: ambiguity (e.g. $O(p,q) = pq \overset{?}{\rightarrow} \hat{p}\hat{q}$ or $\hat{q}\hat{p}$ or $a\hat{p}\hat{q} + (1-a)\hat{p}\hat{p}$)
resolved by experiments.

Ex. $pq \rightarrow \frac{1}{2}(\hat{p}\hat{q} + \hat{q}\hat{p})$ $\Leftarrow$ Hermitian,
but $\hat{p}\hat{q}$ not Hermitian.

Examples:

$$H(p,r) \rightarrow H(\hat{p},\hat{r})$$

1. free particle: $\hat{H} = \frac{\hat{p}^2}{2m} \rightarrow \hat{H} = -\frac{\hbar^2\nabla^2}{2m}$

2. general potential: $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r})$

   e.g. H.O: $V = \frac{1}{2}m\omega^2 r^2$

3. charged particle in EM field:

$$\hat{H} = \frac{|\hat{\vec{p}} - \frac{q}{c}\hat{\vec{A}}|^2}{2m} + qA_0(r,t)$$

under force: $V = -fx$

coord. repr. $\rightarrow$ $$\hat{H} = \frac{1}{2m}\left[-\hbar^2\nabla^2 - \frac{q}{c}(-i\hbar\vec{\nabla}\cdot\vec{A}) - \frac{q}{c}\vec{A}\cdot(-i\hbar\vec{\nabla}) + \right.$$
$$\left. + \frac{q^2}{c^2}\vec{A}\cdot\vec{A}\right] + qA_0(r,t) .$$

$\rightarrow$ Solve (in coord. repres. ... not always best choice) partial linear diff. eqn. with b.c. s.t. ψ is continuous & $\nabla\psi$ also continuous (unless infinite potential somewhere to have ∞ T to cancel ∞ V).

$\rightarrow$ When cannot solve analytically use:
- approximate methods (pert. theory, WKB, variational theory, ...)
- numerics.

$\rightarrow$ quantized eigenvalues due to b.c. & requirements on ψ, $\nabla\psi$, similar to notes for guitar string.

4.17

Time dependence & Energy eigenstates.

$$\hat{H}|\Psi\rangle = i\hbar \partial_t |\Psi\rangle$$

$$|\Psi(t)\rangle = \sum_n |E_n\rangle e^{-\frac{i}{\hbar}E_n t} a_n$$ ← just Fourier representation

$$\Rightarrow \hat{H}|E_n\rangle = E_n|E_n\rangle$$

find eigenstates $|E_n\rangle$ for this t-independent S. Eqn. problem & reconstruct $|\Psi\rangle$ via F.T. above.

Steps to $|\Psi(t)\rangle$:

cf. normal mode analysis of classical mechanics (or any other linear problem)

(1) solve TISE: $\hat{H}|E_n\rangle = E_n|E_n\rangle$

(2) find resolution of initial state $|\Psi(0)\rangle$ in terms of $|E_n\rangle$, i.e. $|\Psi(0)\rangle = \sum_n a_n(0)|E_n\rangle$

where $a_n(0) = \langle E_n|\Psi(0)\rangle$.

(3) $|\Psi(t)\rangle = \sum_n a_n e^{-\frac{i}{\hbar}E_n t}|E_n\rangle$

Lecture 7:

Feynman's Path integral formulation of Q.M.

I. Background:

Invented by Richard Feynman (1940), motivated by original work by P. A. M. Dirac.
"Role of Lagrangian in Q.M.", Dirac.
$\Rightarrow$ now modern language for QFT & Stat Mech

Dirac:

Q. canonical quantization

$$H(p,q) \to H(\hat{p},\hat{q})$$

classical quantum

$$\{\ ,\ \} \to [\ \ ]$$

H-J Eqn $\to$ Sch. Eqn.

... but what role is played by Lagrangian that is so prominent in classical mech.
(may be even more fundamental, since treats t, r on equal footing $\to$ relativity)

$$S = \int dt\, L(q,\dot{q}) \to \ ???$$

$e^{iS/\hbar}$ A. Connection through canonical transformation from $q(t_0) \to q(t) \to$ evolution in time with S the Hamilton's characteristic fnc.

