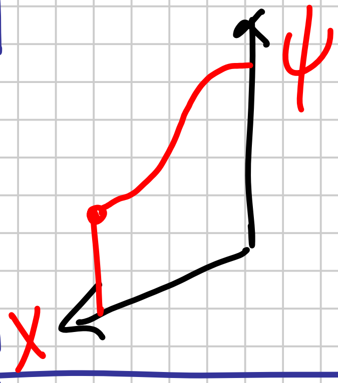
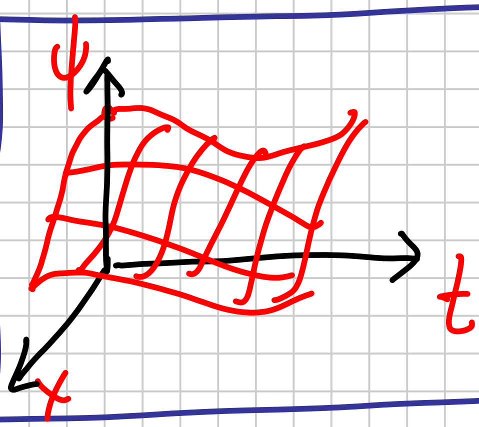
3. Many-Body Functional Field Integral

	Degrees of Freedom	Path Integral
QM	$\bullet\, q$	
QFT		

3.1 Coherent states for Bosons $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$

$|\alpha\rangle \rightarrow$ Construct as eigenstates of $\hat{a}_i$-operator:

$$\underset{\text{Ann. Op.}}{\hat{a}_i}\ \underset{\text{C.S.}}{|\alpha\rangle} = \underset{\text{Complex E.Val.}}{\alpha_i}\ \underset{\text{C.S.}}{|\alpha\rangle}$$

we consider $|\alpha\rangle$ - as a "general" vector in $\mathcal{F}$:

$$|\alpha\rangle = \sum_{n=0}^{\infty} \sum_{i_1 \dots i_n} \overset{\text{coeff.}}{C_{n_{i_1} n_{i_2} \dots}} |n_{i_1} n_{i_2} \dots\rangle \equiv$$

$$\equiv \sum_{\{n_i\}} C_{n_1 n_2 \dots} |n_1 n_2 \dots\rangle$$

$$|n_1 n_2 \dots\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(\hat{a}_2^\dagger)^{n_2}}{\sqrt{n_2!}} \cdots \underset{\text{Vacuum state}}{|0\rangle}$$

Why $\hat{a}_i$ and NOT $\hat{a}_i^+$

Eigenstates of $\hat{a}_i^+$ – can not exist!

if Min number of particle in $|\alpha\rangle$ is n_0,

then Min. number of particle in $\hat{a}_i^+|\alpha\rangle$ is n_0+1

So $\hat{a}_i^+|\alpha\rangle$ is <u>NOT</u> $\sim |\alpha\rangle$

Proof that:

$$|\alpha\rangle = e^{\sum_i \alpha_i \hat{a}_i^+}|0\rangle$$

Since $\hat{a}_i$ commut with All $\hat{a}_j^+$ $(j\neq i)$

we focus only on element i:

since $\hat{a}|0\rangle=0$

$$\hat{a}|\alpha\rangle = \hat{a}\, e^{\alpha \hat{a}^+}|0\rangle \equiv \left[\hat{a}, e^{\alpha\hat{a}^+}\right]|0\rangle$$

$$= \sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\left[\hat{a},(\hat{a}^+)^n\right] = \alpha\sum_{n=1}^{\infty}\frac{\cancel{n}\alpha^{n-1}}{\underbrace{\cancel{n!}}_{(n-1)!}}(\hat{a}^+)^{n-1}|0\rangle = \alpha\,\underbrace{e^{\alpha\hat{a}^+}|0\rangle}_{|\alpha\rangle}$$

$$\left[\hat{a},(\hat{a}^+)^n\right] = n\left(\hat{a}^+\right)^{n-1}$$

Properties of coherent states:

$$\hat{a}_i|\alpha\rangle = \alpha_i|\alpha\rangle \quad , \quad |\alpha\rangle = e^{\sum_i \alpha_i \hat{a}_i^+}|0\rangle$$

1) Hermitian conjugation – $\forall i$:

$$\langle\alpha|\hat{a}_i^+ = \langle\alpha|\alpha_i^* \quad \leftarrow \text{left E. states of } \hat{a}^+$$

α_i^* is complex conjugate of α_i

and

$$\langle\alpha| = \langle 0|e^{\sum_i \hat{a}_i \alpha_i^*}$$

2) Direct application of ∂_{α_i} for $\forall i$

$$\hat{a}_i^\dagger|\alpha\rangle = \partial_{\alpha_i}|\alpha\rangle$$

$$\rightarrow \quad \hat{a}_i^\dagger|\alpha\rangle = \hat{a}_i^\dagger e^{\sum_j \alpha_j \hat{a}_j^\dagger}|0\rangle \equiv \frac{\partial}{\partial\alpha_i}|\alpha\rangle$$

3) Overlap of 2 Coherent states: $\langle\alpha|\beta\rangle$

$$\langle\alpha| = (|\alpha\rangle)^\dagger = \langle 0| e^{\sum_i \hat{a}_i \alpha_i^*}$$

$$|\beta\rangle = e^{\sum_j \beta_j \hat{a}_j^\dagger}|0\rangle \quad \Longrightarrow \quad \hat{a}_i|\beta\rangle = \beta_i|\beta\rangle$$

$$\langle\alpha|\beta\rangle = \langle 0| e^{\sum_i \alpha_i^* \hat{a}_i}|\beta\rangle = e^{\sum_i \alpha_i^* \beta_i}\underbrace{\langle 0|\beta\rangle}_{=1}$$

since: $\langle 0|\beta\rangle = \langle 0|\sum_{n=0}^\infty \frac{\beta_i^n}{n!}(\hat{a}^\dagger)^n|0\rangle = 1$

only: $n=0$ $\qquad \langle 0|0\rangle = 1$

N.B. $\qquad |\alpha\rangle = \sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}|n\rangle$

So:

$$\langle\alpha|\beta\rangle = e^{\sum_i \alpha_i^* \beta_i}$$

4) Norm of C.S.

$$\langle\alpha|\alpha\rangle = e^{\sum_i \alpha_i^* \alpha_i}$$

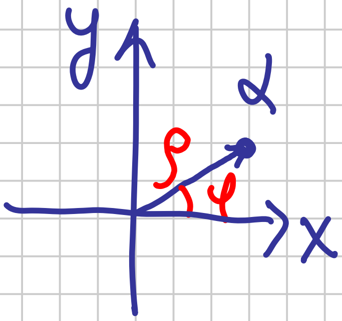
5) Completeness (C.S. is overcomplete!)

