07.01.2019

Hamilton - Jacobi

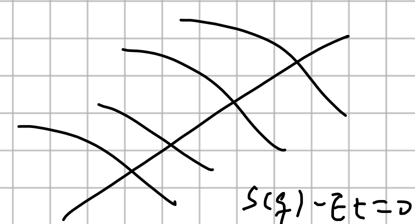
Hamilton funktion: $H(q, \frac{\partial S}{\partial q}, t) + \frac{\partial S}{\partial t} = 0$. $q = q_1, \dots, q_n$

$E = \text{const}$, $H = T + V = E$

$$S(q, t) = S(q) - Et$$

↳ defines surfaces in q

In classical mechanics, we only seeks for $S(q, t)$ with minimal action. (i.e. one particular curve)



In QM we need to consider all

Feynman path integral

Quantum System $\hat{H}(\hat{p}, \hat{x})$

Q: What is amplitude to go from (x_i, t_i) to (x_f, t_f)

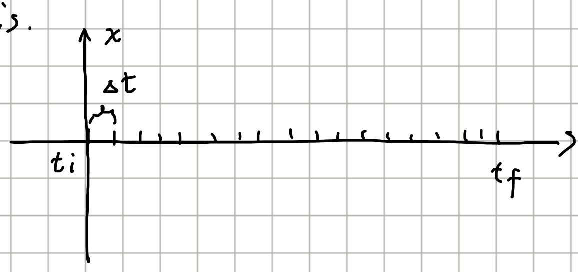
time evolution operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$

$$|\psi(t)\rangle = e^{i\hat{H}(t - t_i)/\hbar} |\psi(t_i)\rangle$$

What we really want to know:

$$\langle x_f | e^{-i\hat{H}(t - t_i)/\hbar} | x_i \rangle$$

It's a hard question in general, since $\hat{H}$ is not diagonal in an arbitary basis.



Trotter - Suzuki decomposition

$$t_k = t_i + \Delta t(k-1) \qquad\qquad \Delta t = \frac{t_f - f_i}{N}$$

$$\longrightarrow \quad t_0 = t_i \quad , \quad t_f = t_N$$

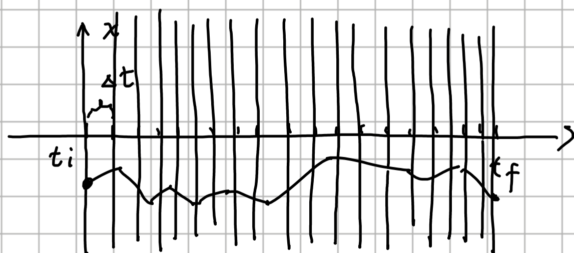
$$x_i = x_0 \quad , \quad x_f = x_N$$

Main idea : Insert $1 = \int |x_k\rangle\langle x_k| \, dx_k$

$$\langle x_f | e^{-i\hat{H}(t_f - t_i)/\hbar} | x_i \rangle = \langle x_f | \left(e^{-i\hat{H}\Delta t/\hbar}\right)^N | x_i \rangle$$

$$= \int \cdots \int \langle x_f | e^{-iH\Delta t/\hbar} | x_{N-1} \rangle \langle x_{N-1} | e^{-i\hat{H}\Delta t/\hbar} | x_{N-2} \rangle$$

$$\langle x_1 | e^{-i\hat{H}\Delta t/\hbar} | x_0 \rangle \, dx_1 \cdots dx_{N-1}$$



Integrate over all paths

Paths are not necessarily smooth.

So far everything is an exact re-writing of the original amplitude! We need an approximation to evaluate :

$$\langle x_k | e^{-i\hat{H}\Delta t/\hbar} | x_{k-1} \rangle$$

Need an approximation to $(\Delta t)^2$

Problem : $[\hat{x}, \hat{p}] \neq 0$

Solve the problem by <u>Normal Order</u>

$$: \hat{O}(\hat{p}, \hat{x}) : \quad \text{all } \hat{p}\text{'s appear only left of any } \hat{x}$$

Example:

$$: \hat{H}(\hat{p}, \hat{x}) : \; = \frac{\hat{p}^2}{2m} + V(\hat{x}) \qquad \text{already in normal order}$$

$$: e^{-iH\Delta t/\hbar} : \; = \sum_{n=0}^{\infty} \left(\frac{-i\Delta t}{\hbar}\right)^n \sum_{j=0}^{n} \frac{1}{j!\,(n-j)!} \left(\frac{\hat{p}^2}{2m}\right)^j \left(V(\hat{x})\right)^{n-j}$$

$n!$

$$e^{-i\hat{H}\Delta t/\hbar} = :e^{-iH\Delta t/\hbar}: - \frac{(\Delta t)^2}{4m\hbar^2}\left(V'' + 2iV'\hat{p}\right) + \cdots$$

$\propto (\Delta t)^2$

$\Rightarrow$

$$\langle x_k | :e^{-i\hat{H}\Delta t/\hbar}: | x_{k-1}\rangle$$

$$= \int \langle x_k | p_k\rangle \langle p_k | :e^{-i\hat{H}\Delta t/\hbar}: | x_{k-1}\rangle \, dp_k$$

$$= \int e^{ip_k(x_k - x_{k-1})} e^{-i\hat{H}(p_k, x_{k-1})\Delta t/\hbar} \, dp_k$$

using eigenvalue equation

<u>Single particle in a potential</u>

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

$$\langle x_k | e^{-i(\hat{p}^2/2m + V(\hat{x}))\Delta t/\hbar} | x_{k-1}\rangle$$

$$= \langle x_k | :e^{-i(\hat{p}^2/2m + V(\hat{x})\Delta t/\hbar)}: | x_{k-1}\rangle + \mathcal{O}(\Delta t^2)$$

$$= \int e^{ip_k(x_k - x_{k-1})\Delta t/\hbar - i\Delta t\, p^2/2m - i\Delta t\, V(x_{k-1})} \frac{dp}{2\pi\hbar} + \mathcal{O}(\Delta t^2)$$

(one-dimensional case)

The integral can be done: (three-dimensional case)

$$\langle x_k | e^{-i\hat{H}\Delta t/\hbar} | x_{k-1}\rangle$$

$$= \left(\frac{m}{2\pi i\Delta t/\hbar}\right)^{3/2} e^{\frac{i}{\hbar}\left(\frac{m}{2\Delta t}(\vec{x}_k - \vec{x}_{k-1})^2 - \Delta t\, V(\vec{x}_{k-1})\right)}$$

$\Rightarrow$ the fine answer

$$\lim_{N\to\infty} \int \cdots \int \left(\frac{m}{2\pi i\Delta t/\hbar}\right)^{3N/2} e^{i\Delta t/\hbar \sum_{k=1}^{N}\left(\frac{m}{2}\left|\frac{\vec{x}_k - \vec{x}_{k-1}}{\Delta t}\right|^2 - V(\vec{x}_{k-1})\right)}$$

