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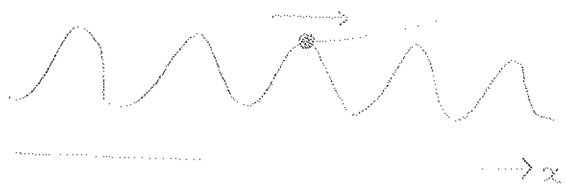
(3) Phase and group velocity

$$|\psi(t)\rangle = \sum_k \underbrace{e^{ikx - iE_k t}}_{\text{plane wave}} a(k) = \int_{-\infty}^{\infty} a(k,t)\, e^{ikx}\, dk$$

$E_k = \frac{k^2}{2m}$ (dispersion relation)

i) Phase velocity



a point on a wave corresponds to

$$e^{i\underbrace{(kx - E_k t)}_{\text{constant}}}$$

$$\boxed{v_{phase} = \frac{x}{t} = \frac{E_k}{k}} = \frac{k}{2m}$$

factor of 2 difference

(classical $\frac{p}{m}$)

ii) Group velocity

$$v_{group} = \frac{\partial \langle x\rangle(t)}{\partial t}$$

Since $|\psi\rangle$ is defined by its momentum composition, $a(k,t)$, let us work within the momentum space

position op. in momentum space

$$\langle x\rangle(t) = \frac{\int a(k,t)^* \left(i\frac{\partial}{\partial k}\right) a(k,t)\, dk}{\underbrace{\int a(k,t)^* a(k,t)\, dk}_{\text{normalization}}}$$

$$i\frac{\partial}{\partial k} a(k,t) = \left(i\frac{\partial}{\partial k} a(k)\right) e^{-iE_k t} + a(k)\left(i\frac{\partial}{\partial k} e^{-iE_k t}\right)$$

$$= \left(i\frac{\partial}{\partial k} a(k)\right) e^{-iE_k t} + a(k)\frac{\partial E_k}{\partial k} t\, e^{-iE_k t}$$

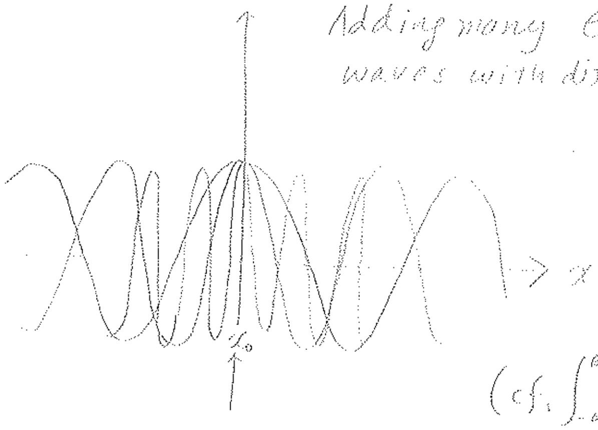
$$= \underbrace{\frac{\int a(k)^* i\frac{\partial}{\partial k} a(k)\, dk}{\int a(k)^* a(k)\, dk}}_{\langle x\rangle(t=0)} + \underbrace{\frac{\int a(k)^* \left(\frac{\partial E_k}{\partial k}\right) t\, a(k)\, dk}{\int a(k)^* a(k)\, dk}}_{\underbrace{\left\langle \frac{\partial E_k}{\partial k}\right\rangle}_{\text{must be } v_{group}} t}$$

$$\boxed{v_{group} = \frac{\partial E_k}{\partial k}} = \frac{k}{m}$$

(agrees w/ classical)

Another way to understand $v_{group} = \frac{\partial \varepsilon_k}{\partial k}$

Adding many $e^{ik(x-x_0)}$ waves with different k's



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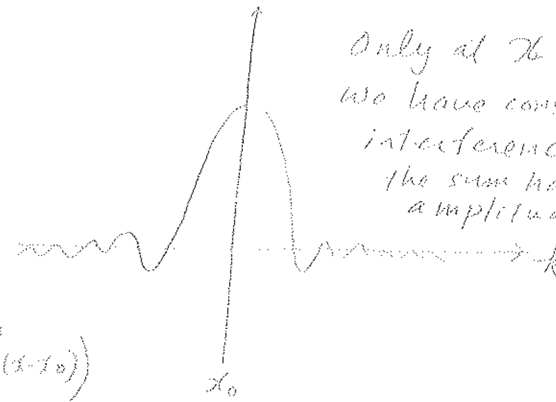