Resolution of $\hat{1}$!

$$\int \prod_i \frac{d\alpha_i^* d\alpha_i}{2\pi i} e^{-\sum_i \alpha_i^* \alpha_i}|\alpha\rangle\langle\alpha| = \mathbb{1}$$

Bosonic P.I. measure

$$\frac{d\alpha^* d\alpha}{2\pi i} \equiv \frac{d(\mathrm{Re}\,\alpha)\, d(\mathrm{Im}\,\alpha)}{\pi}$$



$$\alpha = x + iy$$
$$\alpha^* = x - iy \qquad \alpha^*\alpha = x^2 + y^2 = \rho^2$$
$$\alpha = \rho e^{i\varphi}$$

$$\frac{\partial(\alpha^*,\alpha)}{\partial(x,y)} = \begin{vmatrix} \frac{\partial\alpha^*}{\partial x}, & \frac{\partial\alpha^*}{\partial y} \\ \frac{\partial\alpha}{\partial x}, & \frac{\partial\alpha}{\partial y} \end{vmatrix} = \begin{vmatrix} 1 & -i \\ 1 & i \end{vmatrix} = 2i$$

$$\Rightarrow \quad \frac{d\alpha^* d\alpha}{2\pi i} = \frac{dx\,dy}{\pi} = \frac{\rho\, d\rho\, d\varphi}{\pi} = \frac{d^2\alpha}{\pi}$$

Proof of Unity expansion:

$$\int \frac{d\alpha^* d\alpha}{2\pi i} e^{-\alpha^*\alpha} |\alpha\rangle\langle\alpha| = \int \frac{\rho\, d\rho\, d\varphi}{\pi} e^{-\rho^2} \Big(\sum_n \frac{(\rho e^{i\varphi})^n}{\sqrt{n!}} |n\rangle\Big)\Big(\sum_m \frac{(\rho e^{-i\varphi})^m}{\sqrt{m!}} \langle m|\Big) =$$

$$= \frac{1}{\pi} \int_0^\infty \rho\, d\rho\, e^{-\rho^2} \sum_{n,m} \frac{\rho^{n+m}}{\sqrt{n!m!}} \underbrace{\int_0^{2\pi} d\varphi\, e^{i(n-m)\varphi}}_{= 2\pi\,\delta_{n,m}} |n\rangle\langle m| =$$

$$= \sum_n \frac{2}{\cancel{n!}} \underbrace{\int_0^\infty d\rho\, \rho^{2n+1} e^{-\rho^2}}_{x=\rho^2:\ \frac{1}{2}\int_0^\infty dx\, x^n e^{-x} = \cancel{\frac{1}{2} n!}} |n\rangle\langle n| = \sum_n |n\rangle\langle n| = \hat{\mathbb{1}}$$

B-P.I. measure: $\quad D[\alpha^*,\alpha] \equiv \prod_i \frac{d\alpha_i^* d\alpha_i}{2\pi i} = \prod_i \frac{d^2\alpha}{\pi}$

6) The Trace of Operators – $\hat{A}$!

$$\mathrm{Tr}\,\hat{A} = \sum_n \langle n| \underset{\mathbb{1}}{\uparrow} \hat{A} |n\rangle =$$

$$= \int \mathcal{D}[\alpha^*\alpha]\, e^{-\sum_i \alpha_i^*\alpha_i} \sum_n \langle n|\alpha\rangle\langle\alpha|\hat{A}|n\rangle =$$

$$= \int \mathcal{D}[\alpha^*\alpha]\, e^{-\sum_i \alpha_i^*\alpha_i} \langle\alpha|\hat{A} \underbrace{\sum_n |n\rangle\langle n|}_{= \mathbb{1}} \alpha\rangle =$$

$$= \int \mathcal{D}[\alpha^*,\alpha]\, e^{-\sum_i \alpha_i^*\alpha_i} \langle\alpha|\hat{A}|\alpha\rangle$$

7) Matrix element of normal-ordered operator

$$\langle\alpha| \hat{A}(\hat{a}_i^\dagger, \hat{a}_i) |\beta\rangle = A(\alpha_i^*, \beta_i)\, e^{\sum_i \alpha_i^*\beta_i}$$

Note: Hamiltonian in second-quantization is always in "normal order"!

$$\hat{H} = \sum_{ij} t_{ij}\, \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2}\sum_{ijkl} V_{ijkl}\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

So

$$\langle\alpha|\hat{H}|\beta\rangle = e^{\sum_i \alpha_i^*\beta_i}\, H(\alpha_i^*, \beta_i)$$

3.2 Fermion coherent state: $\{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij}$

$$\hat{c}_i |c\rangle = c_i |c\rangle$$

Anticommutivity of $\{\hat{c}_i, \hat{c}_j\} = 0$ implies that eigenvalues c_i anticommute $c_i c_j + c_j c_i = 0$

$\rightarrow$ $c_i c_j = - c_j c_i$ is not ordinary number!

Grassmann Algebra: $\{c_i\}$

1) Anticommuting number: $c_i c_j + c_j c_i = 0$
2) $c_i^2 = 0$
3) Anticommute with Fermi-operators: $c\hat{c}^+ + \hat{c}^+ c = 0$
4) Can be add to and multiply by complex numbers: (f)
   Functions: $F(c_i) = c_i + \sum_j f_j c_j$
5) Differentiation: $\partial_{c_i} c_j = \delta_{ij}$

   N.B. ordering! $\partial_{c_i} c_j c_i = -c_j$

6) Integration:

$$\left.\begin{aligned} \int dc\, 1 &= 0 \\ \int dc\, c &= 1 \end{aligned}\right\} \quad \int \equiv \partial$$

Fermionic coherent state $|c\rangle = \{c_i\}$

$$|c\rangle = e^{-\sum_i c_i \hat{c}_i^{+}} |0\rangle$$

Proof! $(i=j)$

$$\hat{c}|c\rangle = \hat{c}\, e^{-c\hat{c}^{+}} |0\rangle =$$

$$= \hat{c}\Big(1 - c\hat{c}^{+} \underbrace{+ \cdots}_{0\ (c^2=0)}\Big)|0\rangle = \underbrace{\hat{c}|0\rangle}_{=0} - \hat{c}\, c\, \hat{c}^{+}|0\rangle$$

$$= c\, \underbrace{\hat{c}\hat{c}^{+}}_{1-\hat{c}^{+}\hat{c},\ \hat{c}|0\rangle=0} |0\rangle = c|0\rangle \equiv c\underbrace{(1 - c\hat{c}^{+})}_{c^2=0\ \Rightarrow\ = e^{-c\hat{c}^{+}}}|0\rangle =$$

$$= c\, \underbrace{e^{-c\hat{c}^{+}}|0\rangle}_{|c\rangle} = c|c\rangle$$

Adjoint-States:

$$\langle c| = \langle 0| e^{-\sum_i \hat{c}_i c_i^*} \equiv \langle 0| e^{+\sum c_i^* \hat{c}_i}$$

