

## §1. Many-particle quantum mechanics

\*) Single-particle QM: path integral formulation

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{r})$$

time  $t$ :  $|\vec{r}\rangle$  (not an eigenstate)

time  $t' > t$ :  $e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|\vec{r}\rangle$

Probability of finding the particle at  $\vec{r}'$ ?

$$\begin{aligned} e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|\vec{r}\rangle &= \int d^3\vec{r}' \underbrace{|\vec{r}'\rangle\langle\vec{r}'|}_{\hat{1}} e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|\vec{r}\rangle \\ &= \int d^3\vec{r}' \underbrace{U(\vec{r}', t'; \vec{r}, t)}|\vec{r}'\rangle \end{aligned}$$

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



quantum mechanical amplitude of  
finding the particle at  $\vec{r}'$  after time  $t'-t$

Probability:  $|U(\vec{r}', t'; \vec{r}, t)|^2$

— Path integral formulation (restrict to 1D for ease of notation)

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

time evolution  $t \rightarrow t'$ :

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

$$\hat{U}(t', t) = e^{-\frac{i}{\hbar} \hat{H}(t'-t)}$$

$$= e^{-\frac{i}{\hbar} \hat{H}(t'-t)} |\psi(t)\rangle$$

$$\int dx' \psi(x', t') |x'\rangle$$

$$\int dx \psi(x, t) |x\rangle$$

$$\Rightarrow \psi(x', t') = \langle x' | \psi(t') \rangle$$

$$= \langle x' | \hat{U}(t', t) | \psi(t) \rangle$$

$$= \int dx \underbrace{\langle x' | \hat{U}(t', t) | x \rangle}_{U(x', t'; x, t)} \underbrace{\langle x | \psi(t) \rangle}_{\psi(x, t)}$$

$$U(x', t'; x, t) \quad \psi(x, t)$$

$$= \int dx U(x', t'; x, t) \psi(x, t)$$

complete basis

$$\int dx |x\rangle \langle x| = \hat{1}$$

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

difficult to calculate

since  $[\hat{x}, \hat{p}] \neq 0 \Rightarrow$

exponential does not factorize ...

Feynman's great idea:

Decompose  $t' - t$  into small time intervals

$$t' - t = N \Delta t$$



$$t_k = t + k \Delta t \quad (k = 1, 2, \dots, N-1)$$

$$\begin{aligned} \hat{U}(t', t) &= e^{-\frac{i}{\hbar} \hat{H}(t' - t)} \\ &= e^{-\frac{i}{\hbar} \hat{H}(t' - t_{N-1})} e^{-\frac{i}{\hbar} \hat{H}(t_{N-1} - t_{N-2})} \dots e^{-\frac{i}{\hbar} \hat{H}(t_1 - t)} \\ &= \hat{U}(t', t_{N-1}) \hat{U}(t_{N-1}, t_{N-2}) \dots \hat{U}(t_1, t) \end{aligned}$$

$x$ -representation:

insert resolution of identity

$$\hat{1} = \int dx_k |x_k\rangle \langle x_k| \text{ for each interval}$$

$$\begin{aligned} U(x', t'; x, t) &= \langle x' | \hat{U}(t', t) | x \rangle \\ &= \int dx_{N-1} dx_{N-2} \dots dx_1 \langle x' | \hat{U}(t', t_{N-1}) | x_{N-1} \rangle \\ &\quad \times \langle x_{N-1} | \hat{U}(t_{N-1}, t_{N-2}) | x_{N-2} \rangle \dots \langle x_1 | \hat{U}(t_1, t) | x \rangle \\ &= \int dx_{N-1} \dots dx_1 U(x', t'; x_{N-1}, t_{N-1}) \\ &\quad \times U(x_{N-1}, t_{N-1}; x_{N-2}, t_{N-2}) \dots U(x_1, t_1; x, t) \end{aligned}$$

need to evaluate  $U(x_{k+1}, t_{k+1}; x_k, t_k) = \langle x_{k+1} | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_k \rangle$

Basic idea:

$$\langle x_{k+1} | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_k \rangle \simeq \langle x_{k+1} | \left( 1 - \frac{i}{\hbar} \hat{H} \Delta t \right) | x_k \rangle + O(\Delta t^2)$$

small time interval

$$\Delta t \rightarrow 0$$

need to evaluate  $\langle x_{k+1} | \hat{H} | x_k \rangle$

$$\langle x_{k+1} | \hat{H} | x_k \rangle = \int dp_k \langle x_{k+1} | p_k \rangle \langle p_k | \hat{H} | x_k \rangle$$

$$\frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p_k x_{k+1}}$$

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

$$\langle p_k | \left[ \frac{\hat{p}^2}{2m} + V(\hat{x}) \right] | x_k \rangle$$

$$H(p_k, x_k) = \frac{p_k^2}{2m} + V(x_k)$$

number, NOT an operator!

