Continuous-time impurity solvers

Impurity model: Hamiltonian H

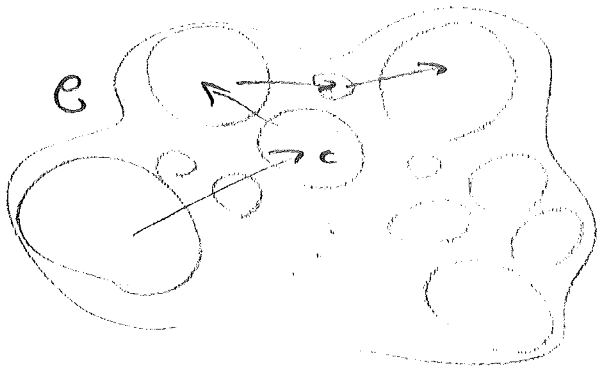
Partition function: $Z = \mathrm{Tr}\, e^{-\beta H}$

Observable: Green function $\quad G(\tau) = \frac{1}{Z}\mathrm{Tr}\left[e^{-(\beta-\tau)H} d\, e^{-\tau H} d^\dagger\right] \quad 0<\tau<\beta$

Define a configuration space $\mathcal{C}$ consisting of configurations c, whose contribution to Z and G is easily computed:

$$Z = \sum_{c\in\mathcal{C}} w_c \leftarrow \text{"weight" of } c$$

$$G = \frac{1}{Z}\sum_{c\in\mathcal{C}} G_c = \frac{1}{Z}\sum_c w_c \underbrace{\frac{G_c}{w_c}}_{\equiv\, g_c}$$



Implement a random walk in $\mathcal{C}$ in such a way that each configuration is visited with a probability $\sim |w_c|$.

Sufficient conditions: i) ergodicity (all c accessible)

ii) detailed balance

$$|w_1|\, p(c_1\to c_2) = |w_2|\, p(c_2\to c_1)$$

$$\Rightarrow G = \frac{\sum_c |w_c|\,\mathrm{sign}_c\, g_c}{\sum_c |w_c|\,\mathrm{sign}_c} \underset{\uparrow}{=} \frac{\langle \mathrm{sign}\cdot c\rangle_{MC}}{\langle \mathrm{sign}\rangle_{MC}}$$

if c is generated with probability $\sim |w_c|$

"sign problem", if $\langle\mathrm{sign}\rangle$ decreases exponentially with system size or β.

Continuous-time Monte Carlo

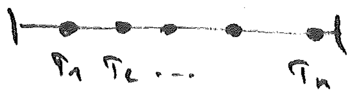
Step 1) Use interaction representation to write Z as a time-ordered exponential:

$$H = H_1 + H_2,\quad O(\tau) = e^{\tau H_1} O\, e^{-\tau H_1}, \quad Z = \mathrm{Tr}\left[e^{-\beta H_1} T_\tau\, e^{-\int_0^\beta d\tau H_2(\tau)}\right]$$

Step 2) Expand time ordered exponential into a power series

$$Z = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{n-1}}^\beta d\tau_n \, \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1} (-H_2) \cdots e^{-(\tau_2-\tau_1)H_1} (-H_2) e^{-\tau_1 H_1} \right]$$

$\Rightarrow \quad c = \{\tau_1, \ldots, \tau_n\} \quad \tau_i \in [0,\beta]$



$$w_c = (d\tau)^n \, \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1} (-H_2) \cdots e^{-(\tau_2-\tau_1)H_1} (-H_2) e^{-\tau_1 H_1} \right]$$

Anderson impurity model:

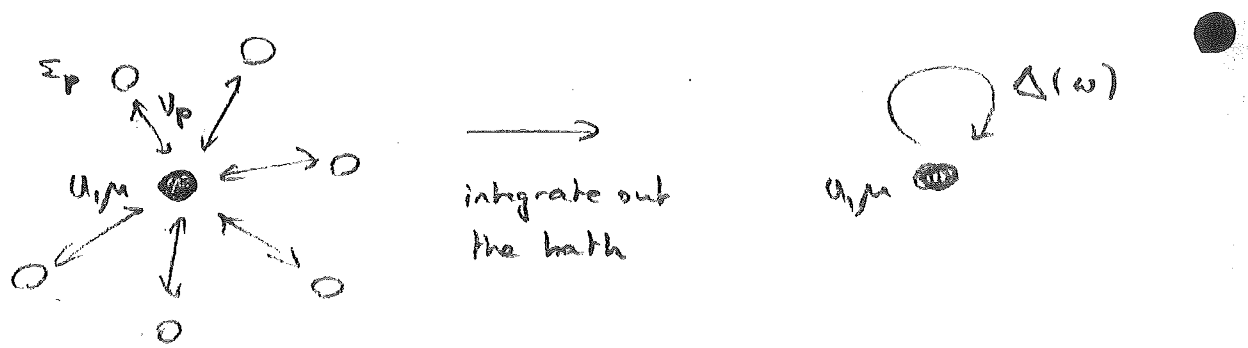
hybridization term — bath

$$H = \underbrace{U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow)}_{\downarrow} + \underbrace{\sum_{p,\sigma} (V_p^\sigma a^\dagger_{p\sigma} d_\sigma + h.c.)}_{\downarrow} + \sum_{p\sigma} \varepsilon_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}$$

$H_2^{\text{weak-coupling}}$ — $H_2^{\text{strong-coupling}}$

expand Z in powers of the interaction — expand Z in powers of the hybridization

Hamiltonian representation: — action formulation:



$$S = \int d\tau [U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow)]$$
$$+ \iint d\tau d\tau' \sum_\sigma d^\dagger_\sigma(\tau) \Delta_\sigma(\tau-\tau') d_\sigma(\tau')$$

Strong-coupling approach (hybridization expansion)

$$H_2 = \underbrace{\sum_{p\sigma} V_p^{\sigma} d^\dagger_\sigma a_{p\sigma}}_{\equiv H_2^{d^\dagger}} + \underbrace{\sum_{p\sigma} V_p^{\sigma *} a^\dagger_{p\sigma} d_\sigma}_{\equiv H_2^{d}}$$

need equal number of $d^\dagger$ and d $\to$ $\frac{2n!}{n!\,n!}$ possibilities for order $2n$

$$Z = \sum_{n=0}^{\infty} \frac{1}{(2n)!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_{2n}\, \mathrm{Tr}\left[e^{-\beta H_1}\, T\, H_2(\tau_{2n}) \ldots H_2(\tau_1)\right]$$

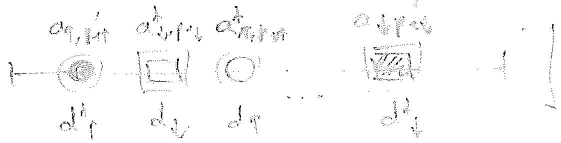
$$= \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \left(\int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n\right)\left(\int_0^\beta d\tau_1' \ldots \int_0^\beta d\tau_n'\right) \mathrm{Tr}\left[e^{-\beta H_1}\, T\, H_2^d(\tau_n) H_2^{d^\dagger}(\tau_n') \ldots H_2^d(\tau_1) H_2^{d^\dagger}(\tau_1')\right]$$

Note that H_2^d, $H_2^{d^\dagger}$ commute, because $d^\dagger a$

separating the d and $d^\dagger$ operators into $\sigma = \uparrow, \downarrow$ ($n = n_\uparrow + n_\downarrow \to \frac{n!}{n_\uparrow!\, n_\downarrow!}$ combinations)