Only at $x = x_0$ we have constructive interference and the sum has significant amplitude

$$\left(\text{cf.} \int_{-\infty}^{\infty} e^{ik(x-x_0)} dk = 2\pi\,\delta(x-x_0)\right)$$

$$|w\rangle = \int_{-\infty}^{+\infty} a(k)\, e^{ikx - i\varepsilon_k t}\, dk$$

; $\varepsilon_k t$ is a function of k

$$\varepsilon_k t = \left(\varepsilon_0 + \frac{\partial \varepsilon_k}{\partial k} k + \cdots\right) t$$

$$= \int_{-\infty}^{+\infty} a(k)\, e^{i\left(x - \frac{\partial \varepsilon_k}{\partial k} t\right) k} \cdot e^{-i\varepsilon_0 t}\, dk$$

no or only small dependence on k

constructive interference occurs at

$$x = \frac{\partial \varepsilon_k}{\partial k} t$$

where $|w\rangle$ should have a peak.

$|w\rangle$'s peak travels at the velocity $\frac{\partial \varepsilon_k}{\partial k} = v_{group}$

⑥ Ehrenfest theorem

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, d\tau$$

$$\frac{d}{dt}\langle \hat{A} \rangle = \int \frac{d\psi^*}{dt} \hat{A} \psi \, d\tau + \int \psi^* \frac{d\hat{A}}{dt} \psi \, d\tau + \int \psi^* \hat{A} \frac{d\psi}{dt} \, d\tau$$

$$-i \frac{\partial \psi^*}{\partial t} = \hat{H}^* \psi^* \qquad\qquad i \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$= -\frac{1}{i} \underbrace{\int (\hat{H}^* \psi^*) \hat{A} \psi \, d\tau} + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i} \int \psi^* \hat{A} (\hat{H} \psi) \, d\tau$$

$$= \int (\hat{A}\psi)(\hat{H}^* \psi^*) \, d\tau$$

$$= \int \psi^* \hat{H} \hat{A} \psi \, d\tau$$

$$= \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i} \langle \psi | [\hat{A}, \hat{H}] | \psi \rangle \qquad [\hat{P}, \hat{Q}] = \hat{P}\hat{Q} - \hat{Q}\hat{P}$$

commutator

When $\hat{A}$ has no explicit time dependence

$$i \frac{d}{dt} \langle \hat{A} \rangle = \langle \psi | [\hat{A}, \hat{H}] | \psi \rangle$$

When $\hat{A}$ and $\hat{H}$ commute, $\langle A \rangle$ is time independent

When $\hat{A} = \hat{p} = -i\nabla$

commute

(☆) $$i \frac{d}{dt} \langle \hat{p} \rangle = \langle \psi | [-i\nabla, \frac{1}{2m}\nabla^2 + \hat{V}] | \psi \rangle$$

$$= \langle \psi | [-i\nabla, \hat{V}] | \psi \rangle$$

$$= -i \langle \psi | (\nabla \hat{V}) + \hat{V}\nabla - \hat{V}\nabla | \psi \rangle$$

$$= -i \langle \psi | (\nabla \hat{V}) | \psi \rangle$$

$$\frac{d}{dt} \langle \hat{p} \rangle = -\langle \nabla \hat{V} \rangle \quad \text{QM}$$

$$m a = -\frac{\partial V}{\partial x} \quad \text{Newton}$$

v_{group}

$$m \frac{d\langle \hat{x} \rangle}{dt} = -\langle \nabla \hat{V} \rangle$$

Wave packet's group velocity satisfies Newtonian mechanics

(7) Correlation function

Fourier convolution theorem

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} f(t)g(t)\, e^{-i\omega t}\, dt$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} f(\omega')\, e^{i\omega' t}\, d\omega'\right)\left(\int_{-\infty}^{\infty} g(\omega'')\, e^{i\omega'' t}\, d\omega''\right) e^{-i\omega t}\, dt$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(\omega')\, g(\omega'')\, \underbrace{\int_{-\infty}^{+\infty} e^{-i(\omega-\omega'-\omega'')t}\, dt}_{2\pi\,\delta(\omega-\omega'-\omega'')}\, d\omega'\, d\omega''$$