$$= \left[ \frac{p_k^2}{2m} + V(x_k) \right] \langle p_k | x_k \rangle$$

$$= H(p_k, x_k) \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} p_k x_k}$$

Full derivation:

$$U(x_{k+1}, t_{k+1}; x_k, t_k) = \langle x_{k+1} | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x_k \rangle$$

$$\simeq \langle x_{k+1} | \left( 1 - \frac{i}{\hbar} \hat{H} \Delta t \right) | x_k \rangle$$

$$= \int dp_k \langle x_{k+1} | p_k \rangle \langle p_k | \left( 1 - \frac{i}{\hbar} \hat{H} \Delta t \right) | x_k \rangle$$

$$\frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p_k x_{k+1}}$$

$$= \int dp_k \langle x_{k+1} | p_k \rangle \langle p_k | x_k \rangle$$

$$\times \left[ 1 - \frac{i}{\hbar} H(p_k, x_k) \Delta t \right]$$

$$\frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} p_k x_k}$$

$$\simeq e^{-\frac{i}{\hbar} H(p_k, x_k) \Delta t} + O(\Delta t^2)$$

$$= \int \frac{dp_k}{2\pi\hbar} e^{\frac{i}{\hbar} p_k (x_{k+1} - x_k) - \frac{i}{\hbar} H(p_k, x_k) \Delta t}$$

Substitute into  $U(x', t'; x, t)$  :

$$U(x', t'; x, t) = \int dx_{N-1} \cdots dx_1 U(x', t'; x_{N-1}, t_{N-1}) \cdots U(x_1, t_1; x, t)$$

$$= \int dx_{N-1} \cdots dx_1 \frac{dP_{N-1}}{2\pi\hbar} \cdots \frac{dP_1}{2\pi\hbar} \frac{dP_0}{2\pi\hbar} \rightarrow \text{initial point: } x_0 = x, t_0 = t$$

$$\times e^{\frac{i}{\hbar} P_{N-1} (x' - x_{N-1}) - \frac{i}{\hbar} H(P_{N-1}, x_{N-1}) \Delta t}$$

$$\times \cdots \times e^{\frac{i}{\hbar} P_0 (x_1 - x) - \frac{i}{\hbar} H(P_0, x_0) \Delta t}$$

final point:

$$x_N = x'$$

$$t_N = t'$$

$$= \int dx_{N-1} \cdots dx_1 \frac{dP_{N-1}}{2\pi\hbar} \cdots \frac{dP_0}{2\pi\hbar} \times e^{\frac{i}{\hbar} \sum_{k=0}^{N-1} [P_k (x_{k+1} - x_k) - H(P_k, x_k) \Delta t]}$$

In the limit  $\Delta t \rightarrow 0$  ( $N \rightarrow \infty$ ):

$$x_{k+1} - x_k \rightarrow \dot{x}(t) \Delta t$$

$$\sum_{k=0}^{N-1} \Delta t \rightarrow \int_t^{t'} dt''$$

$$\Rightarrow U(x', t'; x, t) = \int_{\substack{x(t) = x \\ x(t') = x'}} \mathcal{D}x(t'') \mathcal{D}p(t'')$$

functional integral  
over all possible "paths"  
in phase space

$$\times e^{\frac{i}{\hbar} \int_t^{t'} dt'' [P(t'') \dot{x}(t'') - H(P(t''), x(t''))]}$$

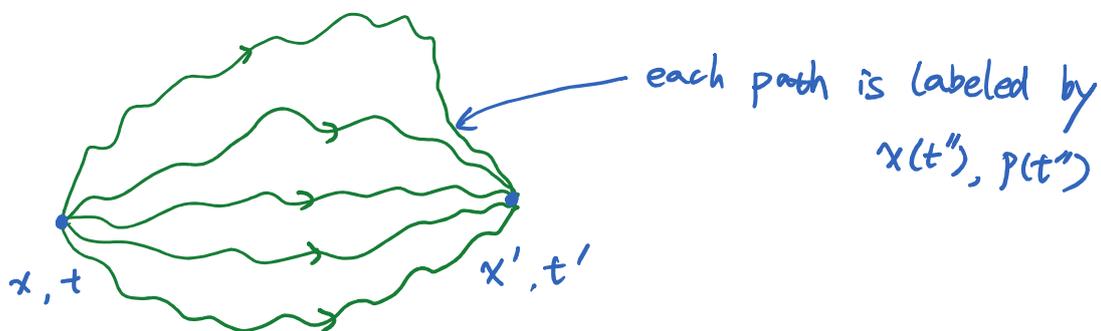
$$U(x', t'; x, t) = \int_{\substack{x(t) = x \\ x(t') = x'}} Dx(t'') Dp(t'')$$