Feynman "pushed"/developed this idea into a concrete theory from which explicit calc's can be done.

How? $\Rightarrow$ focus on evolution operator

$$e^{-i\hat{H}t/\hbar} = \hat{U}(t)$$, whose knowledge is equivalent to solving Schrödinger's Eqn.

Know $\hat{U}(t) \longrightarrow$ everything else follows.

... but need to compute $\hat{U}(t)$ in a specific representation, e.g. coord. repres.

Q: $\langle x|\hat{U}(t)|x'\rangle \equiv \underline{U(x,t;x',t')} = ?$

A: $$U(x,t;x',t') = A \sum_{\text{all paths}} e^{\frac{i}{\hbar} S[X(t)]}$$

where,

- $S[X(t)]$ classical action functional for path $X(t)$ connecting $x' \equiv X(t')$ to $x = X(t)$
- $\sum_{\text{all paths.}}$ — "sum" over all paths $X(t)$ connecting (x',t') to (x,t)

Why? How related to Sch. Eqn? Corresp. princip?

II. Derivation of path-integral form of $U(x,t;x')$

$$U(x,x';t) = \langle x | e^{-\frac{i}{\hbar}\hat{H}t} | x' \rangle \quad \text{(picked } t'=0\text{)}$$

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t} = \Big(e^{-\frac{i}{\hbar}\hat{H}\underbrace{\tfrac{t}{N}}_{\equiv \varepsilon}}\Big)^N$$

$$= \underbrace{\hat{U}(\varepsilon)\hat{U}(\varepsilon)\ldots\hat{U}(\varepsilon)}_{N\text{ - times}} = \big(\hat{U}(\varepsilon)\big)^N$$

infinitesmal evolution operator:

$$\hat{U}(\varepsilon) = e^{-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\varepsilon} \approx e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon}\, e^{-\frac{i}{\hbar}V(\hat{x})\varepsilon}$$

even though $e^{A+B} = e^A e^{B + \frac{1}{2}[A,B] + \ldots} \neq e^A e^B$

if $[A,B] \neq 0$

show for hw4

$$\Rightarrow U(x_N,x_0;t) = \langle x_N | \hat{U}(\varepsilon)\underbrace{\ }_{\int_{-\infty}^{\infty} dx_{N-1} |x_{N-1}\rangle\langle x_{N-1}|}\hat{U}(\varepsilon)\underbrace{\ }_{\int_{-\infty}^{\infty} dx_{N-2} |x_{N-2}\rangle\langle x_{N-2}|}\hat{U}(\varepsilon)\ldots\hat{U}(\varepsilon)\underbrace{\ }_{\int_{-\infty}^{\infty} dx_1 |x_1\rangle\langle x_1|}\hat{U}(\varepsilon)|x_0\rangle$$

$$\Rightarrow U(x_N,x_0;t) = \int_{-\infty}^{\infty} dx_{N-1} \int_{-\infty}^{\infty} dx_{N-2} \int_{-\infty}^{\infty} dx_{N-3} \ldots \int_{-\infty}^{\infty} dx_1 \times$$

$$\times \underbrace{\langle x_N | \hat{U}(\varepsilon) | x_{N-1}\rangle \langle x_{N-1} | \hat{U}(\varepsilon) | x_{N-2}\rangle \ldots \langle x_1 | \hat{U}(\varepsilon) | x_0\rangle}_{N\text{ - factors}}$$

focus of generic one $\langle x_{n+1} | \hat{U}(\varepsilon) | x_n \rangle \equiv U(x_{n+1}, x_n, \varepsilon) = ?$

(7.4)

$$U(x_{n+1}, x_n; \varepsilon) = \langle x_{n+1} | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} e^{-\frac{i}{\hbar}V(\hat{x})\varepsilon} | x_n \rangle = ?$$

$$= \underbrace{\langle x_{n+1} | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | x_n \rangle}_{\equiv U_0 = ?} e^{-\frac{i}{\hbar}V(x_n)\varepsilon}$$

$\equiv U_0 = ?$ $\rightarrow$ free particle evolution operator for $t = \varepsilon$.