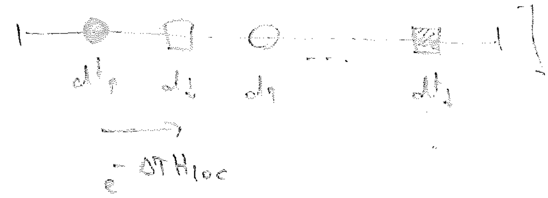
and time ordering the integrals gives

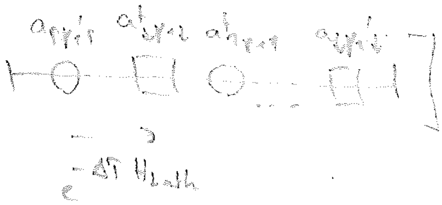
$$Z = \sum_{\{n_\sigma\}} \prod_\sigma \left(\int_0^\beta d\tau_1^\sigma \ldots \int_{\tau^\sigma_{n-1}}^\beta d\tau_n^\sigma\right)\left(\int_0^\beta d\tau_1'^\sigma \ldots \int_0^\beta d\tau_n'^\sigma\right)$$

$$\times\, \mathrm{Tr}\Big[e^{-\beta H_1} \prod_\sigma \sum_{\{p\}} \sum_{\{p'\}} VV^* \ldots VV^*$$  $\Big]$

$H_1 = H_{loc} + H_{bath}$ does not mix impurity and bath states

$\to$ separate $\mathrm{Tr}[\,]$ into impurity (d) and bath (a) states

impurity: $\mathrm{Tr}_d\Big[$  $\Big]$

bath: $Z_a \frac{1}{Z_a} \mathrm{Tr}_a\Big[\prod_\sigma \sum_{\{p\}} \sum_{\{p'\}} VV^* \ldots VV^*$  $\Big]$

H_{bath} is non-interacting $\Rightarrow$ Wick theorem gives $\frac{1}{Z_a}\mathrm{Tr}[\ldots] = \det(\ldots)$

What is det (...) ? $\to$ Compute lowest order $n_\sigma = 1, n_{\bar\sigma} = 0$

$$Z_{bath} = \prod_\sigma \prod_p \big(\underset{\substack{\downarrow \\ |1\rangle_p}}{e^{-\varepsilon_p \beta}} + \underset{\substack{\downarrow \\ |0\rangle_p}}{1} \big)$$

$$\sum_{p_1} \sum_{p_1'} V_{p_1}^\sigma V_{p_1'}^{\sigma *} \frac{1}{Z_{bath}} \operatorname{Tr}_a \left[e^{-\beta H_{bath}} T\, a^\dagger_{\sigma_1 p_1}(\tau_1^\sigma)\, a_{\sigma p_1'}(\tau_1'^\sigma) \right] \quad \to \quad p_1 = p_1'$$

$$= \sum_p \frac{|V_p|^2}{e^{-\varepsilon_p \beta} + 1} \begin{cases} e^{-\varepsilon_p(\beta - (\tau_1^\sigma - \tau_1'^\sigma))} & \tau_1^\sigma > \tau_1'^\sigma \\ -e^{-\varepsilon_p(\tau_1'^\sigma - \tau_1^\sigma)} & \tau_1^\sigma < \tau_1'^\sigma \end{cases}$$

$$\equiv \Delta_\sigma(\tau_1'^\sigma - \tau_1^\sigma) \qquad \text{hybridization function} \qquad \left[\Delta(i\omega_n) = \sum_p \frac{|V_p|^2}{i\omega_n - \varepsilon_p} \right]$$

For higher order, one gets $\frac{1}{Z_{bath}} \operatorname{Tr}_a [\dots] = \prod_\sigma \det M_\sigma^{-1}$, $(M_\sigma^{-1})_{ij} = \Delta_\sigma(\tau_i^\sigma - \tau_j'^\sigma)$