But c_i^* is NOT related to c_i

(not a complex conjugate!) def: $c^* \equiv \bar{c}$

$$\langle c|\hat{c}_i^{+} = \langle c| c_i^*$$

c_i^* is "left e.v. of $\hat{c}_i^{+}$

Arbitrary function of c^*, c

$$f(c^*, c) = f_{00} + f_{01}\, c + f_{10}\, c^* + f_{11}\, c^* c$$

$$\partial_c f(c^*, c) = f_{01} - f_{11}\, c^*, \quad \partial_{c^*} f(c^*, c) = f_{10} + f_{11}\, c$$

$$\vec{\partial}_{c^*} \vec{\partial}_c f(c^*, c) = - f_{11}$$

$$\int dc^* f(c^*, c) = f_{10} + f_{11}\, c$$

$$\int \underset{\substack{\uparrow \\ \text{2nd}}}{dc^*} \underset{\substack{\uparrow \\ \text{1st}}}{dc}\, f(c^*, c) = - f_{11}$$

Gaussian Integral

$$\int dc^* dc\; e^{-c^* c} = 1 \qquad \text{(N.B. no factor } \pi\text{!)}$$

proof:

$$= \int dc^* dc \left(1 - c^* c\right) = \int dc^* \underbrace{dc\, c}_{=1}\, c^* = \int \underbrace{dc^* c^*}_{=1} = 1$$

Fermion P.I. measure:

$$D[c^*, c] = \prod_i dc_i^*\, dc_i$$

Gauß!

$$\int D[c^*, c]\; e^{-\vec{c}^{*T} \hat{M} \vec{c}} = \det \hat{M} \quad (\text{NOT the } \det \hat{M}^{-1})$$

For $\forall$ J^*, J – Grassmann variables.

$$\int D[c^*, c]\; e^{-\vec{c}^{*T} \hat{M} \vec{c} + \vec{J}^{*T} \cdot \vec{c} + \vec{c}^{*T} \cdot \vec{J}} = \det \hat{M} \cdot e^{\vec{J}^{*T} \hat{M}^{-1} \vec{J}}$$

Completness relation (resolution of $\hat{\mathbb{1}}$)

$$\int \mathcal{D}[c^*_i, c]\, e^{-\sum_i c^*_i c_i} |c\rangle\langle c| = \hat{\mathbb{1}}_F$$

Proof: (for 1-Fermion state)

$$\sum_n |n\rangle\langle n| = |0\rangle\langle 0| + |1\rangle\langle 1| = \hat{\mathbb{1}}$$

Overlap (over-complete basis) $\langle c|c\rangle = e^{c^* c}$

$$\langle c|c\rangle = \langle 0| e^{-\hat{c} c^*} e^{-c\hat{c}^+} |0\rangle =$$

$$= \langle 0|(1-\hat{c}c^*)(1-c\hat{c}^+)|0\rangle =$$

$$= 1 + c^* c = e^{c^* c}$$

Since $|c\rangle = e^{-c\hat{c}^+}|0\rangle \equiv e^{\hat{c}^+ c}|0\rangle$

Then:
$$\langle n|c\rangle = \langle n|\big(|0\rangle + |1\rangle c\big) = \underbrace{\langle n|0\rangle}_{=\delta_{n,0}} + \underbrace{\langle n|1\rangle}_{=\delta_{n,1}} c \equiv c^n$$

Identity:
$$\int dc^* dc\, \underbrace{e^{-c^* c}}_{=(1-c^*c)} c^n c^{*m} = \delta_{nm}$$

or

$$\langle n|m\rangle = \int dc^* dc\, e^{-c^* c}\, \underbrace{c^n}_{=\langle n|c\rangle}\, \underbrace{c^{*m}}_{=\langle c|m\rangle}$$

$$\delta_{nm} = \int dc^* dc\, e^{-c^* c} \langle n|c\rangle\langle c|m\rangle$$

Then:
$$\int dc^* dc\, e^{-c^* c} |c\rangle\langle c| = |0\rangle\langle 0| + |1\rangle\langle 1| = \hat{\mathbb{1}}.$$

N. b.: normalization: $e^{-c^* c} |c\rangle\langle c| \equiv \frac{|c\rangle\langle c|}{\langle c|c\rangle}$

Then: $\sum_{c^* c} \frac{|c\rangle\langle c|}{\langle c|c\rangle} = \mathbb{1} = \int D[c^* c] e^{-c^* c} |c\rangle\langle c|$

Trace of Normal Odered operator $H[\hat{c}^{+}, \hat{c}]$

$$\langle c| H[\hat{c}^{+}, \hat{c}] |c\rangle = \langle c|c\rangle H[c^*, c]$$

$$\mathrm{Tr}\, \hat{H} = \sum_n \langle n| \hat{H} |n\rangle = \int dc^* dc\, e^{-c^* c} \langle -c^* | H | c\rangle$$

Proof (2 possibilities)

a) $$\hat{H} = \sum_{\{n,m\}} |n\rangle H_{nm} \langle m|$$

$$\int dc^* dc\, e^{-c^* c} \langle -c| \hat{H} |c\rangle = \sum_{n,m} \int dc^* dc\, e^{-c^* c} \langle -c|n\rangle H_{nm} \langle m|c\rangle$$

$$= \sum_{\underset{0,1}{n,m}} H_{nm} \int dc^* dc\, e^{-c^* c} (-c^*)^n (c)^m = \sum_n H_{nn}$$

$\ominus$

$= \delta_{n,m}$

b) $$\sum_n \langle n| \underset{\mathbb{1}}{\uparrow} \hat{H} |n\rangle = \sum_n \int dc^* dc\, e^{-c^* c} \langle n|c\rangle\langle c| \hat{H} |n\rangle =$$

$= \langle -c|H|n\rangle\langle n|c\rangle$, $\sum_n = \mathbb{1}$

$$= \int dc^* dc\, e^{-c^* c} \langle -c| H |c\rangle$$

Why?

$$|n\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger \cdots \hat{c}_n^\dagger |0\rangle$$

$$\langle n|c\rangle = \langle 0|\hat{c}_n \cdots \hat{c}_2 \hat{c}_1|c\rangle = c_n \cdots c_2 c_1 \underbrace{\langle 0|c\rangle}_{=1}$$

$$\langle c|n\rangle = c_1^* c_2^* \cdots c_n^*$$

Then:

$$\langle n|c\rangle\langle c|n\rangle = c_n \cdots c_2 c_1 c_1^* c_2^* \cdots c_n^* =$$

$$= (-c_1^* c_1)(-c_2^* c_2)\cdots(-c_n^* c_n) \equiv \langle -c|n\rangle\langle n|c\rangle$$