Intepretation:

$$\lim_{N\to\infty} \Delta t \sum_{k=1}^{N} \frac{m}{2}\left(\frac{\vec{x}_n - \vec{x}_{n-1}}{\Delta t}\right)^2 \xrightarrow{???} \int_{t_i}^{t_f} \frac{m}{2}\left(\frac{d\vec{x}}{dt}\right)^2 dt$$

$\vec{x}(t)$ not always differentiable !!!

$$\lim_{N\to 0} \Delta t \sum_{k=1}^{N} V(\vec{x}_{k-1}) \longrightarrow \int_{t_i}^{t_f} V(\vec{x}(t))\, dt$$

$$\int_{(x_i,t_i)}^{(x_f,t_f)} (\qquad\qquad) \, \mathcal{D}[x(t)]$$

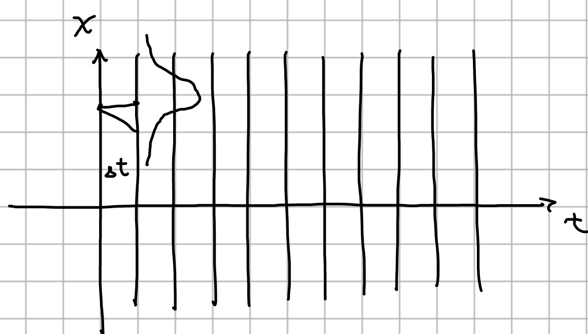
$$\Rightarrow \langle x_f | \hat{U}(t_f - t_i) | x_i \rangle = \int_{(x_i,t_i)}^{(x_f,t_f)} \exp(iS[x(t)]/\hbar)\, \mathcal{D}[x(t)]$$

Simplest case $V(x) = 0$

$$\langle x_f | \hat{U}(t_f - t_i) | x_i \rangle = \left(\frac{m}{2\pi i\hbar (t_f - t_i)}\right)^{3/2} e^{i\frac{m}{2\hbar}\frac{(x_i - x_f)^2}{t_f - t_i}}$$

solution of diffusion equation

Brownian motion:



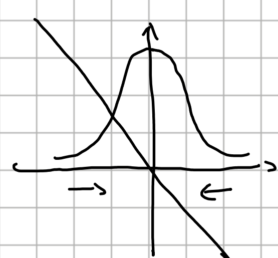
Langevian equation

$$\dot{x} = f(x) + \eta(t)$$

external field/force

random number

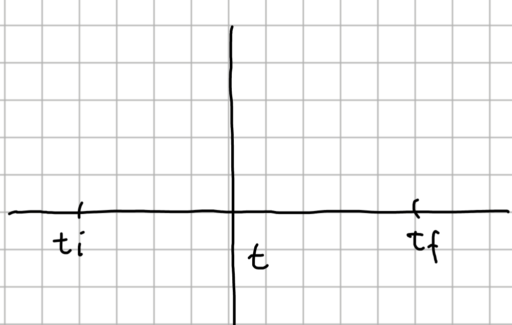
example :



Orenstein - Uhlembecken

Superposition principle:

$$S[x(t)] = \int_{t_i}^{t_f} L[x(t)]\, dt$$



$$U(x_f t_f, x_i t_i)$$
$$= \int U(x_f t_f ; x t)\, U(x t ; x_i t_i)\, dx$$

$$\int_{(x_i,t_i)}^{(x_f,t_f)} \exp\left(i/\hbar \int_{t_i}^{t_f} L[x(t)]\, dt\right) \mathcal{D}(x(t))$$

$$= \int \int_{(x_i,t_i)}^{(x_f,t_f)} \exp\left(i/\hbar \int_{t_i}^{t_f} L[x(t')]\, dt'\right) \mathcal{D}(t') \times \int_{t_i}^{t}$$

$$\int_{(x_i,t_i)}^{(x_f,t_f)} \exp\left(\tfrac{i}{\hbar}\int_{t_i}^{t_f} L[x(t)]\,dt\right) \mathcal{D}(x(t))$$

$$= \int \left\{ \int_{(x,t)}^{(x_f,t_f)} \exp\left(\tfrac{i}{\hbar}\int_{t}^{t_f} L[x(t')]\,dt'\right) \mathcal{D}(t') \times \right.$$

$$\left. \int_{(x_i,t_i)}^{(x,t)} \exp\left(\frac{i}{\hbar}\int_{t_i}^{t} L[x(t'')]\,dt''\right) \mathcal{D}[x(t'')] \right\} dx$$

09.01.2019

Weierstrass function

$$f(x) = \sum_{n=0}^{\infty} a^n \cos(b^n \pi x), \qquad b \geq 7 \text{ odd number}$$
$$0 < a < 1$$

continuous but nowhere differentiable

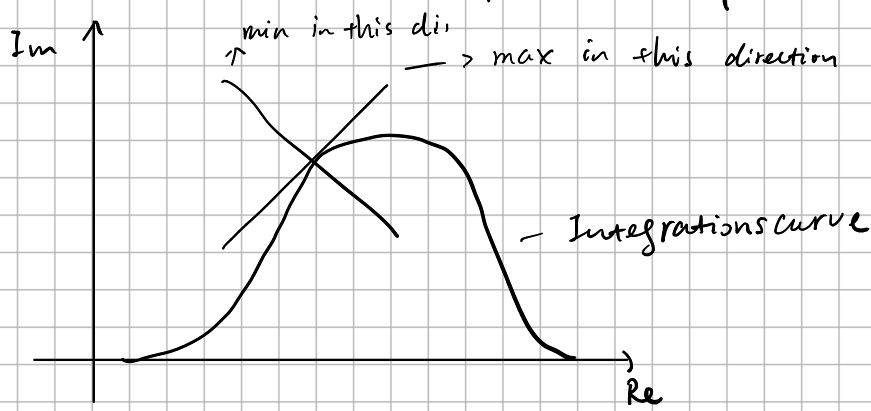
Approximation methods for path integrals

$$\int_{-\infty}^{\infty} dx\, e^{-iaf(x)} \qquad a \in \mathbb{R},\ a > 0 \text{ very large}$$

A complex function $f(z)$ cannot have maximum/minimum except at its boundaries. $\rightarrow$ only saddle point

$$f(z) = f(x+iy) = u(x,y) + i\,v(x,y). \qquad f \text{ analytic} \rightarrow \Delta u = 0$$

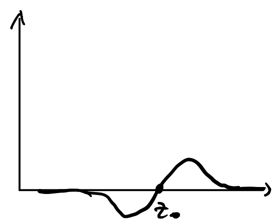
Main contribution comes from the $f(x)$ at saddle point.