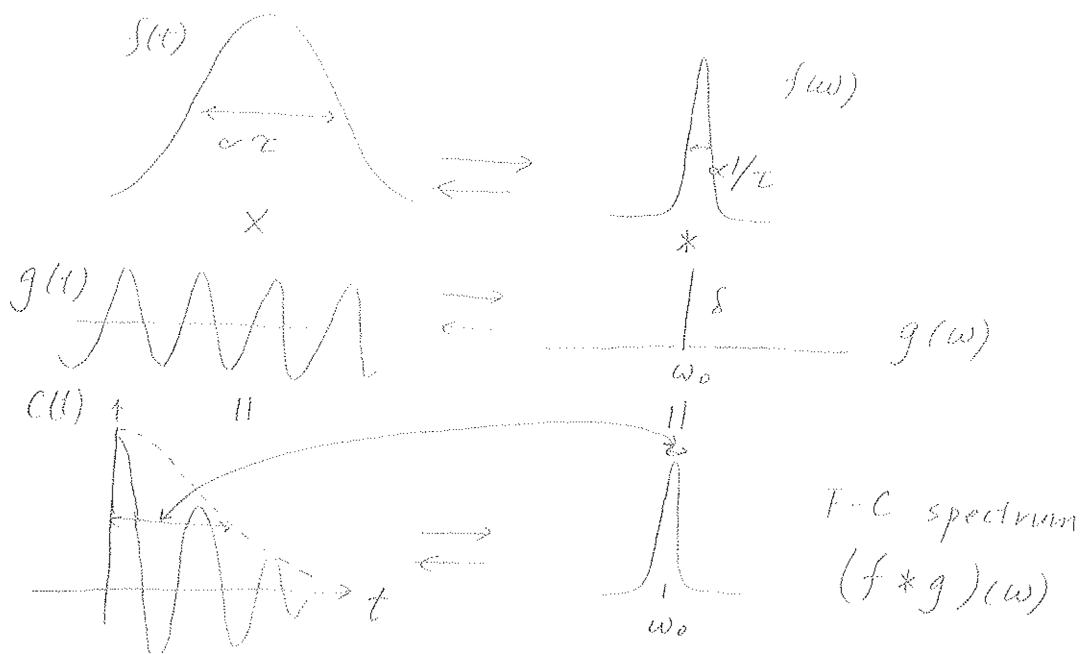
$$= \int_{-\infty}^{+\infty} f(\omega')\, g(\omega-\omega')\, d\omega'$$

$$\equiv (f * g)(\omega) \quad \text{convolution}$$

$$f(t) \underset{\longleftarrow}{\xrightarrow{FT}} f(\omega)$$

$$g(t) \underset{\longleftarrow}{\xrightarrow{FT}} g(\omega)$$

$$f(t)g(t) \underset{\longleftarrow}{\xrightarrow{FT}} (f * g)(\omega)$$



$$* \int_{-\infty}^{+\infty} \delta(\omega-\omega_0)\, e^{i\omega t}\, d\omega = e^{i\omega_0 t}$$

(8) Evolution operator

$$\hat{H}\psi = i\frac{\partial}{\partial t}\psi \qquad \frac{\partial}{\partial t}\psi = \frac{\hat{H}}{i}\psi = -i\hat{H}\psi$$

$$\frac{\partial^2}{\partial t^2}\psi = (-i\hat{H})^2\psi$$

$$\frac{\partial^3}{\partial t^3}\psi = (-i\hat{H})^3\psi$$

$$\vdots$$

Taylor series

$$\psi(t+\Delta t) = \psi(t) + \frac{\partial\psi}{\partial t}\Delta t + \frac{1}{2!}\left(\frac{\partial^2\psi}{\partial t^2}\right)\Delta t^2 + \frac{1}{3!}\left(\frac{\partial^3\psi}{\partial t^3}\right)\Delta t^3 +$$

$$= \psi(t) + (-i\hat{H})\psi\Delta t + \frac{1}{2!}(-i\hat{H})^2\psi\Delta t^2 + \frac{1}{3!}(-i\hat{H})^3\psi\Delta t^3 + \cdots$$