Summary: $\zeta = \begin{cases} +1 & \text{Boson} \\ -1 & \text{Fermion} \end{cases}$ $[\hat{c}_i, \hat{c}_j^\dagger]_\zeta = \delta_{ij}$

$$\hat{c}_i|c\rangle = c_i|c\rangle \quad \text{with} \quad |c\rangle = e^{\zeta\sum_i c_i \hat{c}_i^\dagger}|0\rangle$$

$$\langle c|\hat{c}_i^\dagger = \langle c|c_i^* \quad \text{with} \quad \langle c| = \langle 0|e^{\zeta\sum_i \hat{c}_i c_i^*}$$

$$\hat{c}_i^\dagger|c\rangle = \zeta\partial_{c_i}|c\rangle \quad \text{and} \quad \langle c|\hat{c}_i = \partial_{c_i^*}\langle c|$$

Overlap: $\langle \bar{c}|c\rangle = e^{\sum_i \bar{c}_i^* c_i}$

Completness: $\int dc^* dc\, e^{-\sum_i c_i^* c_i}|c\rangle\langle c| = \hat{\mathbb{1}}_F$

Trace: $\forall \hat{H}$ $\mathrm{Tr}\,\hat{H} = \sum_n \langle n|\hat{H}|n\rangle = \int dc^* dc\, e^{-\sum_i c_i^* c_i}\langle \zeta c|\hat{H}|c\rangle$

P.I. measure: $\mathcal{D}[c^*, c] \equiv \lim_{N\to\infty} \prod_i \frac{dc_i^* dc_i}{(2\pi i)^{(1+\zeta)/2}}$

3.3 Coherent State Path Integral

Quantum Partition funktion (Grand Canonical)

$\beta = \frac{1}{k_B T}$, $k_B = 1$

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_{n\in\mathcal{F}} \langle n| e^{-\beta(\hat{H}-\mu\hat{N})} |n\rangle =$$

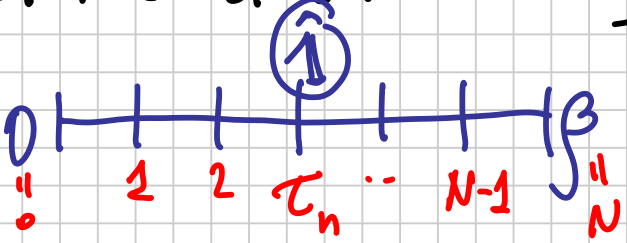
$$= \int dc^* dc\, e^{-\sum_i c_i^* c_i} \langle \zeta c| e^{-\beta(\hat{H}-\mu\hat{N})} |c\rangle$$

General Hamiltonian (normal-odered!)

$$\hat{H} - \mu\hat{N} = \sum_{ij} (h_{ij} - \mu\delta_{ij}) \hat{c}_i^+ \hat{c}_j + \frac{1}{2}\sum_{ijkl} V_{ijkl}\, c_i^+ c_j^+ c_l c_k$$

Following Feynman's strategy!

1) Divide "time interval" β $[0,\beta)$ into N segments:



$$\Delta\tau = \frac{\beta}{N} \Rightarrow \Delta\tau \ll 1$$

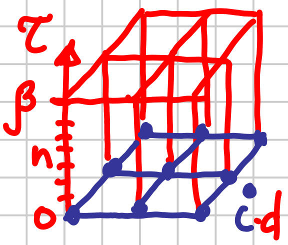
$$\tau_n = n\cdot\Delta\tau$$

$$e^{-\beta(\hat{H}-\mu\hat{N})} = \left[e^{-\Delta\tau(\hat{H}-\mu\hat{N})}\right]^N$$

$$\langle \zeta c| e^{-\beta(\hat{H}-\mu\hat{N})} |c\rangle = \langle \zeta c| e^{-\Delta\tau(\hat{H}-\mu\hat{N})} \underset{\hat{1}}{\cdot} e^{-\Delta\tau(\hat{H}-\mu\hat{N})} \underset{\hat{1}}{\cdot} \cdots \underset{\hat{1}}{} e^{-\Delta\tau(\hat{H}-\mu\hat{N})} |c\rangle$$

2) At each $\hat{1}$ insert $\hat{\mathbb{1}}_F$ - resolution

$\hat{1}_n$:
$$\hat{\mathbb{1}}_F = \int dc_n^* dc_n\, e^{-\sum_i c_{n_i}^* c_{n_i}} |c_n\rangle\langle c_n|$$



i.e. N-independent sets: $|\vec{c}_n\rangle = \{c_n^i\}$ "d+1" lattice

3) Expand the exp for $\Delta\tau \ll 1$

$$\langle c_n | e^{-\Delta\tau(\hat{H}-\mu\hat{N})} | c_{n-1}\rangle \approx \langle c_n | 1 - \Delta\tau(\hat{H}-\mu\hat{N}) \cancel{+ O(\Delta\tau^2)} | c_{n-1}\rangle$$

$$= \langle c_n | c_{n-1}\rangle - \Delta\tau \langle c_n | H(\hat{c}^+, \hat{c}) - \mu N(\hat{c}^+, \hat{c}) | c_{n-1}\rangle =$$

$$= \langle c_n | c_{n-1}\rangle \left[1 - \Delta\tau\left(H(c_n^*, c_{n-1}) - \mu N(c_n^*, c_{n-1})\right)\right] \approx$$

$$\simeq e^{c_n^* c_{n-1} - \Delta\tau[H(c_n^*, c_{n-1}) - \mu N(c_n^*, c_{n-1})]}$$

with: $H(c^*, c) = \dfrac{\langle c | \hat{H} | c\rangle}{\langle c | c\rangle} = \sum_{ij} h_{ij} c_i^* c_j + \frac{1}{2}\sum_{ijkl} V_{ijkl} c_i^* c_j^* c_l c_k$

Then we will get for Z: (for simplicity: $H - \mu N \to \tilde{H}$)

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \int \prod_{n=0}^{N-1} dc_n^* dc_n\, e^{-\sum_n c_n^* c_n} \langle \zeta c_0 | e^{-\Delta\tau\hat{H}} | c_{N-1}\rangle \cdots \langle c_1 | e^{-\Delta\tau\hat{H}} | c_0\rangle$$

$$= \int \prod_{n=0}^{N-1} dc_n^* dc_n\, e^{-\sum_n c_n^* c_n}\, e^{\zeta c_0^* c_{N-1} - \Delta\tau H(\zeta c_0^*, c_{N-1})} \cdot$$

$$\cdot\, e^{c_{N-1}^* c_{N-2} - \Delta\tau H(c_{N-1}^*, c_{N-2})} \cdots e^{c_1^* c_0 - \Delta\tau H(c_1^*, c_0)} =$$

$$= \int \prod_{n=0}^{N-1} dc_n^* dc_n\, e^{-\sum_{n=1}^{N}\left[c_n^*(c_n - c_{n-1}) + \Delta\tau H(c_n^*, c_{n-1})\right]}$$

$$+\, c_N^* c_{N-1} + c_{N-1}^* c_{N-2} + \cdots + c_1^* c_0$$
$$-\, c_N^* c_N \qquad c_{N-1}^* c_{N-1} \qquad c_1^* c_1 + c_0^* c_0$$