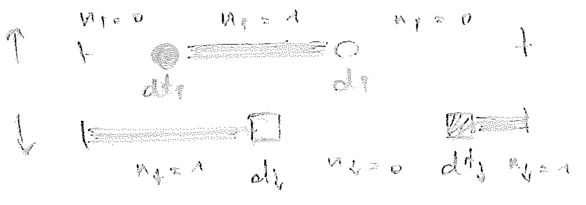
Monte Carlo configurations : $c = \{ \underbrace{\tau_1^\uparrow, \dots, \tau_{n_\uparrow}^\uparrow}_{n_\uparrow \times d_\uparrow} ; \underbrace{\tau_1'^\uparrow \dots \tau_{n_\uparrow}'^\uparrow}_{n_\uparrow \times d^\dagger_\uparrow} \mid \underbrace{\tau_1^\downarrow, \dots, \tau_{n_\downarrow}^\downarrow}_{n_\downarrow \times d_\downarrow} ; \underbrace{\tau_1'^\downarrow, \dots, \tau_{n_\downarrow}'^\downarrow}_{n_\downarrow \times d^\dagger_\downarrow} \}$

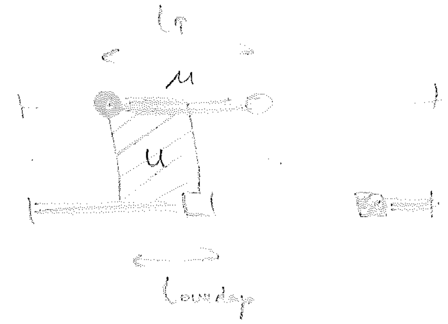
$$w_c = \underbrace{Z_{bath} \operatorname{Tr}_d \left[e^{-\beta H_{loc}} T \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d_\sigma^\dagger(\tau_{n_\sigma}'^\sigma) \dots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\tau_1'^\sigma) \right]}_{\text{impurity contribution}} \times \underbrace{\prod_\sigma \det M_\sigma^{-1}}_{\text{bath contribution}}$$

Impurity contribution must be evaluated explicitly.

Simple case : density-density interactions (occupation number basis is eigenbasis of H_{loc})

alternating $d_\sigma^\dagger$ and d_σ operators $\Rightarrow$ $c \mathrel{\hat=}$ collection of segments on $[0, \beta]$





Segment picture allows cheap calculation of $\operatorname{Tr}_d [\dots] = e^{\mu(l_\uparrow + l_\downarrow) - U l_{overlap}} \cdot s$

from time-ordering

Sampling procedure

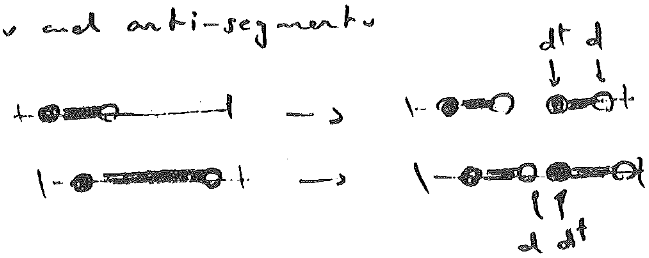
Z = sum over all segment conf.

local updates in the segment configurations

insertion / removal of segments and anti-segments

ex: insertion of segment

insertion of anti-segment



detailed balance

insertion: i) choose $d^\dagger, d$ randomly in $[0,\beta]$

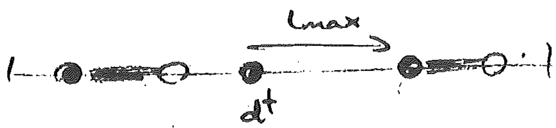
$$p^{prop}(n_\sigma \to n_\sigma+1) = \frac{d\tau}{\beta}\frac{d\tau}{\beta}$$