$$= e^{-i\hat{H}\Delta t}\psi(t)$$

$$\psi(t) = \underbrace{e^{-i\hat{H}t}}_{\text{evolution operator}}\psi(0)$$

Alternatively

$$\hat{H}\psi = i\frac{\partial\psi}{\partial t} \longrightarrow \frac{\partial\psi}{\psi} = -i\hat{H}\,dt \longrightarrow \int_{\psi(0)}^{\psi(t)}\frac{\partial\psi}{\psi} = \int_0^t -i\hat{H}\,dt$$

$$\left[\ln\psi\right]_{\psi(0)}^{\psi(t)} = -i\hat{H}t$$

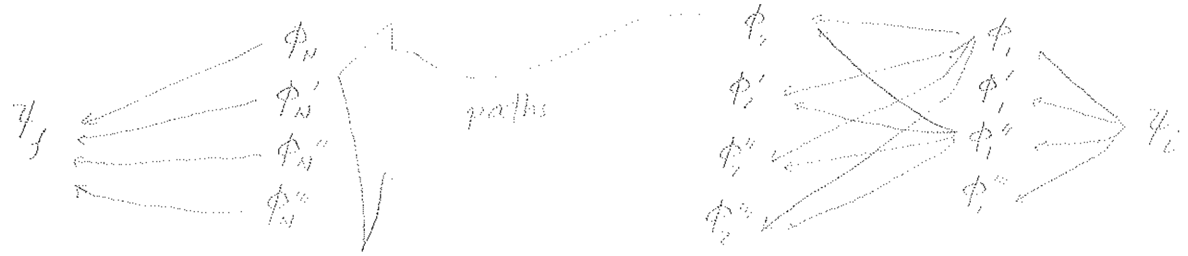
$$\frac{\psi(t)}{\psi(0)} = e^{-i\hat{H}t}$$

$$\psi(t) = e^{-i\hat{H}t}\psi(0)$$

⑨ Path integral

$Z = \langle \psi_f | e^{-i\hat{H}t} | \psi_i \rangle \qquad |Z|^2 \propto$ probability of $\psi_i \to \psi_f$ in time t

$$= \sum_{\text{path}} \langle \psi_f | e^{-i\hat{H}\Delta t} | \phi_N \rangle \langle \phi_N | e^{-i\hat{H}\Delta t} | \phi_{N-1} \rangle \cdots \langle \phi_2 | e^{-i\hat{H}\Delta t} | \phi_1 \rangle \langle \phi_1 | e^{-i\hat{H}\Delta t} | \psi_i \rangle$$



When $|\psi_i\rangle, |\psi_f\rangle, |\phi_n\rangle$ are positions in space,

$$Z = \langle x_f | e^{-i\hat{H}t} | x_i \rangle$$

$$= \int dx_1 dx_2 \cdots dx_N \langle x_f | e^{-i\hat{H}\Delta t} | x_N \rangle \langle x_N | e^{-i\hat{H}\Delta t} | x_{N-1} \rangle \cdots \langle x_1 | e^{-i\hat{H}\Delta t} | x_i \rangle$$

$$e^{-i\hat{H}\Delta t} = e^{-i(\hat{T}+\hat{V})\Delta t} \approx e^{-i\hat{T}\Delta t} \cdot e^{-i\hat{V}\Delta t}$$

Only approximate ☆
because $[\hat{T}, \hat{V}] \neq 0$
exact as $\Delta t \to 0$

$$e^{(x+y)} = 1 + (x+y) + \frac{1}{2!}(x+y)^2 + \frac{1}{3!}(x+y)^3 + \cdots$$

$$e^{x} = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots$$

$$e^{y} = 1 + y + \frac{1}{2!}y^2 + \frac{1}{3!}y^3 + \cdots$$

$$e^{x} \cdot e^{y} = 1 + x + y + \frac{1}{2!}(x^2 + \underline{2xy} + y^2) + \cdots$$

$$e^{(x+y)} = 1 + x + y + \frac{1}{2!}(x^2 + xy + \underline{yx} + y^2) + \cdots$$