With boundary condition: $\begin{cases} c_N = \zeta c_0 \\ c_N^* = \zeta c_0^* \end{cases}$ B ⇒ periodic, F ⇒ antiperiodic

Finally for Grand Canonical Z:

$$Z = \int_{\substack{c_N=\zeta c_0 \\ c_N^*=\zeta c_0^*}} \prod_{n=0}^{N-1} dc_n^*\, dc_n\; e^{-\Delta\tau \sum_{n=1}^{N}\left[c_n^* \frac{(c_n-c_{n-1})}{\Delta\tau} + H(c_n^*, c_{n-1}) - \mu N(c_n^*, c_{n-1})\right]}$$

Continuum limit: $N\to\infty$, $\Delta\tau \to 0$:

$$\Delta\tau\sum_{n=1}^{N} \longrightarrow \int_0^\beta d\tau, \qquad \frac{c_n-c_{n-1}}{\Delta\tau}\longrightarrow \partial_\tau c$$

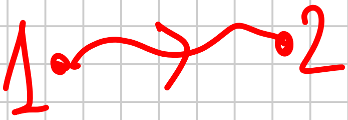
P.I. Measure: $D[c^*,c] = \lim_{N\to\infty}\prod_{n=0}^{N-1}\prod_i dc_{ni}^*\, dc_{ni}$

General Path-Integral representation:

$$Z = \int_{c(\beta)=\zeta c(0)} D[c^*,c]\; e^{-\int_0^\beta d\tau\left[c^*\frac{\partial}{\partial\tau}c + H(c^*,c) - \mu N(c^*,c)\right]}$$

analogy: Feynman: $\int_1^2 dp\,dq\; e^{i\int_1^2 dt\,(p\,\partial_t q - H(p,q))}$

Coherent state: $\int_1^2 dc^*\, dc\; e^{i\int_1^2 dt\,(c^*\partial_t c - H(c^*,c))}$



$\Rightarrow$ $c^* \leftarrow$ conjugate $\rightarrow c$

with boundary condition:

Boson

$$c(\beta) = c(0)$$
$$c^*(\beta) = c^*(0)$$

Fermion

$$c(\beta) = -c(0)$$
$$c^*(\beta) = -c^*(0)$$

For our Hamiltonian: $Z = \int D[c^*,c]\; e^{-S[c^*,c]}$

with Action:

$$S[c^*,c] = \int_0^\beta d\tau \left\{\sum_{ij} c_i^*(\tau)\left[(\partial_\tau-\mu)\delta_{ij} + h_{ij}\right]c_j(\tau) + \frac{1}{2}\sum_{ijkl} V_{ijkl}\, c_i^*(\tau)\,c_j^*(\tau)\,c_l(\tau)\,c_k(\tau)\right\}$$

Fourier transformation of fields:

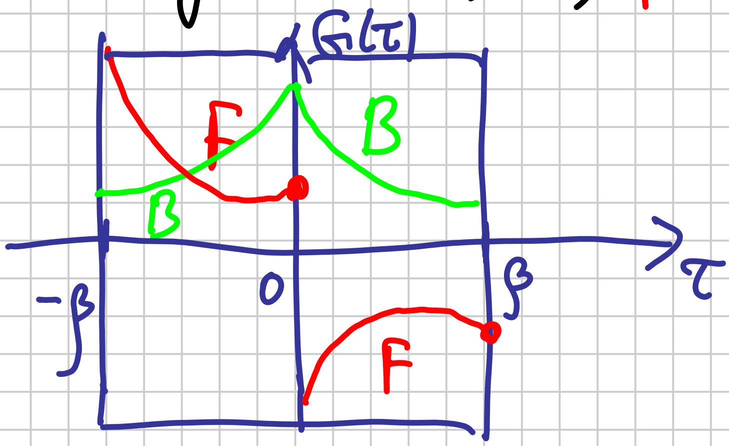
$$\begin{cases} c(\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\tau} c(\omega_n) \\ c^*(\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{i\omega_n\tau} c^*(\omega_n) \end{cases}$$

Inverse FT:

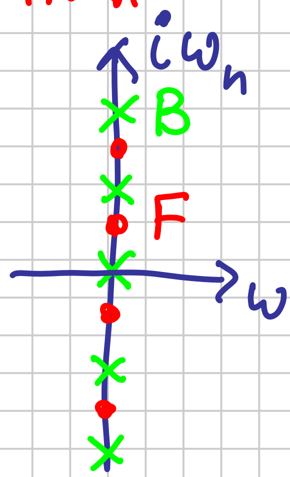
$$\begin{cases} c(\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} c(\tau) \\ c^*(\omega_n) = \int_0^\beta d\tau\, e^{-i\omega_n\tau} c^*(\tau) \end{cases}$$

Since: $[0,\beta)$

$$c(\tau+\beta) = \{ c(\tau) \quad \begin{matrix} B: \text{periodic} \\ F: \text{antiperiodic} \end{matrix}$$



$\Rightarrow$



then:

Matsubara frequencies:

$$\omega_n = \begin{cases} 2n\frac{\pi}{\beta} & \text{- Boson} \\ (2n+1)\frac{\pi}{\beta} & \text{- Fermion} \end{cases}$$

$n = -\infty \cdots -1, 0, 1 \cdots \infty$
integer Numbers

Using:

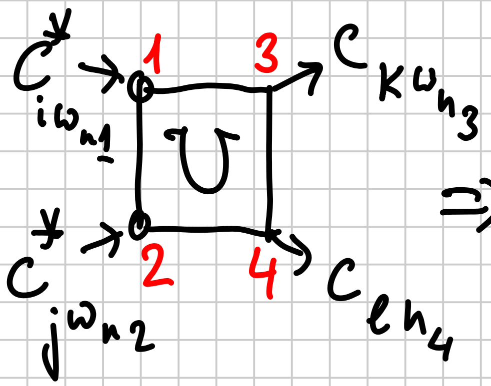
$$\int_0^\beta d\tau\, e^{-i(\omega_n-\omega_m)\tau} = \beta\,\delta_{n,m}$$

We obtain action in Fourier space:

$$S[c^*,c] = -\frac{1}{\beta}\sum_{ij,\omega_n} c^*_{i,\omega_n}\overbrace{[i\omega_n+\mu-h_{ij}]}^{=G_0^{-1}}c_{j,\omega_n} \; +$$

$$+\frac{1}{2\beta^3}\sum_{ijkl}\sum_{\omega_{n_1}\ldots\omega_{n_4}} V_{ijkl}\, c^*_{i\omega_{n_1}} c^*_{j\omega_{n_2}} c_{l\omega_{n_4}} c_{k\omega_{n_3}}\, \delta_{\omega_{n_1}+\omega_{n_2},\,\omega_{n_3}+\omega_{n_4}}$$