$$\times e^{\frac{i}{\hbar} \int_t^{t'} dt'' [P(t'') \dot{x}(t'') - H(P(t''), x(t''))]}$$

//  
action  $S$

$$S[x(t''), p(t'')] = \int_t^{t'} dt'' [P(t'') \dot{x}(t'') - H(P(t''), x(t''))]$$

Natural link to classical mechanics!



amplitude for the path  $\{x(t''), p(t'')\}$ :  $e^{\frac{i}{\hbar} S[x(t''), p(t'')]}$

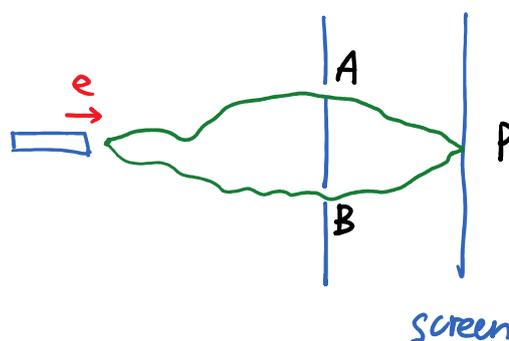
Remark:  $P(t'')$  not necessarily the same as  $m\dot{x}(t'')$ !

↑  
This can be seen from the "infinite-time-interval" derivation.

Example: electron double-slit experiment

amplitude  $a_A$  &  $a_B$

$$\frac{a_A}{a_B} = \left| \frac{a_A}{a_B} \right| e^{i\varphi}$$



Probability (intensity of the wave)

$$\begin{aligned} |a_A + a_B|^2 &= |a_B|^2 \cdot \left| \frac{a_A}{a_B} + 1 \right|^2 \\ &= |a_B|^2 \left[ \left( 1 + \left| \frac{a_A}{a_B} \right| \cos \varphi \right)^2 + \left| \frac{a_A}{a_B} \right|^2 \sin^2 \varphi \right] \\ &= |a_A|^2 + |a_B|^2 + 2 |a_A| \cdot |a_B| \cos \varphi \end{aligned}$$

Interference!

Path integral viewpoint:

$a_A$ : amplitude from a summation over all paths  
passing through slit A

( Similar for  $a_B$ : summing over all paths  
passing through slit B )

- Imaginary time formulation & partition function

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

Partition function at temperature  $T = \frac{1}{\beta}$  (take  $k_B = 1$ )

$$Z = \text{Tr} e^{-\beta H}$$

$$= \int dx \langle x | e^{-\beta H} | x \rangle$$

$$\beta = \frac{\tau}{\hbar} = \frac{i t}{\hbar}$$

↓  
imaginary time  $\tau = i t$

$$\langle x' | e^{-H\tau/\hbar} | x \rangle = \int_{\substack{x(0)=x \\ x(\tau)=x'}} \mathcal{D}x(\tau') \mathcal{D}p(\tau') e^{-\frac{1}{\hbar} S[x(\tau'), p(\tau')]}$$

$$S[x(\tau'), p(\tau')] = \int_0^\beta d\tau' \left[ -i p(\tau') \dot{x}(\tau') + H(p(\tau'), x(\tau')) \right]$$

Exercise: Derive the path integral form of the partition function.

$$\Rightarrow Z = \int_{\substack{x(0)=x(\tau)}} \mathcal{D}x(\tau') \mathcal{D}p(\tau') e^{-\frac{1}{\hbar} S[x(\tau'), p(\tau')]}$$

↓  
 $i p \dot{x}$  term is a Berry phase (why?  $\Rightarrow$  go back to "time-interval" picture)

(geometric phase arising from evolving  $|x\rangle$  back to itself)

Deep insight: d-dimensional quantum problem at finite temperature



(d+1)-dimensional classical statistical problem

Note, however, Berry phase has no classical analog!