$$\underbrace{e^{-i\hat{T}\Delta t}}_{\substack{\text{conveniently}\\ \text{expressed in}\\ \text{momentum}\\ \text{space}}} \cdot \underbrace{e^{-i\hat{V}\Delta t}}_{\substack{\text{conveniently}\\ \text{expressed in}\\ \text{position}\\ \text{space}}}$$

$$|k_0\rangle = \frac{e^{ik_0x}}{\sqrt{2\pi}} \quad (A)$$

$$\hat{T}|k_0\rangle = -\frac{1}{2m}\frac{\partial^2}{\partial x^2}\frac{e^{ik_0x}}{\sqrt{2\pi}} = \frac{k_0^2}{2m}|k_0\rangle$$

$$|x_0\rangle = \delta(x-x_0)$$

$$\hat{V}|x_0\rangle = V(x_0)|x_0\rangle$$

$$\langle k_1|k_0\rangle = \int_{-\infty}^{+\infty}\frac{e^{i(k_0-k_1)x}}{2\pi}dx = \frac{1}{2\pi}2\pi\delta(k_0-k_1) = \delta(k_0-k_1)$$

(orthonormality)

$$\langle x_1|x_0\rangle = \int_{-\infty}^{+\infty}\delta(x-x_1)\delta(x-x_0)\,dx = \delta(x_1-x_0)$$

(orthonormality)

$$\langle x_0|k_0\rangle = \int_{-\infty}^{+\infty}\delta(x-x_0)\frac{e^{ik_0x}}{\sqrt{2\pi}}dx = \frac{e^{ik_0x_0}}{\sqrt{2\pi}}$$

(unitary basis transformation matrix element)

(cf. $|k_0\rangle = \sum_{x_0}|x_0\rangle\langle x_0|k_0\rangle$)

$$\langle x_2|e^{-i\hat{H}\Delta t}|x_1\rangle \approx \langle x_2|e^{-i\hat{T}\Delta t}\cdot e^{-i\hat{V}\Delta t}|x_1\rangle$$

$$= \int \underbrace{\langle x_2|k\rangle}_{\frac{e^{ikx_2}}{\sqrt{2\pi}}}\underbrace{\langle k|e^{-i\hat{T}\Delta t}|k\rangle}_{e^{-i\frac{k^2}{2m}\Delta t}}\underbrace{\langle k|x_1\rangle}_{\frac{e^{-ikx_1}}{\sqrt{2\pi}}}\underbrace{\langle x_1|e^{-i\hat{V}\Delta t}|x_1\rangle}_{e^{-iV(x_1)\Delta t}}dk$$

$$\overset{(A)}{=} \int\frac{e^{ik(x_2-x_1)}}{2\pi}e^{-i\frac{k^2}{2m}\Delta t}dk\cdot e^{-iV(x_1)\Delta t}$$

$$\int_{-\infty}^{+\infty}e^{-ax^2+ibx}dx = \sqrt{\frac{\pi}{a}}\,e^{-\frac{b^2}{4a}}$$

$$a = \frac{i\Delta t}{2m},\quad b = x_2-x_1$$

$$= \frac{1}{2\pi}\sqrt{\frac{2\pi m}{i\Delta t}}\,e^{-\frac{m}{2i\Delta t}(x_2-x_1)^2}\cdot e^{-iV(x_1)\Delta t}$$