in the neighborhood of saddle point ($f'(z)=0$): $z = z_0 + \rho e^{i\alpha}$, $\rho \in \mathbb{R}$, $\alpha \in \mathbb{C}$

$$f(z) = f(z_0) + \frac{1}{2} f''(z_0)\rho^2 e^{2i\alpha} + O(\rho^3)$$

$z_0 \in \mathbb{R}$ $\rightarrow$



$$\int_{-\infty}^{\infty} e^{-iaf(x)} dx = e^{-af(x_0)} \int e^{-\frac{1}{2}\alpha |f''(x_0)|\rho^2} d\rho + O(\rho^3)$$

$a = i\pi/4$ $$= e^{af(x_0)} \sqrt{2\pi / a|f''(x_0)|}$$

Stirling's formula

Hamilton principle from QM:

$$U(x_f, t_f, x_i, t_i) = \int_{(x_i, t_i)}^{(x_f, t_f)} \exp(i/\hbar\, S[x(t)])\, D[x(t)]$$

The most important parts to the time evolution operator come from paths at which the action is minimal!

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\bar{x}}} = -\partial_x V(\bar{x})$$

$\bar{x}(t)$ the path minimises the action $\hat{=}$ classical path

We expand around the classical path:

$$\eta(t) = (x(t) - \bar{x}(t))/\hbar$$

$\Rightarrow U(x_f, t_f, x_i, t_i)$

$$= e^{iS[\bar{x}(t)]/\hbar} \int_{(0,t_i)}^{(0,t_f)} \exp[i \int_{t_i}^{t_f} \{\tfrac{1}{2}\eta(t) [-m \tfrac{d^2}{dt^2} - V''(\bar{x}(t))]\eta(t)\} dt\, D[\eta(t)]$$

+ higher order in $\eta(t)$

14.01.2019

Gaussian integral:

$$\vec{x} = (x_1, \dots, x_n)^T, \qquad \vec{J} = (J_1, \dots, J_n)^T$$

$$\int \exp\Big(\underbrace{-\tfrac{1}{2}\vec{x}^T A \vec{x} + \vec{J}\cdot\vec{x}}_{= -\frac{1}{2}(\vec{x}^T A \vec{x} - 2\vec{J}\cdot\vec{x})}\Big) \frac{d^n x}{(2\pi)^{n/2}}$$

$$(\vec{x}+\vec{d})^T A (\vec{x}+\vec{d}) = \vec{x}^T A \vec{x} + \vec{x}^T A \vec{d} + \vec{d}^T A \vec{x} + \vec{d}^T A \vec{d}$$

$$\vec{x}^T A \vec{x} + (\vec{d}^T A^T)\cdot\vec{x} + (\vec{d}^T \vec{A})\cdot\vec{x} + \vec{d}^T \vec{A} \vec{d}$$

$$\Big[\quad x_i A_{ij} d_j = d_j A_{ij} x_i = d_j (A^T)_{ji} x_j = \vec{d}^T A^T \vec{x}$$

$$\vec{x}^T A \vec{x} + \underbrace{\vec{d}^T (A^T + A)}_{-2\vec{J}} \vec{x} + \vec{d}^T A \vec{d} \quad\Big]$$

For A symmetric $\quad A^T = A \quad$ and $\det A \neq 0$

$$2\vec{d}^T A = -2\vec{J} \longrightarrow \vec{d} = -A^{-1}\vec{J}$$

$$(\underbrace{\vec{x} - A^{-1}\vec{J}}_{\vec{x}'})^T A (\vec{x} - A^{-1}\vec{J}) - (A^{-1}\vec{J})^T A (A^{-1}\vec{J})$$

$$= \vec{x}^T A \vec{x} - 2\vec{J}\cdot\vec{x}$$

$$\Rightarrow \int \exp\Big(-\tfrac{1}{2}\vec{x}^T A \vec{x} + \vec{J}\,\vec{x}\Big) \frac{d^n x}{(2\pi)^{n/2}}$$

$$= \exp\Big(\tfrac{1}{2}\vec{J}^T A^{-1}\vec{J}\Big) \int \exp\Big(-\tfrac{1}{2}(x - A^{-1}\vec{J})^T A (x - A^{-1}\vec{J})\Big) \frac{d^n x}{(2\pi)^{n/2}}$$

$$= \exp\Big(\tfrac{1}{2}\vec{J}^T A^{-1}\vec{J}\Big) \int \exp\Big(-\tfrac{1}{2}\vec{x}^T A \vec{x}\Big) \frac{d^n x}{(2\pi)^{n/2}}$$

Linear transformation: $\quad U A U^{-1} = \Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$, $\det(U) = 1$

$$\vec{y} = U^{-1} \vec{x}, \quad \det(\mathrm{Jac}) = 1$$

$$\Rightarrow \quad I = \int \exp(-\tfrac{1}{2} \vec{x}^T U U^{-1} A U U^{-1} \vec{x}) \frac{d^n x}{(2\pi)^{n/2}}$$

$$= \int \exp(-\tfrac{1}{2}(\lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots \lambda_n y_n^2)) \frac{dy_1 \cdots dy_n}{(2\pi)^{n/2}}$$

$$= \prod_{j=1}^{n} \lambda_j^{-\frac{1}{2}} = \frac{1}{\sqrt{\det(A)}}$$

(A positiv definite, $\lambda_i > 0, \ \forall i$)

$$\Rightarrow \quad \int \exp(-\tfrac{1}{2} \vec{x}^T A \vec{x} + \vec{J} \cdot \vec{x}) = \frac{\exp(\frac{1}{2} \vec{J}^T A^{-1} \vec{J})}{\sqrt{\det(A)}}$$

Complex case:

$$\int \exp(-z^* a z) \frac{dz\, dz^*}{2\pi i} = \int e^{-a(x^2+y^2)} \frac{dx\, dy}{\pi}$$

$$= \frac{1}{\pi} \int_0^\infty \int_0^{2\pi} e^{-ar^2} d\varphi\, dr = \frac{1}{a}$$

$$\int \exp(-\vec{z}^+ H \vec{z} + \vec{J}^+ \vec{z} + \vec{J} \vec{z}^+) \prod_{k=1}^{\infty} \left(\frac{dz_k^* dz_k}{2\pi i} \right)$$

$$= (\det H)^{-1} e^{\vec{J}^+ H^{-1} \vec{J}}$$

Grassmann case:

$$\int \exp(-\vec{\eta}^+ H \vec{\eta} + \vec{\xi}^+ \vec{\eta} + \vec{\xi} \vec{\eta}^+) \prod_{j=1}^{n} d\eta_j^* d\eta_j$$

$$\left[\iint d\xi^* d\xi \ e^{-\xi^* a \xi} = \iint d\xi^* d\xi (1 - \xi^* a \xi) = a \right]$$

$$= (\det H)\, e^{\vec{\xi}^+ H \vec{\xi}}$$

Path integral of harmonic oszillation

The action of the HOZ is a quadratic form:

$$\frac{1}{\hbar}\int_{(x_i,\,t_i)}^{(x_f,\,t_f)} \mathcal{L}[x(t)]\,dt$$

$$= \text{"}\lim_{N\to\infty}\text{"} \frac{i}{\hbar} \underbrace{\frac{t_f - t_i}{N}}_{\Delta t} \sum_{k=1}^{N} \left\{ \frac{m}{2}\left(\frac{x_k - x_{k-1}}{\Delta t}\right)^2 - \frac{m}{2}\omega^2 x_{k-1}^2 \right\}$$