this will propose many unphysical conf. with weight 0

better: ii) choose $d^\dagger$ randomly in $[0,\beta]$

if it falls on a segment $\to$ reject move

if it falls on an empty space $\to$ compute l_{max}



choose d randomly in interval of length l_{max}

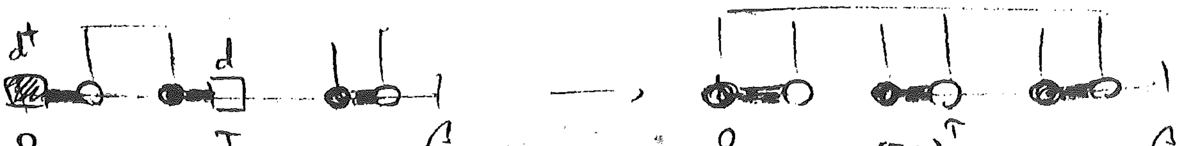
$$p^{prop}(n_\sigma \to n_\sigma+1) = \frac{d\tau}{\beta}\frac{d\tau}{l_{max}}$$

removal: choose a random segment:

$$p^{prop}(n_{\sigma+1} \to n_\sigma) = \frac{1}{n_\sigma+1}$$

$$\frac{p^{acc}(n_\sigma \to n_\sigma+1)}{p^{acc}(n_\sigma+1 \to n_\sigma)} = \underbrace{\frac{p^{prop}(n_\sigma+1 \to n_\sigma)}{p^{prop}(n_\sigma \to n_\sigma+1)}}_{\frac{\beta\, l_{max}}{(n_\sigma+1)\cancel{(d\tau)^2}}} \underbrace{\frac{|w_c(n_\sigma+1)|}{|w_c(n_\sigma)|}}_{\frac{|\det(M_\sigma^{(n_\sigma+1)})^{-1}|}{|\det(M_\sigma^{(n_\sigma)-1})|}\cancel{(d\tau)^2}}$$

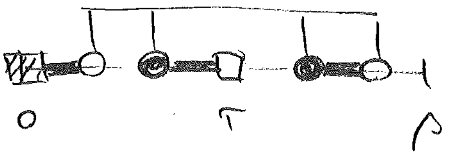
Measurement of the GF



$w_c^{d(\tau)d^\dagger(0)}$ $\qquad\qquad$ $w_c^{(\tau,0)}$ ↑

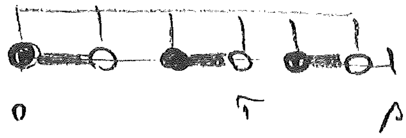
GF $\qquad\qquad$ Z

Measurement of the GF



$w_c^{d(\tau)d^\dagger(0)}$

diagram which appear in the expansion of $G(0,\tau)$



$w_c^{(0,\tau)}$

diagram with $d^\dagger$ at 0 and d at τ which appear in the expansion of Z

$$G(0,\tau) = \frac{1}{Z}\sum_c w_c^{d(\tau)d^\dagger(0)} = \frac{1}{Z}\sum_c w_c^{(0,\tau)} \underbrace{\frac{w_c^{d(\tau)d^\dagger(0)}}{w_c^{(0,\tau)}}}$$

$\mathrm{Tr}[\ldots]$ identical $\Rightarrow$ $\dfrac{\det M_c^{-1}}{\det (M_c^{(0,\tau)})^{-1}} =$

$(\quad) = (M_c^{(0,\tau)})^{-1}$

$d^\dagger$ (column j)

$$= \frac{\det\left(\;\begin{array}{c|c} & \\ \hline & \end{array}\;\right)}{\det\left(\quad\right)}\;(-1)^{i+j}$$

$\leftarrow d$ (row i)

minor ij $\leftrightarrow$ element of the inverse matrix

$$= \left(M_c^{(0,\tau)}\right)_{ji}$$

Want to go from $\sum_c w_c^{(0,\tau)}\left(M_c^{(0,\tau)}\right)_{ji}$ (with fixed operators at $0,\tau$) to