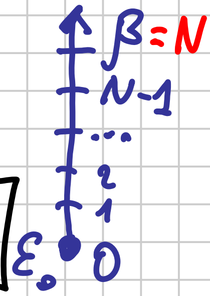
(rule: $\frac{1}{\beta}\sum_{\omega_n}$)



$$\Rightarrow \omega_{n_1}+\omega_{n_2} = \omega_{n_3}+\omega_{n_4}$$

3.4 Partition function for free particles

a) 1-particle: $\hat{H}_0 = \varepsilon_0\,\hat{c}^{\dagger}\hat{c}$



$$Z_0 = \int \mathcal{D}[c^*,c]\, e^{-\int_0^\beta d\tau\left[c^*(\tau)\frac{\partial}{\partial\tau}c(\tau)+H_0(c^*(\tau),c(\tau))-\mu N\right]}$$

$$= \lim_{N\to\infty}\int\prod_{n=1}^{N} dc^*_n dc_n\, e^{-\sum_{n=1}^{N}\left[c^*_n(c_n-c_{n-1})+\Delta\tau(\varepsilon_0-\mu)c^*_n c_{n-1}\right]} \equiv$$

$$\equiv \lim_{N\to\infty}\int\prod_{n=1}^{N} dc^*_n dc_n\, e^{-\sum_{n,k=1}^{N} c^*_n M_{nk} c_m} \underset{\text{Gauß}}{=} \lim_{N\to\infty}\left[\det M\right]^{-\zeta}$$

where:

$$\underline{M}_{nk} = \begin{array}{c|c} & \begin{array}{cccccc} 1 & 2 & \ldots & & & N \end{array} \\ \begin{array}{c} 1 \\ 2 \\ \vdots \\ \\ \\ N \end{array} & \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 & -\zeta\alpha \\ -\alpha & 1 & 0 & \ldots & 0 & 0 \\ 0 & -\alpha & 1 & \ldots & 0 & 0 \\ 0 & 0 & -\alpha & & & \\ & & \cdots & & 1 & 0 \\ 0 & 0 & 0 & \ldots & -\alpha & 1 \end{bmatrix} \end{array} \quad \text{with} \quad c_n = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ c_N \end{pmatrix}$$

with: $$\alpha = 1 - \Delta\tau(\varepsilon_0 - \mu) \quad , \quad \Delta\tau = \frac{\beta}{N}$$

The $\det \hat{M}$ is evaluated by expanding over 1^{st}-row

$$Z_0 = \lim_{N\to\infty} [\det \hat{M}]^{-\zeta} = \lim_{N\to\infty} \left[1 + (-\zeta\alpha)(-\alpha)^{N-1}(-1)^{N-1}\right]^{-\zeta}$$

$$= \lim_{N\to\infty} \left[1 + (-1)^{N-1}\zeta(-\alpha)^N\right]^{-\zeta} =$$

$$= \lim_{N\to\infty} \left[1 - \zeta\left(1 - \frac{\beta(\varepsilon_0 - \mu)}{N}\right)^N\right]^{-\zeta} =$$

$$= \left[1 - \zeta e^{-\beta(\varepsilon_0 - \mu)}\right]^{-\zeta}$$

b) Non-interacting particles:

$$\hat{H}_0 = \sum_i \varepsilon_i \hat{c}_i^{+} \hat{c}_i$$

$$Z_0 = \lim_{N\to\infty} \int \prod_i \prod_n dc^*_{in} dc_{in} \, e^{-\sum_{inm} c^*_{in} M^i_{nk} c_{ik}} =$$

$$= \prod_i \left[1 - \zeta e^{-\beta(\varepsilon_i - \mu)}\right]^{-\zeta}$$

Free energy: $(k_B = 1, \; T = \frac{1}{\beta})$

$$F_0 = -T \ln Z_0 = \frac{\zeta}{\beta} \sum_i \ln\left(1 - \zeta e^{-\beta(\varepsilon_i - \mu)}\right)$$

– is standart free-energy of Bose (Fermi) gas.

c) One-electron non-interacting Green-Function

$$G(i\tau, j\tau') \overset{\text{def}}{=} -\langle T_\tau\, \hat{c}_i(\tau)\, c_j^\dagger(\tau') \rangle$$

P.I.:

$$\langle A(\hat{c}^+\hat{c}) \rangle_S \overset{\text{def}}{=} \frac{\int D[c^*,c]\, A(c^*,c)\, e^{-S}}{\int D[c^*,c]\, e^{-S}} = \frac{1}{Z}\int D[c^*,c] A(c^*,c) e^{-S}$$

$\hat{H}_0 = \sum_\ell \varepsilon_\ell \hat{c}^+_\ell \hat{c}_\ell$

$$\Rightarrow\; G_0(i\underset{q}{\tau}, j\underset{r}{\tau'}) = \frac{-1}{Z_0}\int D[c^*,c]\, c_i(\tau)\, c_j^*(\tau')\, e^{-S_0}$$

Discretize version: $\tau_q = q\cdot\Delta\tau, \quad q = 0, 1, \dots, N$

$$G_0(i\tau_q, j\tau_r) = \frac{-1}{Z}\lim_{N\to\infty}\int \prod_\ell \prod_{n=1}^{N} dc^*_{\ell n}\, dc_{\ell n}\, c_{iq}\, c^*_{jr}\, e^{-\sum_{\ell n k} c^*_{\ell n} M^{(\ell)}_{nk} c_{\ell k}} =$$

(Skip: ℓ)

$$= -\delta_{ij}\, \frac{\int \prod_{n=1}^{N} dc_n^*\, dc_n\, c_q\, c_r^*\, e^{-\sum_{nk} c_n^* M^{(i)}_{nk} c_k}}{\int \prod_{n=1}^{N} dc^*_n\, dc_n\, e^{-\sum_{n,k} c^*_n M^{(i)} c_k}}$$

Introduce "source terms": J^*, J

it is easy to see that:

$$G_0(i\tau_q, j\tau_r) = -\delta_{ij}\, \frac{\partial^2}{\partial J^*_q \partial J_r}\left[\frac{\int \prod_n dc^*_n dc_n\, e^{-\sum_{nk} c^*_n M^{(i)}_{nk} c_k + \sum_k (J^*_k c_k + c^*_k J_k)}}{\int \prod_n dc^*_n dc_n\, e^{-\sum_{nk} c^*_n M^{(i)}_{nk} c_k}}\right]_{\substack{J=0\\ J^*=0}} =$$

Gauß

$$= -\delta_{ij}\, \frac{\partial^2}{\partial J^*_q \partial J_r}\, e^{\sum_{n,k} J^*_n M^{-1}_{nk} J_k}\Bigg|_{\substack{J=0\\ J^*=0}} = -\delta_{ij}\, {M^{(i)}_{qr}}^{-1}$$