$T = t_f - t_i$

$$= \text{"}\lim_{N\to\infty}\text{"} \frac{mi}{\hbar\Delta t} \sum_{k=1}^{N} \left\{ \frac{1}{2}(x_k - x_{k-1})^2 - \frac{1}{2}\underbrace{(\omega\Delta t)}_{=:a}{}^2 x_{k-1}^2 \right\}$$

$$= \text{"}\lim_{N\to\infty}\text{"} \left(\frac{mi}{\hbar\Delta t} \frac{1}{2} \vec{x}^T A \vec{x} \right)$$

$$A = \begin{pmatrix} 1-a^2 & -1 & & & \\ -1 & 2-a^2 & -1 & & 0 \\ & -1 & \ddots & \ddots & \\ & & \ddots & \ddots & \\ 0 & & & 2-a^2 & -1 \\ & & & -1 & 1 \end{pmatrix}$$

$0 \; - - - - \; N$

$x_0 = x_i\,, \quad x_N = x_f$

For example: $N = 5$

$$\frac{1}{2}(x_0 - x_1)^2 + \frac{1}{2}(x_1 - x_2)^2 + \dots + \frac{1}{2}(x_5 - x_4)^2 - \frac{1}{2}a^2 x_0^2 - \frac{1}{2}a^2 x_1^2 \dots - \frac{1}{2}a^2 x_4^2$$

$$= \frac{1}{2}(x_0^2 + 2x_1^2 + \dots + 2x_4^2 + x_5^2 - \underbrace{2x_0 x_1}_{x_0x_1 + x_1x_0} - 2x_1x_2 \dots - 2x_4 x_5) - \frac{1}{2}a^2 x_0^2 \dots - \frac{1}{2}a^2 x_4^2$$

$$= \frac{1}{2}\underset{i}{x_0^2} + \frac{1}{2}\underset{f}{x_5^2} + x_1^2 + x_2^2 + \dots x_4^2 - x_1x_2 \dots - x_3x_4$$

$$- x_0x_1 - x_4x_5 - \frac{1}{2}a^2x_0^2 \quad - \frac{1}{2}a^2 x_1^2 - \frac{1}{2}a^2 x_2^2 \dots - \frac{1}{2}a^2 x_4^2$$

$$\hookrightarrow \qquad \underbrace{\qquad\qquad\qquad}_{\text{Integrate } x_1, \ldots x_4}$$

$$2 \begin{pmatrix} x_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ x_5 \end{pmatrix}$$

$$\vec{J}$$

We need the determinant of

$$B = \begin{bmatrix} 2-a^2 & -1 & & 0 \\ -1 & 2-a^2 & \ddots & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 2-a^2 \end{bmatrix}$$

$$1 \qquad\qquad\qquad N-1$$

$$\det(B) = d_{N-1}, \quad \underset{\substack{\uparrow \\ \text{Laplace}}}{d_k =} (2-a^2)\, d_{k-1} + \det \begin{bmatrix} -1 & 0 & \cdots & \\ -1 & 2-a^2 & -1 & \\ & -1 & \ddots & -1 \\ & & -1 & 2-a^2 \end{bmatrix}$$

$$d_k = (2-a^2)\, d_{k-1} - d_{k-2}$$

$$\rightarrow d_{k+1} - (2-a^2)\, d_k + d_{k-1} = 0$$

Ansatz: $\quad d_k = \lambda^k$

Plug in the Ansatz: $\quad \lambda^{k+1} - (2-a^2)\lambda^k + \lambda^{k-1} = 0$

$$\hookrightarrow \quad \lambda^2 - (2-a^2)\lambda + 1 = 0 \quad \rightarrow \lambda = \lambda_1, \lambda_2$$

general solution of the recursion: $\quad d_k = c_1 \lambda_1^k + c_2 \lambda_2^k$

$$d_1 = 2-a^2, \quad d_2 = (2-a^2)^2 - 1, \quad \lambda_{1,2} = 1 - \tfrac{1}{2}a^2 \pm \tfrac{1}{2} i a \sqrt{4-a^2}$$

$$= 1 \pm ia + O(a^2)$$

$$\rightarrow \lim_{N\to\infty} \left(1 \pm \frac{i\omega T}{N}\right)^N = e^{\pm i\omega T}$$

$$d_k = i \frac{2-a^2 - ia\sqrt{4-a^2}}{2a\sqrt{4-a^2}} \lambda_1^k - i \frac{2-a^2+ia\sqrt{4-a^2}}{2a\sqrt{4-a^2}} \lambda_2^k$$

classical path

$$\bar{x}(t) = A\cos(\omega t) + B\sin(\omega t)$$

$$\left.\begin{aligned} x(t_i) &= A\cos(\omega t_i) + B\sin(\omega t_i) \\ x(t_f) &= \quad - \quad - \quad - \end{aligned}\right\} \longrightarrow A, B$$

$$\Rightarrow A = \frac{x_i \sin(\omega t_f) - x_f \sin(\omega t_i)}{\sin(\omega T)}$$

$$B = \frac{x_f \cos(\omega t_i) - x_i \cos(\omega t_f)}{\sin(\omega t)}$$

$$\eta(t) = \sum_{k=1}^{\infty} a_n \sin\left(\frac{\pi}{T} k t\right)$$ integration over an

16.04.2019

Born Series: (Dyson series) (three pictures of QM!)

$$\hat{U}(t, t_0) = \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{i}{\hbar}\right)^k \int_{t_0}^{t} \cdots \int_{t_0}^{t} \hat{T} \hat{H}_1(t_1)\hat{H}_1(t_2)\cdots\hat{H}_1(t_k)\, dt_1 \cdots dt_k$$

$$= \hat{T} \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t} \hat{H}_1(t)\, dt\right)$$