$$U(x_{n+1}, x_n; \varepsilon) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}(x_{n+1}-x_n)^2} e^{-\frac{i}{\hbar}V(x_n)\varepsilon}$$

$$= \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{1/2} e^{\underbrace{\frac{i}{\hbar}\underset{\Delta t}{\underset{\sim}{\varepsilon}}\underbrace{\left(\frac{1}{2}m\left(\overbrace{\frac{x_{n+1}-x_n}{\varepsilon}}^{\dot{x}_n}\right)^2 - V(x_n)\right)}_{L(x_n)}}_{\frac{i}{\hbar}S_\varepsilon = \frac{i}{\hbar}\int_{t_n}^{t_{n+1}=t_n+\varepsilon} dt\, L(x(t))}}$$

$$\boxed{\begin{aligned} U(x_N, x_0; t) &= \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx_{N-1} A \int_{-\infty}^{\infty} dx_{N-2} A \ldots \int_{-\infty}^{\infty} dx_1 A \times \\ &\times e^{\frac{i}{\hbar}\varepsilon \sum_{n=1}^{N}\left[\frac{1}{2}m\left(\frac{x_n - x_{n-1}}{\varepsilon}\right)^2 - V(x_{n-1})\right]} \\ U(x_N, x_0; t) &\equiv \int_{x_0,0}^{x_N,t} \underbrace{\mathcal{D}x(t)}_{} \, e^{\frac{i}{\hbar} S(x(t))} \end{aligned}}$$

$S(x(t))$ ← Action functional

(sum over all paths connecting x_N, t & $x_0, 0$.)

<u>coordinate</u> <u>form</u> <u>of</u> <u>a</u> <u>path-integral</u>
(configuration space)

Show:

A. $U_0(x_{n+1}, x_n; \varepsilon) = \langle x_{n+1} | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | x_n \rangle$

B. phase-space path-integral form

C. How it works for: • free particle

hw4 { • harmonic oscillator
• linear potential

D. Physical picture

E. Classical limit & F. Semiclassical expansion

A. $U_0(x_{n+1}, x_n; \varepsilon) = \langle x_{n+1} | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | x_n \rangle$

$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} |p_n\rangle\langle p_n|$$

$$= \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \underbrace{\langle x_{n+1} | p_n \rangle}_{e^{\frac{i}{\hbar} p_n x_{n+1}}} \underbrace{\langle p_n | x_n \rangle}_{e^{-\frac{i}{\hbar} p_n x_n}} e^{-\frac{i}{\hbar}\frac{p_n^2}{2m}\varepsilon}$$

$$\Rightarrow U_0(x_{n+1}, x_n; \varepsilon) = \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} e^{-\frac{i}{\hbar}\frac{p_n^2}{2m}\varepsilon + \frac{i}{\hbar} p_n (x_{n+1} - x_n)}$$

$$= \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{1/2} e^{\frac{i}{\hbar} \underset{\uparrow}{\varepsilon} \frac{1}{2} m \Big(\underbrace{\frac{x_{n+1} - x_n}{\varepsilon}}_{\dot{x}_n}\Big)^2}$$

$\Delta t = t_{n+1} - t_n$

B. phase-space P-I.:

$$U(x_N, x_0; t) = \int_{-\infty}^{\infty} dx_{N-1} \int_{-\infty}^{\infty} dx_{N-2} \ldots \int_{-\infty}^{\infty} dx_1 \times$$

$$\times \prod_{n=1}^{N} \Big[\underbrace{\langle x_n | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | x_{n-1}\rangle}_{U_0(x_n, x_{n-1}; \varepsilon)} e^{-\frac{i}{\hbar} V(x_{n-1})\varepsilon} \Big]$$

insert $\prod_{n=1}^{N} \left(\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} |p_n\rangle\langle p_n| \right)$