The inverse of M-matrix:

$$\left(M^{(i)}\right)^{-1} = \frac{1}{1-\zeta\alpha^N} \begin{array}{c} \quad \xrightarrow{r} \\ q\downarrow \begin{bmatrix} 1 & \zeta\alpha^{N-1} & \zeta\alpha^{N-2} & \cdots & \zeta\alpha \\ \alpha & 1 & \zeta\alpha^{N-1} & \cdots & \zeta\alpha^2 \\ \alpha^2 & \alpha & 1 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha^{N-1} & \alpha^{N-2} & \alpha^{N-3} & \cdots & 1 \end{bmatrix} \end{array}$$

Hence, for $q \geq r$

$$G_0(i\tau_q, j\tau_r) = -\delta_{ij} \lim_{N\to\infty} \left(M^{-1}_{(i)}\right)_{q,r} = -\delta_{ij} \lim_{N\to\infty} \frac{\alpha^{q-r}}{1-\zeta\alpha^N} =$$

$$= -\delta_{ij} \lim_{N\to\infty} \left(1-\frac{\beta}{N}(\varepsilon_i-\mu)\right)^{q-r} \left(1+\frac{\zeta}{\left(1-\frac{\beta}{N}(\varepsilon_i-\mu)\right)^N-\zeta}\right) =$$

$$= -\delta_{ij}\, e^{-(\varepsilon_i-\mu)(\tau_q-\tau_r)} \left(1+\frac{\zeta}{e^{\beta(\varepsilon_i-\mu)}-\zeta}\right) \equiv$$

$$\equiv -\delta_{ij}\, e^{-(\varepsilon_i-\mu)(\tau_q-\tau_r)} \left(1+\zeta n_i\right)$$

where $n_i \overset{\text{def}}{=} \dfrac{1}{e^{\beta(\varepsilon_i-\mu)}-\zeta}$ Boson-Fermion ocupation probability

Similar, for $q < r$

$$G_0(i\tau_q, j\tau_r) = -\delta_{ij} \lim_{N\to\infty} \frac{\zeta \alpha^{N+q-r}}{1-\zeta\alpha^N} =$$

$$= -\delta_{ij} \lim_{N\to\infty} \left(1-\frac{\beta}{N}(\varepsilon_i-\mu)\right)^{q-r} \frac{\zeta}{\left(1-\frac{\beta}{N}(\varepsilon_i-\mu)\right)^{-N}-\zeta} =$$

$$= -\delta_{ij}\, e^{-(\varepsilon_i-\mu)(\tau_q-\tau_r)} \zeta n_i$$

Combining:

$$G_0(i\tau, j\tau') = -\langle T_\tau\, \hat{c}_i(\tau)\, \hat{c}_j^{\dagger}(\tau')\rangle =$$

$$= -\delta_{ij}\, e^{-(\varepsilon_i-\mu)(\tau-\tau')} \left[\theta(\tau-\tau'-\delta)(1+\zeta n_i) + \zeta\,\theta(\tau'-\tau+\delta)\, n_i\right]$$

Fourier Transform $\quad \omega_n = \begin{cases} 2n\pi/\beta & \to B \\ (2n+1)\pi/\beta & \to F \end{cases}$

$$G_0^i = \int_0^\beta d\tau\, e^{i\omega_n\tau} G_0^i(\tau) = -\int_0^\beta d\tau\, e^{[i\omega_n-(\varepsilon_i-\mu)]\tau} \left[\theta(\tau)(1+\zeta n_i) + \zeta\,\theta(-\tau) n_i\right]$$

$$= -\frac{e^{\beta(i\omega_n-\varepsilon_i+\mu)}-1}{i\omega_n-\varepsilon_i+\mu} \frac{e^{\beta(\varepsilon_i-\mu)}}{e^{\beta(\varepsilon_i-\mu)}-\zeta} = + \frac{\cancel{\zeta - e^{\beta(\varepsilon_i-\mu)}}}{[i\omega_n-\varepsilon_i+\mu]\cancel{\left(e^{\beta(\varepsilon_i-\mu)}-\zeta\right)}} =$$

$$= \frac{1}{i\omega_n+\mu-\varepsilon_i}$$

– Matsubara Green Function non-interacting.

Back FT:

$$G_0^i(\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n \tau} \frac{1}{i\omega_n + \mu - \varepsilon_i}$$

Problem: $\sum_{\omega_n}$ is NOT converges

Convergence Factor: $\delta \to 0$

$$G_0^i(\tau) = \frac{1}{\beta}\sum_{\omega_n} \frac{e^{-i\omega_n(\tau-\delta)}}{i\omega_n + \mu - \varepsilon_i}$$

Matsubara Summation: $S = \frac{1}{\beta}\sum_{\omega_n} f(\omega_n)$

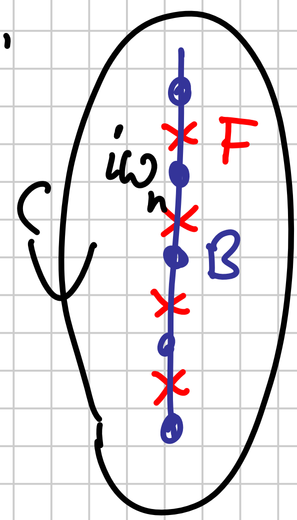
e.g.

$$F_0 = -\frac{1}{\beta}\ln Z_0 = \frac{\zeta}{\beta}\sum_{\substack{\omega_n \\ i}} \ln\left[-i\omega_n + \varepsilon_i\right]$$

Transform to contour integral:

$$\frac{1}{\beta}\sum_n \to \int \frac{d\omega}{2\pi} \to \oint_C \frac{dz}{2\pi i}$$

Introduce auxiliary function:



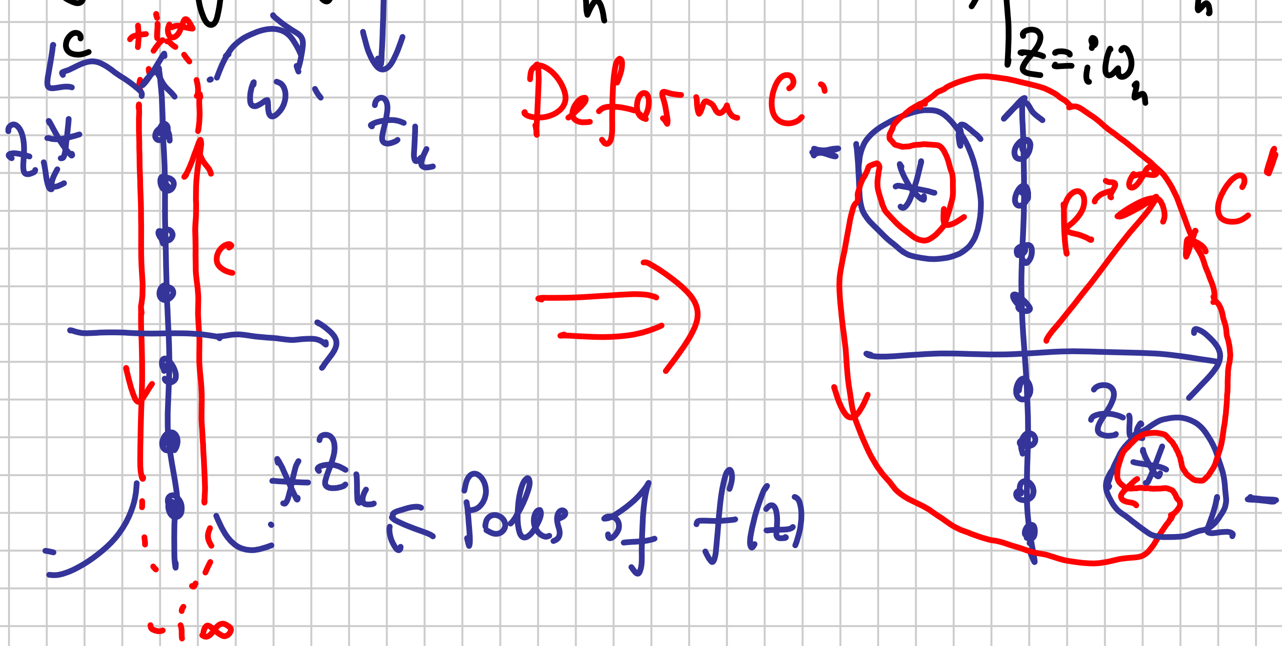
$$g(z) = \frac{1}{e^{\beta z} - \zeta}$$