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad (\text{in general } [\hat{H}_0, \hat{H}_1] \neq 0)$$

$$\hat{O}_S \longrightarrow e^{iH_0 t} \hat{O} e^{-i\hat{H}_0 t}$$ (interaction pic.)

$$\langle x_f | \hat{T} \hat{A}(t_1) \hat{B}(t_2) \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}_1(t)\, dt\right) | x_i \rangle$$

Heisenberg evolution here, two general operator, e.g. creation/annilation

$$= \langle x_f | \hat{T} e^{-i/\hbar \int_{t_1}^{t_f} \hat{H}(t) dt} \hat{A}\, e^{-i/\hbar \int_{t_2}^{t_1} \hat{H}(t) dt} \hat{B} e^{-i/\hbar \int_{t_i}^{t_1} \hat{H}(t) dt} | x_i \rangle$$

$$= \lim_{N \to 0} \int \cdots \int \langle x_f | e^{-i/\hbar \hat{H} \Delta t} \cdots | x_m \rangle \langle x_m | \hat{A} | x_{m-1} \rangle \langle x_{m-1} | e^{-i/\hbar \hat{H} \Delta t} | x_{m-2} \rangle$$

$$\dots \langle x_n|\hat{B}|x_{n-1}\rangle\langle x_{n-1}|e^{-i/\hbar \hat{H}\Delta t}|x_{n-2}\rangle \dots |x_i\rangle$$

$$= \int_{(x_i,t_i)}^{(x_f,t_f)} \underbrace{A(x(t_1))}_{\substack{\langle x_m|\hat{A}|x_{m-1}\rangle \\ \text{matrix element}}} B(x(t_2)) \exp\left(-\frac{i}{\hbar}\int_{t_i}^{t_f} \mathcal{L}(x(t))\, dt\right) \mathcal{D}[x(t)]$$

Path integral in Hamiltonian form:

$$\langle x_k| :e^{-i/\hbar \hat{H}\Delta t}: |x_{k-1}\rangle$$

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

$p\cdot\dot{x}$, Legendre Trafo!

$$U(x_f, t_f; x_i, t_i) = \int \exp\left(i/\hbar \int_{t_i}^{t_f} \left(p(t)\frac{dx}{dt}(t) - H(x(t), p(t)\right) dt\right) \mathcal{D}[x(t)]\mathcal{D}[p(t)]$$

21.01.2019

Linear response and Green's function

small perturbation, only linear term

System described by a Hamiltonian $\hat{H}$

perturbation:

$$e\hat{\rho}(\vec{r})\phi(\vec{r},t), \qquad \hat{\rho}(\vec{r}) = \sum_{a\in\{\uparrow,\downarrow\}} \hat{\psi}_a^+(\hat{r})\hat{\psi}_a(\hat{r})$$

$$\frac{e}{c}\vec{j}(\vec{r})\cdot\vec{A}(\vec{r},t), \qquad \vec{j}(\vec{r}) = \frac{\hbar}{2mi}\sum_\alpha \left(\hat{\psi}_\alpha^+(\vec{r})\vec{\nabla}\hat{\psi}_\alpha(\vec{r}) - \hat{\psi}_\alpha(\vec{r})\vec{\nabla}\hat{\psi}_\alpha^+(\vec{r})\right)$$

Time evolution:

$$|\psi(t)\rangle = \hat{U}(t,t_i)|\psi(t_i)\rangle$$

Interaction picture:

$$\hat{U}_I(t,t_i) = \mathbb{1} - \frac{i}{\hbar}\int_{t_i}^{t_f} \hat{H}_I(t')\hat{U}_I(t',t_i)\,dt'$$

$\hat{H}_{1,I}$

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \qquad \hat{O}_I(t) = e^{i\hat{H}_0 t/\hbar}\,\hat{O}\,e^{-i\hat{H}_0 t/\hbar}$$

$$|\psi(t_f)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t_f}\,\hat{U}_I(t_f,t_i)\,|\psi(t_i)\rangle$$

Plug in the first two terms of $\hat{U}_I$

$$\langle\psi(t_f)|\hat{A}(t_f)|\psi(t_f)\rangle$$

$$= \langle\psi(t_i)|\left(\mathbb{1}+\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{H}_I(t')dt'\right)e^{\frac{i}{\hbar}\hat{H}_0 t_f}\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}_0 t_f}\cdot$$

$$\cdot\left(1-\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{H}_I(t')dt'\right)|\psi(t_i)\rangle$$

$$= \langle\hat{A}(t_f)\rangle + \frac{i}{\hbar}\int_{t_i}^{t_f}\langle\psi(t_i)|[\hat{H}_I(t'),\hat{A}_I(t_f)]|\psi(t_i)\rangle dt'$$

$$+\,\mathcal{O}(H_I^2)$$

$t_i = 0$, $t_f = t$, $\hat{H}_I \longrightarrow \hat{B}$

$$\Rightarrow \quad \delta\langle\hat{B}(t)\rangle = \frac{i}{\hbar}\int_0^t\langle[\hat{B}(t'),\hat{A}(t)]\rangle dt'$$

$\hat{A}$

ground state expectation value

Define Green's function:

$$G_{AB}(t,t') = -i\,\Theta(t-t')\langle[\hat{A}(t),\hat{B}(t')]\rangle$$

Examples:

with α,β: spin

$$G^R_{\alpha\beta}(\vec{r},t;\vec{r}',t') = -i\Theta(t-t')\langle[\hat{\psi}_\alpha(\vec{r},t),\hat{\psi}^+_\beta(\vec{r}',t')]\rangle$$

single particle Green's function

take out one particle

put in a particle

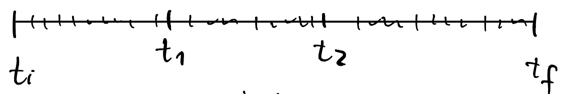
current-current-correlation $\quad -i\,\Theta(t-t')\langle[\hat{\vec{J}}(r,t),\hat{\vec{J}}(r',t)]\rangle$

density-density-correlation $\quad -i\,\Theta(t-t')\langle[\hat{\rho}(r,t),\hat{\rho}(\vec{r}',t')]\rangle$

physical!, $\rightarrow$ causality

with time ordering $\hat{T} \longrightarrow$ two Θ, with reverse sign

$$\langle x_f | \hat{T} \hat{A}(t_1) \hat{B}(t_2) \exp\left(-\frac{i}{\hbar}\int_{t_i}^{t_f} \hat{H}(t)\,dt\right) | x_i \rangle$$



$$= \langle x_f | e^{-\frac{i}{\hbar}\hat{H}\underbrace{(t_N - t_{N-1})}_{\Delta t}} e^{-\frac{i}{\hbar}\hat{H}(t_{N-1}-t_{N-2})} \cdots e^{-\frac{i}{\hbar}\hat{H}(t_2+\Delta t - t_2)} e^{\frac{i}{\hbar}\hat{H}t_2}$$