$\sum_{\tilde c} w_{\tilde c}\,(M_{\tilde c})_{ji}\,(\ldots)$ (no restriction on operator positions)

$$\downarrow$$

$$\sum_{ij}\frac{1}{\beta}\,\delta(\tau,\tau_i-\tau_j')$$

sum over n^2 $(d^\dagger,d)$ pairs, because we go from $\frac{1}{(n-1)!}\int_0^\beta d\tau_1\ldots d\tau_{n-1}\frac{1}{(n-1)!}\int_0^\beta d\tau_1'\ldots d\tau_{n-1}'$ $\leftarrow c$

to $\frac{1}{n!}\int_0^\beta d\tau_1\ldots d\tau_n\frac{1}{n!}\int_0^\beta d\tau_1'\ldots d\tau_n'$ $\leftarrow \tilde c$

$\Rightarrow$ $n^2\,\delta(\tau,\tau_1-\tau_1')$ or $\sum_{ij}\delta(\tau,\tau_i-\tau_j')$

$$G(\tau) = \frac{1}{\beta}\left\langle \sum_{ij}\delta(\tau,\tau_i-\tau_j')(M_c)_{ji}\right\rangle_{MC}$$

average perturbation order

kinetic energy per flavor $= \int_0^\beta d\tau \, G(\tau) F(\tau)$ $\qquad F(\tau) = -\Delta(\beta-\tau)$

$$\int_0^\beta d\tau \, G(\tau) F(\tau) = \frac{1}{\beta} \Big\langle \sum_{ij} M_{ji} \underbrace{\int d\tau \, \delta(\tau, \tau_i - \tau_j') F(\tau)}_{F(\tau_i-\tau_j')} \Big\rangle$$

$F(\tau_i - \tau_j')$

$$\begin{array}{c} j \\ \downarrow \end{array}$$

$$\frac{\det\left(\quad \right) \leftarrow i}{\det\left(F \right)} \, (-1)^{i+j} \qquad (M^{-1}) = (F)$$

For i fixed, this is the expansion of $\det\left(F \right)$ along row i

$$= \frac{1}{\beta} \Big\langle \sum_i \frac{\det(F)}{\det(F)} \Big\rangle = \frac{1}{\beta} \langle n \rangle$$

$\uparrow$ perturbation order

Same for multiband models

$\Rightarrow \quad E_{kin} = \frac{1}{\beta} \langle n \rangle$

In an action formulation:

$$Z = \mathrm{Tr}\Big[T e^{-\int_0^\beta d\tau \underbrace{(U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow))}_{H_{loc}} - \int_0^\beta d\tau d\tau' \sum_\sigma d_\sigma^\dagger(\tau)\Delta(\tau-\tau') d_\sigma(\tau')}\Big]$$

let us first consider spinless particles:

$$Z = \mathrm{Tr}\Big[T e^{+\mu\int_0^\beta d\tau\, n(\tau) - \int_0^\beta\int_0^\beta d\tau d\tau' d^\dagger(\tau)\Delta(\tau-\tau') d(\tau')}\Big]$$

$= \mathrm{Tr}[\qquad]$

$- \frac{1}{1!}\int\int_0^\beta d\tau d\tau' \; \mathrm{Tr}\Big[\; d^\dagger \; e^{\mu(\tau'-\tau)} \; d \;\Big] \, \mathrm{sign}(\tau,\tau')$ ← time ordering

$\Delta(\tau-\tau')$; (-1) in this example

$+ \frac{1}{2!}\int\int\int\int_0^\beta d\tau_1 d\tau_2 d\tau_1' d\tau_2' \; \mathrm{Tr}\Big[\qquad\Big] \, \mathrm{sign}(\tau_1,\tau_2,\tau_1',\tau_2')$

$(+1)$ in this example

$- \ldots$

let us rewrite this term:

i) time ordering the position of the creation operators gets rid of the $\frac{1}{2!}$

$\left(\frac{1}{2!}\int_0^\beta d\tau_1 d\tau_2 \rightarrow \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2\right)$

ii) time ordering the annihilation operators gives $2!$ topologically distinct diagrams