dimensionless

$$\boxed{\begin{gathered} \Rightarrow U(x_N, x_0; t) = \int_{-\infty}^{\infty} dx_{N-1} \frac{dp_{N-1}}{2\pi\hbar} \int_{-\infty}^{\infty} dx_{N-2} \frac{dp_{N-2}}{2\pi\hbar} \ldots \int \overbrace{dx_1 \frac{dp_1}{2\pi\hbar}} \cdot \\ \prod_{n=1}^{N} \left(e^{\varepsilon \frac{i}{\hbar}\left[p_n \underbrace{\left(\frac{x_n - x_{n-1}}{\varepsilon}\right)}_{\dot{x}_n} - \frac{p_n^2}{2m} - V(x_{n-1}) \right]} \right) \\ N \to \infty, \quad \varepsilon \to 0 \\ U(x_N, x_0; t) = \int \mathcal{D}x(t) \mathcal{D}p(t)\, e^{\frac{i}{\hbar}\int_0^t dt [p\dot{x} - H(x(t), p(t))]} \end{gathered}}$$

phase-space path-integral.

$$H = \frac{p^2}{2m} + V(x)$$

integrating over $\int \mathcal{D}p(t) \rightarrow$ configurational path-integral.

Note: (for the most part) can only do Gaussian path integrals $\Rightarrow$ can only solve probs with $H = \frac{p^2}{2m} + ax + bx^2$

C. How it works for free particle.
(more examples later)

$$U_0(x_N, x_0; t) = \int_{x_0, 0}^{x_N, t} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_0^t dt' \frac{1}{2} m \dot{x}(t)^2}$$

Actual integral done in discrete form:

Note "closure" property of Gaussian P-I:

$$\int_{-\infty}^{\infty} dx_n\, U_0(x_{n+1}, x_n; t_{n+1}, t_n)\, U_0(x_n, x_{n-1}, t_n, t_{n-1})$$

$$= \int_{-\infty}^{\infty} dx_n \left(\frac{m}{2\pi i \hbar (t_{n+1}-t_n)}\right)^{1/2} e^{\frac{i}{\hbar}\frac{1}{2} m \frac{(x_{n+1}-x_n)^2}{t_{n+1}-t_n}} \times$$

$$\times \left(\frac{m}{2\pi i \hbar (t_n - t_{n-1})}\right)^{1/2} e^{\frac{i}{\hbar}\frac{1}{2} m \frac{(x_n - x_{n-1})^2}{t_n - t_{n-1}}}$$

$$= \left(\frac{m}{2\pi i \hbar (t_{n+1}-t_{n-1})}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_{n+1}-x_{n-1})^2}{t_{n+1}-t_{n-1}}}$$

easiest to show through phase space P-I. (hw 4)

$$= U_0(x_{n+1}, x_{n-1}; t_{n+1}, t_{n-1})$$

This way integrate all $\int dx_{N-1}, \int dx_{N-2}, \ldots \int dx_1$

$$\Rightarrow \boxed{U_0(x_N, x_0; t) = \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_N - x_0)^2}{t}}}$$