$$\hat{B} e^{-\frac{i}{\hbar}\hat{H}t_2/\hbar} e^{-\frac{i}{\hbar}\hat{H}(t_2-(t_2-\Delta t))} \cdots e^{-\frac{i}{\hbar}\hat{H}(t_1+\Delta t - t_1)} e^{\frac{i}{\hbar}\hat{H}t_1} \hat{A}$$

$$e^{-\frac{i}{\hbar}\hat{H}t_1} e^{-\frac{i}{\hbar}\hat{H}(t_1-(t_1-\Delta t))} \cdots e^{-\frac{i}{\hbar}\hat{H}(t_1+\Delta t - t_i)} | x_i \rangle$$

$$\vdots$$

$$= \int_{(x_i,t_i)}^{(x_f,t_f)} A(x(t_1))\, B(x(t_2)) \exp\left(-\frac{i}{\hbar} S[x(t)]\right) \mathcal{D}[x(t)]$$

<u>Coherent states path integral</u>

$$\hat{U}(\phi_f, t_f; \phi_i, t_i) := \langle \phi_f | \hat{U}(t_f, t_i) | \phi_i \rangle$$

$$\lim_{N\to\infty} \langle \phi_f | (e^{-i/\hbar \hat{H}\Delta t})^N | \phi_i \rangle$$

$$= \lim_{N\to\infty} \int e^{-\sum_{k=1}^{N-1} \phi^*_{\alpha k}\phi_{\alpha k}} \langle \phi_f | : e^{-\frac{i}{\hbar}\hat{H}\Delta t} : | \phi_{N-1}\rangle \langle \phi_{N-1} | \ldots : e^{-\frac{i}{\hbar}\hat{H}\Delta t} : | \phi_i \rangle$$

$$\cdot \prod_{k=1}^{N-1} d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}$$

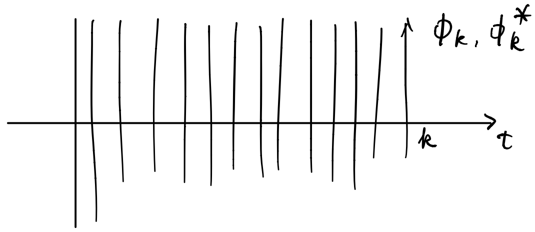
$$\langle \phi_k | : \exp(-\frac{i}{\hbar}\hat{H}\Delta t) : | \phi_{k-1} \rangle = \langle \phi | \exp(-\frac{i}{\hbar}\hat{H}(\hat{\phi}^*_k, \hat{\phi}_{k-1})\Delta t) | \phi_{k-1} \rangle$$

numbers now!

$$= \exp(-\frac{i}{\hbar} H(\phi^*_k, \phi_{k-1})\Delta t) \langle \phi_k | \phi_{k-1} \rangle$$

$$= \exp(-\frac{i}{\hbar} H(\phi^*_k, \phi_{k-1})\Delta t) \exp(\sum_\alpha \phi^*_{\alpha k}\phi_{\alpha, k-1})$$

$\hat{H} = \sum_p \epsilon_p b_p^\dagger b_p$, $\quad \epsilon_p = p^2/2m \qquad \langle \phi_k | b_p^\dagger$ replaced by eigenvalue



$k=1 \qquad \phi_{\alpha 1} - \phi_{\alpha,0}$

$k=2 \qquad \phi_{\alpha 2} - \phi_{\alpha,1}$

$U(\phi_f, t_f ; \phi_i, t_i)$

$$= \lim_{N\to\infty} \int \exp\Big(-\sum_\alpha \Big(\sum_{k=1}^{N-1} \phi^*_{\alpha k}\, \phi_{\alpha,k-1} + \frac{i}{\hbar} \hat{H}(\phi^*_k, \phi_{k-1})\Delta t\Big) + \sum_\alpha \phi^*_{\alpha N}\, \phi_{\alpha N}\Big)$$

$$\prod_{k=1}^{N-1} d\phi^*_{\alpha k}\, d\phi_{\alpha k}$$

$$= \lim_{N\to\infty} \int \exp\Big(\sum_\alpha \phi^*_{\alpha N}\, \phi_{\alpha N} - \sum_{k=1}^{N-1} \Big(\sum_\alpha \phi^*_{\alpha k} \frac{\phi_{\alpha k} - \phi_{\alpha k-1}}{\Delta t}$$

$$+ \frac{i}{\hbar} H(\phi^*_{\alpha k}, \phi_{\alpha k-1})\Big) \Delta t\Big) \prod_{k=1}^{N-1} d\phi^*_{\alpha k}\, d\phi_{\alpha k}$$

$$= \int_{(\phi_t, \phi_t)}^{(\phi_f, \phi_f)} \exp\Big(\sum_\alpha \phi^*_\alpha(t_f)\, \phi_\alpha(t_f) + \frac{i}{\hbar} \int_{t_i}^{t_f} \Big(\sum_\alpha (i\hbar\, \phi^*_\alpha(t) \partial_t \phi_\alpha(t))$$

$$+ H(\phi^*(t), \phi(t))\Big) \mathcal{D}[\phi^*(t), \phi(t)]$$

Functional derivatives

vector space of functions

$$f(x) = \sum_k f(\Delta x \cdot k)\, \delta(x - \Delta x \cdot k)$$

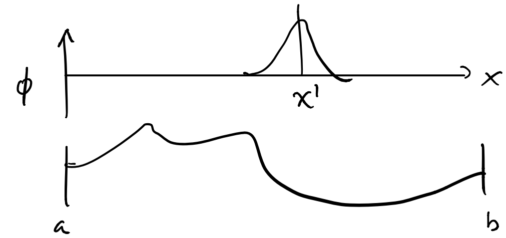
$$f(x) = \int_{-\infty}^{\infty} e^{ikx}\, \check{f}(k)\, dk$$

$$\| f - g \| = \int_a^b (f(x) - g(x))^2 dx \quad , \quad f, g \in L_2$$

$$F[\phi] = \int \phi^2(x)\, dx$$

$$\left[\frac{\delta F[\phi]}{\delta \phi(x')} = 2\phi(x') \right]$$

x' is a particular x



$$\frac{\delta F[\phi]}{\delta \phi(x')} = \lim_{\varepsilon \to 0} \frac{\int (\phi(x) + \varepsilon \delta(x-x'))^2 dx - \int \phi^2(x) dx}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} \frac{\int (2\varepsilon\, \delta(x-x')\phi(x) + \varepsilon^2 \delta(x-x')^2)\, dx}{\varepsilon}$$