$\left(\int_0^\beta d\tau_1' d\tau_2' \; \mathrm{Tr}\Big[\; \tau_1 \;\; \tau_1' \;\; \tau_2 \;\; \tau_2' \;\Big]\, s\right.$

$$= \int_0^\beta d\tau_1' \int_{\tau_1'}^\beta d\tau_2' \Big(\underbrace{\mathrm{Tr}\Big[\; l_1 \;\; l_2\;\Big] 1 + \mathrm{Tr}\Big[\qquad\Big](-1)}_{e^{\mu(l_1+l_2)}\left(\Delta(\tau_1-\tau_1')\Delta(\tau_2-\tau_2') - \Delta(\tau_1-\tau_2')\Delta(\tau_2-\tau_1')\right)}\Big)$$

from time ordering of operators

$$= e^{\mu(l_1+l_2)} \det\begin{pmatrix}\Delta(\tau_1-\tau_1') & \Delta(\tau_1-\tau_2') \\ \Delta(\tau_2-\tau_1') & \Delta(\tau_2-\tau_2')\end{pmatrix}$$

$F(\tau_1'-\tau)$
$\shortparallel$

Note: • $\Delta(\tau) < 0$ for $0 < \tau < \beta$, in the above example, $\tau_1 - \tau_1' < 0 \Rightarrow \Delta(\tau_1 - \tau_1') > 0$ etc

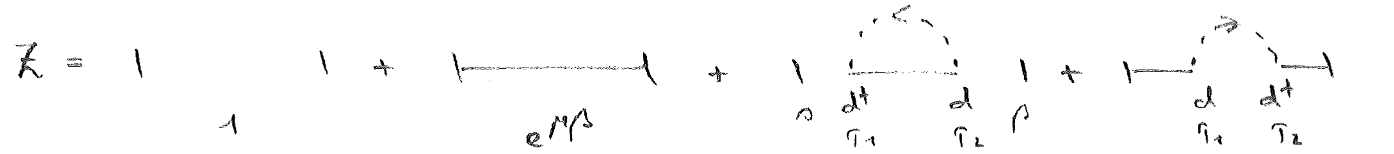
• $\mathrm{Tr}[\ldots]$ enforces alternation of creation and annihilation operators

$\Rightarrow$ segment picture

NCA

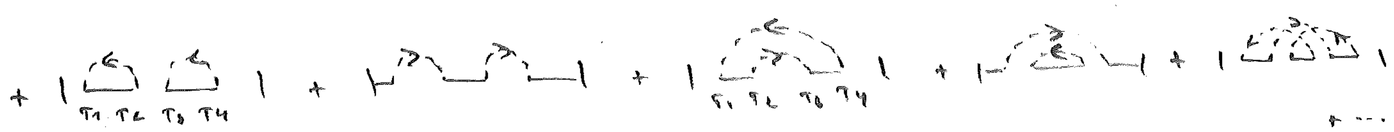
$\Delta(\tau)<0, \quad 0<\tau<\beta$

Noninteracting model : $Z = \mathrm{Tr}\, T e^{\int_0^\beta d\tau \mu n(\tau) - \int_0^\beta \int_0^\beta d\tau d\tau' d^\dagger(\tau) \Delta(\tau-\tau') d(\tau')}$



$e^{\mu(\tau_2-\tau_1)}\Delta(\tau_1-\tau_2)(-1)(-1)$ $\qquad$ $e^{\mu((\tau_1-0)+(\beta-\tau_2))} \times \Delta(\tau_2-\tau_1)(-1)$

expansion $\quad$ time-ordering $\qquad$ expansion



$e^{\mu((\tau_2-\tau_1)+(\tau_4-\tau_3))}\Delta(\tau_1-\tau_2)\Delta(\tau_3-\tau_4)(-1)^2(-1)^2$ $\qquad$ $e^{\mu((\tau_2-\tau_1)+(\tau_4-\tau_3))}\Delta(\tau_1-\tau_4)\Delta(\tau_3-\tau_2)(-1)^2(-1)$