D. Physical picture

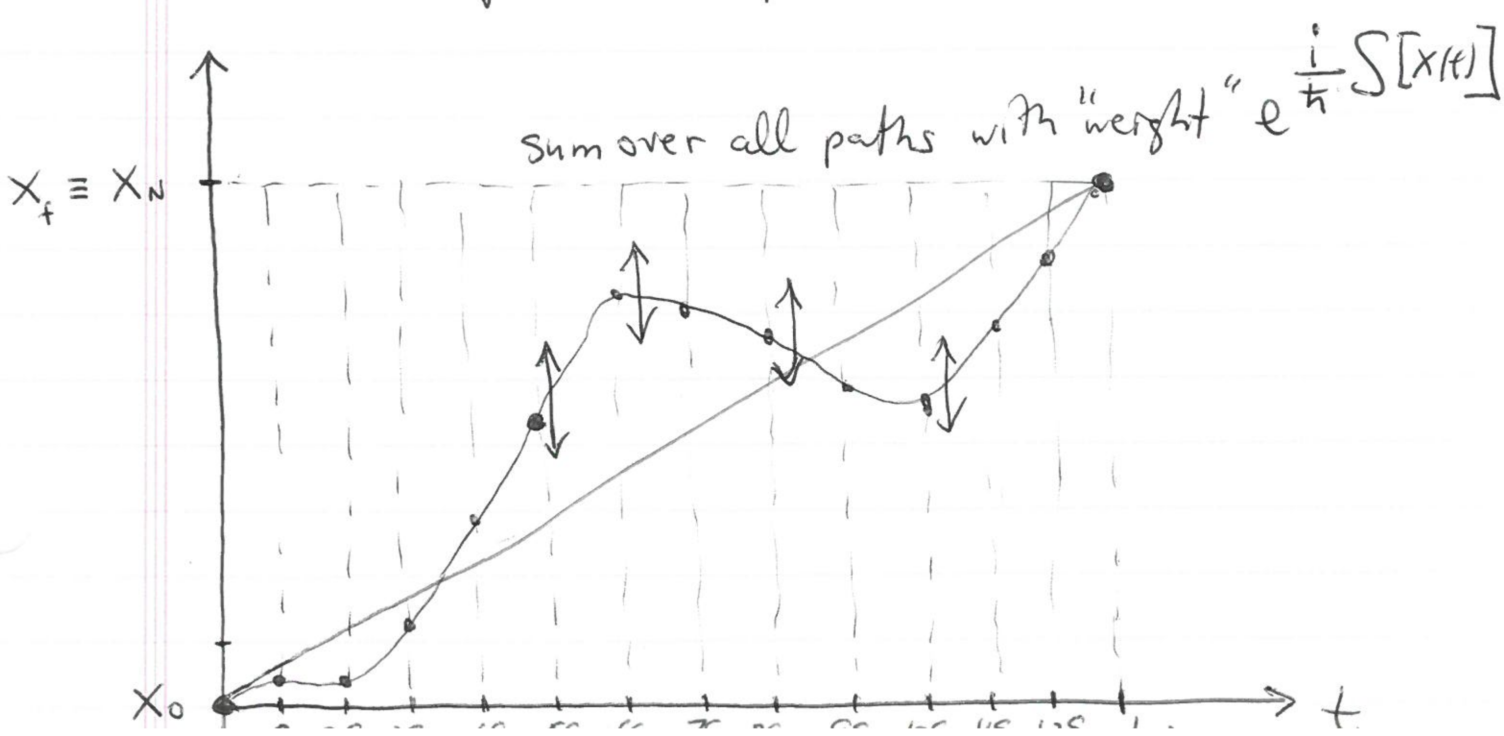
Feynman: There are no waves, only particles!

... but these quantum particles can follow <u>any</u> trajectory $x(t)$ from $x_0, 0$ to x_N, t <u>not</u> just the classical one (from Newton's law)!
(also true for photons, etc.)

$$U(x_f, x_0; t) = \int_{x(0)=x_0}^{x(t)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_0^t dt'\, L(x(t), \dot{x}(t))}$$

$$= \int_{-\infty}^{\infty} dx_{N-1} \int_{-\infty}^{\infty} dx_{N-2} \cdots \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_1\, U(x_N, x_{N-1}; \varepsilon)\, U(x_{N-1}, x_{N-2}; \varepsilon) \times \cdots U(x_2, x_1; \varepsilon)\, U(x_1, x_0; \varepsilon)$$

"sum" over all intermediate $x_1, x_2, \ldots, x_{N-1}$, i.e., sum over all possible paths:



E. <u>Classical</u> <u>limit</u>:

$$U(x_f, x_0; t) = \int_{x(0)=x_0}^{x(t)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar} S[x(t)]}$$

All paths contribute in general →
sum bunch of complex #'s $e^{\frac{i}{\hbar} S[x(t)]}$

...but for $\hbar \to 0$ this sum is that of fast "oscillating" complex #'s, i.e.
<u>small</u> change in <u>path</u> → <u>small</u> change in $S[x]$
⟹ great change in phase of $\frac{1}{\hbar} S[x(t)]$

⟹ $e^{\frac{i}{\hbar} S}$ oscillates a lot

⟹ sum → ≈ 0 from most paths' contributions cancelling out.