Do this by using representation of delta function

$$\delta_\eta(x) = \frac{1}{\pi} \frac{1}{x^2+\eta^2}$$

interchange of limits is not permitted

$$G[\phi] = \int \phi'^2(x) dx \qquad \phi \in C^2$$

$$\frac{\delta G[\phi]}{\delta \phi(x')} = \lim_{\eta \to 0} \lim_{\varepsilon \to 0} \frac{\int [(\phi'(x) + \varepsilon \frac{d}{dx} \delta_\eta(x-x'))^2 - \phi'(x)^2]\, dx}{\varepsilon}$$

$$= \lim_{\eta \to 0} \lim_{\varepsilon \to 0} \int (2\phi'(x)\delta_\eta'(x-x')\, dx + O(\varepsilon))\, dx = -2\phi''(x')$$

23.01.2019

Path integral with interaction

$\langle f | i \rangle$

$$= C \int \exp \frac{i}{\hbar} \int_{t_i}^{t_f} \left(\sum_\alpha i\hbar\, \phi_\alpha^*(t)\, \partial_t \phi_\alpha(t) - H(\phi^*(t), \phi(t))\right) D[\phi^*(t), \phi(t)]$$

$$C = \exp\left(\sum_\alpha \phi_\alpha^*(t)\, \phi_\alpha(t)\right)$$

$\hat{H} = \hat{H}(\hat{a}^+, \hat{a})$ ← can be $\hat{a}_k$, $\hat{a}_\sigma$, ...

Kinetic Energy: $\hat{T}(\hat{a}_k^+, \hat{a}_k) = \sum_k \epsilon_k a_k^+ a_k$ e.g. ϵ_k single particle energy

k = wave number; in general quantum numbers of particle

Interaction term: $V(a^+, a) = \sum_{k_1 k_2 k_3 k_4} V_{k_1 k_2 k_3 k_4}\, \hat{a}_{k_4}^+ \hat{a}_{k_3}^+ a_{k_2} a_{k_1}$

with constraints, e.g. energy conservation $\epsilon_{k_1} + \epsilon_{k_2} = \epsilon_{k_3} + \epsilon_{k_4}$

momentum conservation $p_1 + p_2 = p_3 + p_4$

translate to coherent states $\quad \sum V_{1234}\, \phi_1^* \phi_2^* \phi_3 \phi_4$

$$\langle f|i\rangle = \frac{\int \exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f} \sum_\alpha \left(i\hbar\, \phi_\alpha^*(t)\,\partial_t \phi_\alpha(t) - T(\phi^*(t),\phi(t)\right) dt\right) \times \exp\left(-\frac{i}{\hbar}\int_{t_i}^{t_f} V(\phi^*(t),\phi(t))\,dt\right) \mathcal{D}[\phi^*(t),\phi(t)]\, \langle f|i\rangle_0}{\underbrace{\int \exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f} \sum_\alpha \left(\phi_\alpha^*(t)\partial_t \phi_\alpha(t) - T(\phi^*(t),\phi(t)\right)\right)}_{\langle f|i\rangle_0}\mathcal{D}[\phi^*(t),\phi(t)]}$$

as a normalization

as a distribution

$$= \langle \exp\left(-\frac{i}{\hbar}\int_{t_i}^{t_f} V(\phi^*(t),\phi(t))\,dt\right) \rangle \, \langle f|i\rangle_0$$

[equivalent to $\quad \langle w^2\rangle = \dfrac{\int f(w)\, w^2\, dw}{\int f(w)\, dw}$ $\leftarrow$ (in case) $f(w)$ is not normalized

$\langle f|i\rangle_0 = \cdots$ without V term, ground states / free particle]

$$\langle \quad \rangle = \langle \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int\cdots\int_{[t_i,t_f]^n} V(\phi^*(t),\phi(t))\, V(\phi^*(t),\phi(t)) \ldots dt_1 \ldots dt_n \rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int\cdots\int_{[t_i,t_f]^n} \langle V(\phi^*(t_1)\phi(t_1))\, V(\phi^*(t_2)\phi(t_2)) \cdots V(\phi^*(t_n)\phi(t_n)) \rangle$$

[$$\int_0^\infty e^{-x^2} x^n\, dx = \lim_{t\to 0} \frac{d^n}{dt^n}\int_0^\infty e^{-x^2+tx}\, dx$$

using generating function $\sum_{n=0}^{\infty} a_n t^n$ for the integrals]

↳ reduce the expression to generating functions and use gaussian integrals

28.01.2019

Wick theorem, Green's function and Feynman-diagrams

$$\langle \exp(-\tfrac{i}{\hbar}\int_{t_i}^{t_f} V(\phi^*(t)\,\phi(t)\,dt)\rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \underset{[t_i,t_f]^n}{\int\cdots\int} \langle V(\phi^*(t_1)\phi(t_1)\ldots V(\phi^*(t_n)\,\phi(t_n)\rangle\, dt_1\ldots dt_n$$

$$\langle A\rangle = \frac{\int A\exp(\frac{i}{\hbar}\sum_\alpha (i\hbar\,\phi_\alpha^*(t)\partial_t\phi_\alpha(t) - T(\phi^*(t)\phi(t)))\,\mathcal{D}[\phi^*(t)\,\phi(t)]}{\int \exp(\frac{i}{\hbar}\ \cdots\ )\,\mathcal{D}[\phi^*(t)\,\phi(t)]}$$

not trivial

$$\boxed{\begin{aligned}&\frac{\int \phi_{i_1}\cdots\phi_{i_n}\phi^*_{j_n}\cdots\phi^*_{j_1}\exp(-\sum_{ij}\phi_i^*A_{ij}\phi_j)\,\mathcal{D}[\phi^*\phi]}{\int\exp(-\sum_{ij}\phi^*_i A_{ij}\phi_j)\,\mathcal{D}[\phi^*\phi]}\\ &= \varsigma^P\,(A^{-1})_{i_{P(n)}j_n}(A^{-1})_{i_{P(n-1)}j_{n-1}}\cdots(A^{-1})_{i_{P(1)}j_1}\\ &\text{zeta} \longrightarrow \varsigma = \begin{cases}-1 & \text{fermions}\\ +1 & \text{Bosons}\end{cases}\end{aligned}}$$