$\to$ has poles at $i\omega_n$ $\nearrow$ B $\searrow$ F

Then

$$\oint \frac{dz}{2\pi i} g(z) \to \mathrm{Res}\left(g(i\omega_n)\right) = \frac{\zeta}{\beta}$$

$$\frac{\zeta}{2\pi i}\oint dz\, g(z) f(-iz) = \zeta \sum_n \mathrm{Res}\left(g(z) f(-iz)\right)\Big|_{z=i\omega_n} = \frac{1}{\beta}\sum_{\omega_n} f(\omega_n) = S$$



if: $f\cdot g \xrightarrow[|z|\to\infty]{} \infty$ faster as $\frac{1}{z}$, then

$$S = \frac{-\zeta}{2\pi i}\oint_{C'} dz\, f(-iz)\, g(z) = -\zeta \sum_k \mathrm{Res}\left[f(-iz)\, g(z)\right]_{z=z_k}$$

For example: $f(i\omega_n) = \dfrac{-\zeta e^{i\omega_n\delta}}{i\omega_n - \varepsilon}$

$\Rightarrow\ z_k = \varepsilon$

$$\frac{1}{\beta}\sum_{\omega_n} f(\omega_n) = -\zeta\, \mathrm{Res}\left(f(-iz)\, g(z)\right)_{z=\varepsilon} = \frac{1}{e^{\beta\varepsilon} - \zeta}$$

For $\delta \to 0$

$$-\frac{\zeta}{\beta}\sum_{\omega_n}\frac{e^{i\omega_n\delta}}{i\omega_n - \varepsilon} = \begin{cases} n_B(\varepsilon) = \dfrac{1}{e^{\beta\varepsilon}-1} & \text{- B} \\[2ex] n_F(\varepsilon) = \dfrac{1}{e^{\beta\varepsilon}+1} & \text{- F}\end{cases}$$

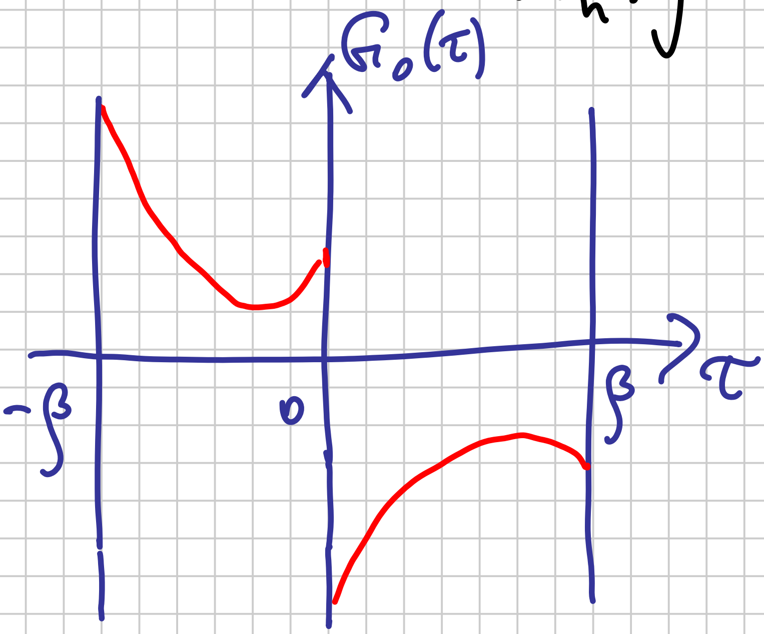
Continuous limit of Green's function

For fermions we have found:

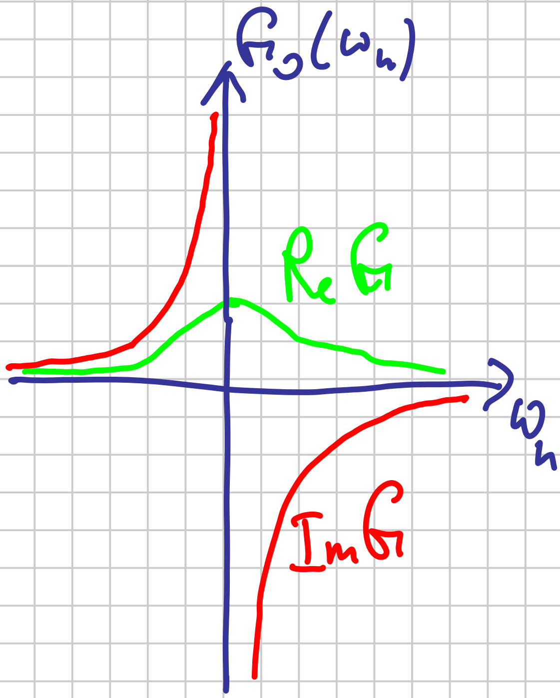
$$G_0^i(\tau) = -e^{-(\varepsilon_i-\mu)\tau}\left[\theta(\tau)(1-n_i) - \theta(-\tau)n_i\right]$$

$$\Big\updownarrow \text{FT}$$

$$G_0^i(\omega_n) = \frac{1}{i\omega_n+\mu-\varepsilon_i}$$



FT $\longleftrightarrow$



Equation:

$$(\partial_\tau - \varepsilon_i - \mu)\, G_0^i(\tau,\tau') = -\delta(\tau-\tau')$$

with boundary condition.

$$G^i(\beta,\tau') = \zeta\, G^i(0,\tau')$$

or:

$$G^i(\tau+\beta,\tau') = G^i(\tau,\tau'+\beta) = \zeta\, G^i(\tau,\tau')$$