Path-integral is dominated by $x(t)$ that extremizes $S[x(t)]$, since then $S[x(t)]$ changes more slowly ⟹
main contribution from paths $x_c(t)$

s.t. $\boxed{\left.\frac{\delta S}{\delta x(t)}\right|_{x_c(t)} = 0}$ ⟺ Euler-Lagrange Eqn
⟺ Newton's 2nd law

$$\Rightarrow U(x_f, x_0; t) = \int_{x(0)=x_0}^{x(t)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar} S[x(t)]}$$

$$\boxed{U \approx e^{\frac{i}{\hbar} S[x_c(t)]}}$$

x_c satisfies Newton's / Euler-Lagrange eqns. with b.c. $x(t) = x_f$, $x(0) = x_0$

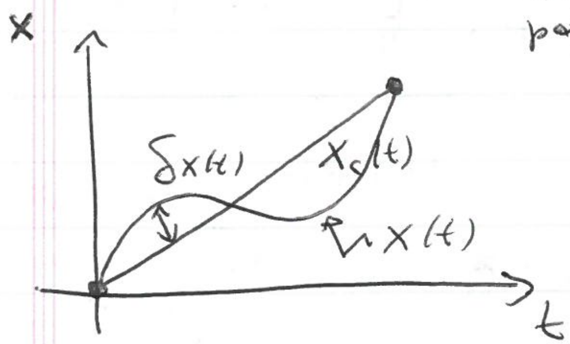
wow !!!

F. <u>Semiclassical expansion</u>:

$$U(x_f, x_0; t) = \int_{x(0)=x_0}^{x(t)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar} S[x(t)]}$$

<u>change vars</u>: $x(t) = x_c(t) + \delta x(t)$

$x(t)$: arbitrary path; $x_c(t)$: classical path; $\delta x(t)$: fluct. about classical path.



$\Rightarrow$ <u>Note</u>: $\left.\begin{array}{l}\delta x(t_f) = 0 \\ \delta x(0) = 0\end{array}\right\}$ simple b.c.'s.

$$\Rightarrow U(x_f, x_0, t_f) = \int_{\delta x(0)=0}^{\delta x(t_f)=0} \mathcal{D}\delta x(t)\, e^{\frac{i}{\hbar} S[\underbrace{x_c(t) + \delta x(t)}_{\text{Taylor expand in } \delta x(t)}]}$$

$$S[x_c + \delta x] = \underbrace{\int_0^{t_f} dt \left[\frac{m}{2}\dot{x}_c^2 - V(x_c)\right.}_{S_c[x_c(t)]} + \frac{m}{2}\delta\dot{x}^2 - \frac{1}{2}V''(x_c(t))\,\delta x_{(t)}^2 + \ldots \Big]$$

<u>Note</u>: $\left.\frac{\delta S}{\delta x(t)}\right|_{x_c} = 0 \Rightarrow$ <u><u>no</u></u> <u>linear</u> terms in $\delta x(t)$!

- Easy to do for any quadratic action, i.e harmonic oscillators; see Feynman & Hibbs.
- Note: $$U(x, x'; t) = \sum_n \psi_n^*(x)\,\psi_n(x')\,e^{-\frac{i}{\hbar}E_n t}$$

this decomposition allows us to find eigenstates $\psi_n(x)$ & E_n (spectrum)

<u>Note</u> connection to classical stat mech.

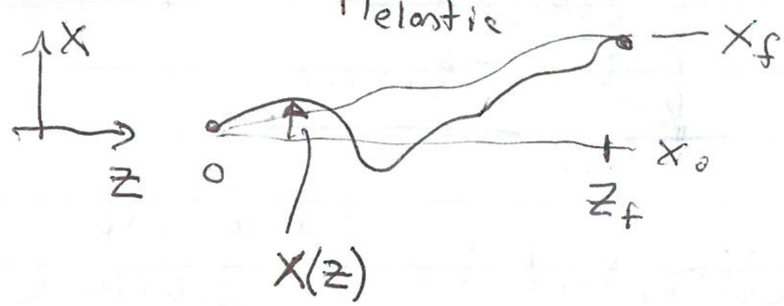
$T=0$ quantum <u>particle</u>

$$U(x_f, x_i; t_f) = \int \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_0^{t_f} dt' \left(\frac{(\partial_{t'} x)^2}{2m} - V(x)\right)}$$

$\Longleftrightarrow$ $T\neq 0$ classical stat mech of a "string"

$$Z(x_f, x_0; z_f) = \int \mathcal{D}x(z)\, e^{-\frac{1}{k_BT}\int_0^{z_f} dz' \underbrace{\left[\frac{\kappa}{2}(\partial_{z'} x)^2 + V(x)\right]}_{H_{elastic}}}$$

polymer, fluxline, guitar string.