Derivation using generating functional:

$$Z(J,J^*) = \frac{\int\exp(-\sum_{ij}\phi_i^*A_{ij}\phi_j + \sum_i(J_i^*\phi_i + J_i\phi_i^*))\,\mathcal{D}[\phi^*\phi]}{\int\exp(-\sum_{ij}\phi_i^*A_{ij}\phi_j)\,\mathcal{D}[\phi^*\phi]}$$

$$\frac{1}{(2\pi i)^n}\int\cdots\int\exp(-\sum_{ij}\phi_i^*A_{ij}\phi_j + \sum_i(J_i^*\phi_i + J_i\phi_i^*))\prod_i d\phi_j^*d\phi_i$$

$$= C\,(\det(A))^{-\varsigma}\exp(\sum_{ij}J_i^*(A^{-1})_{ij}J_j)$$

$$\boxed{Z(J, J^*) = \exp\left(\sum_{ij} J_i^* (A^{-1})_{ij} J_j\right)}$$

J : functional of time

$$\frac{\delta^2 Z(J, J^*)}{\delta J_{i_1}^* \, \delta J_{j_1}} = (A^{-1})_{ij} \exp\left(\sum_{ij} J_i^* (A^{-1})_{ij} J_j\right)$$

$$+ \sum_{\ell} (A^{-1})_{i,\ell} J_i \sum_k J_k^* (A^{-1})_{kj} \exp\left(\sum_{ij} J_i^* (A^{-1}) J_j\right)$$

$$\left.\frac{\delta^{2n} Z(J, J^*)}{\delta J_{i_1}^* \cdots \delta J_{i_n}^* \, \delta J_{j_n} \cdots \delta J_{j_1}}\right|_{J=0} = \sum_P \zeta^P (A^{-1})_{i_{p(n)}, j_n} \cdots (A^{-1})_{i_{p(1)} j_1}$$

The action is a quadratic functional (excluding V):

$$\sum_k \left(\sum_\alpha \left(i\hbar \phi_{k\alpha}^* (\phi_{k\alpha} - \phi_{k-1,\alpha}) - \sum_{\alpha\alpha'} \phi_{k\alpha}^* T_{\alpha\alpha'} \phi_{k-1,\alpha} \Delta t \right) \right)$$

$$= -\sum_{ij} \phi_i^* S_{ij} \phi_j \Delta t$$

Need one more building block: $\boxed{\text{Propagator}}$

$$G_{\xi\eta}(t, t') = \langle T \, \hat{a}_\xi(t) \, \hat{a}_\xi^+(t') \rangle$$

single particle Green's function

$\Downarrow$

n-particle GF

Single particle Green's function:

$$G_{\xi\eta}(t, t') = \frac{\hbar}{i} (S^{-1})_{ij}$$

$$G^{(n)}_{\alpha_1 \cdots \alpha_n \, \alpha_1' \cdots \alpha_n'}(t_1, \ldots, t_n; t_n', \ldots, t_n')$$

$$= \sum_P \zeta^P G_{\alpha_{p(n)} \alpha_n'}(t_{p(n)}, t_n') \cdots G_{\alpha_{p(1)}, \alpha_1'}(t_{p(1)}, t_1')$$

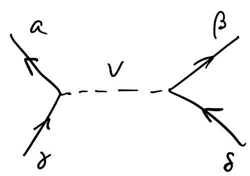
(decomposition into single particle propagator)

Look back:

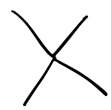
$$\langle f | i \rangle = \sum \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \int_{[t_i,t_f]^n} \cdots \int \langle V(\phi^*(t_1)\phi(t_1)) \ldots V(\phi^*(t_n)\phi(t_n)) \rangle \, dt_1 \ldots dt_n$$

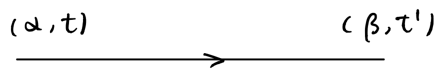
$$\hat{V} = \hat{V}(\hat{a}^+, \hat{a}) = \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta,\gamma\delta} \, a_\alpha^+ a_\beta^+ a_\gamma a_\delta$$

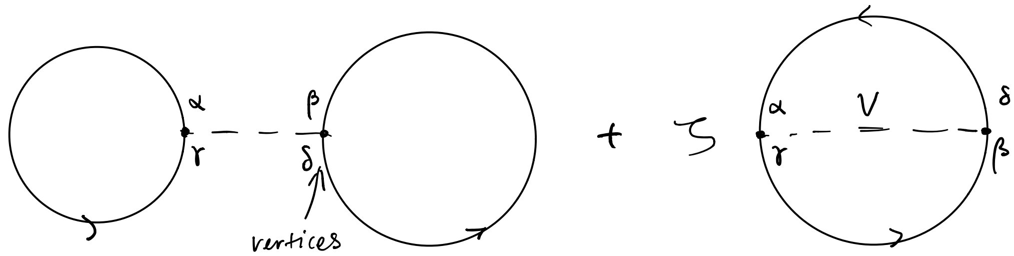
$$\langle f | i \rangle \overset{\text{1. Order}}{=} \langle f | i \rangle_0 \Big(1 - \frac{i}{\hbar} \int \sum_{\alpha\beta\gamma\delta} \big(\varsigma^0 \, G_{\gamma\alpha}(t,t) V_{\alpha\beta,\gamma\delta} G_{\delta\beta}(t,t) + \varsigma^1 \, G_{\delta\alpha}(t,t) V_{\alpha\beta,\gamma\delta} G_{\gamma\beta}(t,t) \big) dt \Big)$$

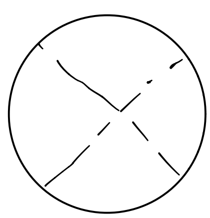
$V_{\alpha\beta,\gamma\delta}$ $\Leftrightarrow$ 

(not relly accurate, V not time dependent)

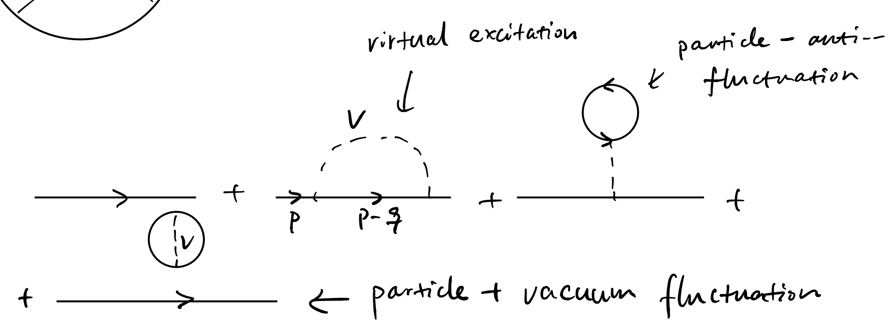
rather 

$G_{\alpha\beta}(t,t')$ $\Leftrightarrow$ 



second order:  → Vaccuum fluctuations

Perturbation in G

first order terms: 

Rules drawing diagrams (n-th order):

1) draw n-vertices and label the states at the vertices
2) connect all of the vertices in all possible ways with propagators
3) Each vertex corresponds to an iteration
4) For each closed loop add a factor ξ
5) Multiply with a factor $\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n$