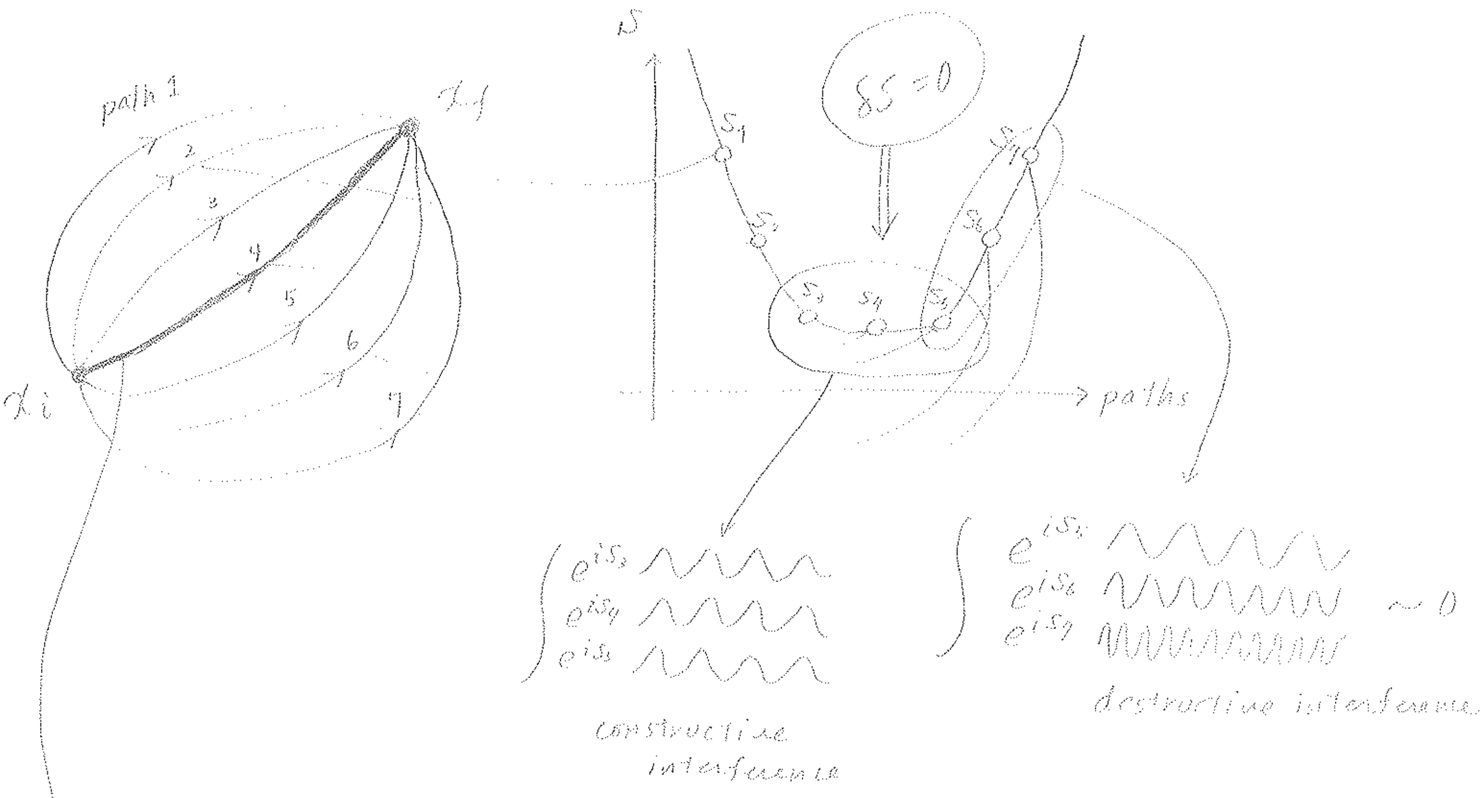
$$= \sqrt{\frac{m}{2\pi i\Delta t}}\,e^{i\underbrace{\left(\frac{1}{2}m\left(\frac{x_2-x_1}{\Delta t}\right)^2-V(x_1)\right)}_{\sim\frac{1}{2}mv^2-V\,\equiv\,L\text{ (Lagrangian)}}\Delta t}$$

$$\mathcal{K} = \langle x_f | e^{-i\hat{H}t} | x_i \rangle = \int_{path} \langle x_f | e^{-i\hat{H}\Delta t} | x_N \rangle \langle x_N | e^{-i\hat{H}\Delta t} | x_{N-1} \rangle \cdots \langle x_1 | e^{-i\hat{H}\Delta t} | x_i \rangle \, dx_N dx_{N-1} \cdots dx_1$$

$$= \int_{path} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} e^{iL_N \Delta t} \cdot e^{iL_{N-1}\Delta t} \cdots e^{iL_1 \Delta t}$$

$$= \int_{path} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} e^{i\left(\sum_k L_k \Delta t\right)} \dashrightarrow \text{Action } S = \int_{t_i}^{t_f} L \, dt$$

$$= \int_{path} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} e^{iS} \quad \text{Feynman path integral}$$



Classical path is one and $\delta S = 0$

$\delta S = 0 = \delta \int L \, dt$