See: Feynman & Hibbs, "PI's" & Feynman, "Stat Mech"

7.1

$$U(x_f, x_0; t_f) \simeq e^{\frac{i}{\hbar} S[x_c(t)]} \times \underbrace{\int_0^0 \mathcal{D}\delta x(t)\, e^{\frac{i}{\hbar}\int_0^{t_f} dt' \left[\frac{1}{2} m \delta\dot{x}^2 - \frac{1}{2} V''(x_c(t))\delta x(t)^2 + \cdots\right]}}$$

do Gaussian integral over $\delta x(t)$. If want to go to higher order expand exponential in $\delta x^3, \delta x^4, \ldots$

$\Rightarrow$ moments of Gaussian integral.

$\rightarrow$ path-integral pert. theory.

effective harmonic oscillator about classical path $x_c(t)$

Ex: free particle

$$S[x(t)] = \int_0^{t_f} dt' \, \frac{1}{2} m \dot{x}(t)^2$$

$$\ddot{x}_c(t) = 0 \quad \Rightarrow \quad x_c(t) = \frac{x_f - x_0}{t_f} t + x_0$$

Note: $x_c(0) = x_0$, $x_c(t_f) = x_f$

~~exactly~~:

$$S[x(t)] = \underbrace{\int_0^{t_f} dt' \, \frac{1}{2} m \dot{x}_c(t)^2}_{S[x_c(t)]} + \underbrace{\int_0^{t_f} dt' \, \frac{1}{2} m \delta\dot{x}(t)^2}_{\text{Gauss. fluctuations.}}$$

$$\Rightarrow U(x_f, x_0; t_f) = \underbrace{e^{\frac{i}{\hbar} S[x_c(t)]}}_{= \, ?} \underbrace{\int_0^0 \mathcal{D}\delta x(t)\, e^{\frac{i}{\hbar}\int_0^{t_f} dt' \frac{1}{2} m \delta\dot{x}(t)^2}}_{N(t_f)}$$

$N(t_f)$ just a #, independent of x_0, x_f; just depends on t_f.

$$S[x_c(t)] = \int_0^{t_f} dt' \frac{1}{2} m \left(\frac{x_f - x_0}{t_f}\right)^2 = \frac{1}{2} m \left(\frac{x_f - x_0}{t_f}\right)^2 t_f$$

$$\Rightarrow \boxed{U(x_f, x_0; t_f) = N(t_f)\, e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x_f - x_0)^2}{t_f}}}$$

$= \left(\frac{m}{2\pi i \hbar t_f}\right)^{1/2}$

fix by $U(0,0,t_f)$

G. Connection/equivalence with Schrödinger Eqn

local $\left\{ \begin{array}{l} \text{Schrödinger Eqn.} \longleftrightarrow \text{Feynman Path integral} \\ \qquad\qquad \text{similar to:} \\ \text{Newton's Eqn} \longleftrightarrow \text{Least action principle. } \dfrac{\delta S}{\delta x(t)} = 0 \end{array} \right\}$ global

$$H|\psi\rangle = i\hbar\, \partial_t |\psi\rangle$$

infinitesimal evolution of time ε:

$$\Leftrightarrow \quad -\frac{i\varepsilon}{\hbar} H|\psi(0)\rangle = |\psi(\varepsilon)\rangle - |\psi(0)\rangle$$

In $|x\rangle$ basis to lowest order in ε $(\Theta(\varepsilon))$:

$$\psi(x,\varepsilon) - \psi(x,0) = \frac{-i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right]\psi(x,0)$$

$$\psi(x,\varepsilon) = \psi(x,0) - \frac{i\varepsilon}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right]\psi(x,0)$$

compare to evolution from 0 to ε

$$\psi(x,\varepsilon) = \int_{-\infty}^{\infty} U(x,\varepsilon;x')\,\psi(x',0)\,dx'$$

where:

$$U(x;\varepsilon;x') = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} e^{i\left[\frac{m(x-x')^2}{2\varepsilon} - \varepsilon V\left(\frac{x+x'}{2},0\right)\right]/\hbar}$$

$$\psi(x,\varepsilon) = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}\underbrace{(x-x')^2}_{\eta}} e^{-\frac{i\varepsilon}{\hbar} V\left(\frac{x+x'}{2}, 0\right)} \psi(x',0)\, dx'$$

$$x' = x + \eta$$

change vars $x' \to \eta$

does not matter i.e. $\eta/2 = 0$ since $\varepsilon \to 0$ & $\eta \sim \mathcal{O}(\varepsilon^{1/2})$

$$\psi(x,\varepsilon) = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} d\eta\, e^{\underbrace{\frac{i}{\hbar}\frac{m}{2\varepsilon}\eta^2}_{\lesssim \mathcal{O}(\pi)} - \frac{i\varepsilon}{\hbar} V\left(x+\frac{\eta}{2}, 0\right)} \psi(x+\eta, 0)$$

$$\Rightarrow \eta \lesssim \sqrt{\frac{\pi\varepsilon\hbar}{m}} \to 0 \text{ as } \varepsilon \to 0$$

Taylor expand in ε to $\mathcal{O}(\varepsilon^1)$

$$\psi(x,\varepsilon) = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} d\eta\, e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}\eta^2} e^{-\frac{i\varepsilon}{\hbar} V(x,0)} \times \left(\psi(x,0) + \eta\frac{\partial}{\partial x}\psi(x,0) + \frac{1}{2}\eta^2\frac{\partial^2}{\partial x^2}\psi(x,0) + \dots\right)$$

$$\psi(x,\varepsilon) = \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} d\eta\, e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}\eta^2} \left(1 - \frac{i}{\hbar}\varepsilon V(x,0) + \dots\right) \times \left(\psi(x,0) + \eta\frac{\partial}{\partial x}\psi(x,0) + \frac{1}{2}\eta^2\frac{\partial^2}{\partial x^2}\psi(x,0) + \dots\right)$$

$$\simeq \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} d\eta\, e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}\eta^2} \left[\left(1 - \frac{i}{\hbar}\varepsilon V(x,0)\right)\psi(x,0) + \cancel{\eta}\frac{\partial\psi(x,0)}{\partial x} + \eta^2\frac{1}{2}\frac{\partial^2\psi(x,0)}{\partial x^2} + \dots\right]$$

0

$$\psi(x,\varepsilon) = \psi(x,0) - \frac{i}{\hbar}\varepsilon V(x,0)\psi(x,0) + \underbrace{\langle \eta^2 \rangle}_{\frac{\hbar\varepsilon}{im}} \frac{1}{2}\frac{\partial^2\psi(x,0)}{\partial x^2}$$

$$\psi(x,\varepsilon) = \psi(x,0) - \frac{i}{\hbar}\varepsilon\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,0)}{\partial x^2} + V(x,0)\psi(x,0)\right)$$

$$\Rightarrow \quad \underline{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\,\partial_t\psi(x,t)}$$

- Harmonic Oscillator:

$$U(x,t;x',0) = A(t)\, e^{\frac{i}{\hbar}S_{cl}}$$

$$S_{cl} = \frac{m\omega_0}{2\sin\omega_0 t}\left[(x^2+x'^2)\cos\omega_0 t - 2xx'\right]$$

$$A(t) = \left(\frac{m\omega_0}{2\pi i\hbar \sin\omega_0 t}\right)^{1/2} \qquad \left(\underline{\text{Note}}:\ A(t) \xrightarrow[\omega_0\to 0]{} \left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\right)$$

- Linear potential $V(x) = -fx$:

$$U(x,t;x',0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{i}{\hbar}S_{cl}}$$

where $S_{cl} = S[x_c(t)]$ & $x_c(t) = x_0 + v_0 t + \frac{1}{2}\left(\frac{f}{m}\right)t^2$

chosen s.t. $x(t_f) = x_f$.