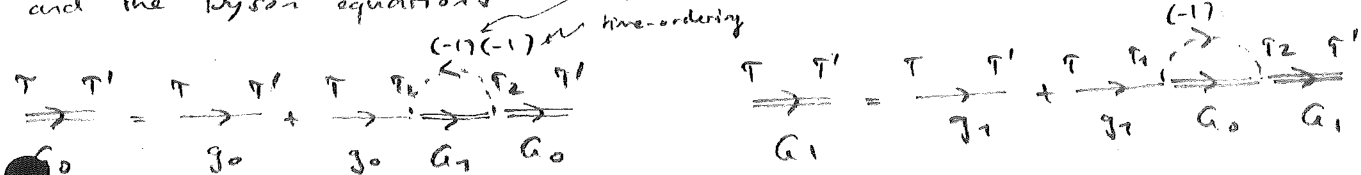
expansion $\quad$ time-ordering $\qquad$ expansion $\quad$ time-ordering

We can generate the terms of this series which do not contain crossing hybridization lines by introducing the bare pseudoparticle propagators

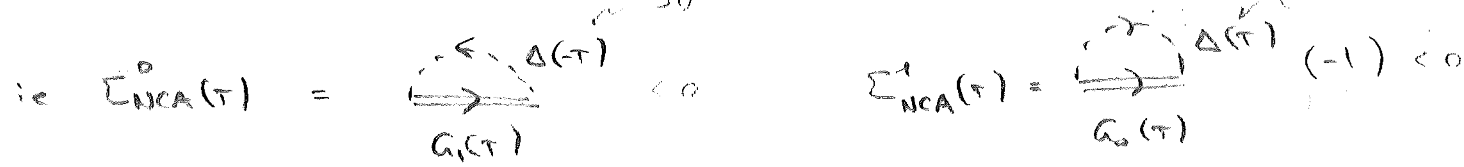
$\underset{g_0}{\longrightarrow}$ $\quad g_0(\tau) = -e^{-\epsilon_0 \tau}$, $\quad \epsilon_0 = 0$ $\qquad$ $\underset{g_1}{\longrightarrow}$ $\quad g_1(\tau) = -e^{-\epsilon_1\tau}$, $\quad \epsilon_1 = \mu$

convention

and the Dyson equations



$\tau<\tau_1<\tau_2<\tau'$ $\qquad\qquad$ $\tau<\tau_1<\tau_2<\tau'$



$$G_0(\tau) = g_0(\tau) + \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1\, g_0(\tau_1)\, \Sigma^0_{NCA}(\tau_2-\tau_1)\, G_0(\tau-\tau_2)$$

$\rightarrow G_\alpha(0) = -1$

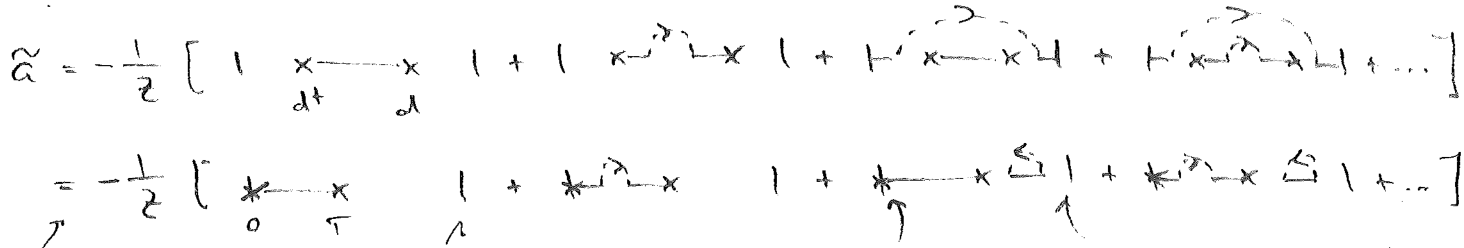
$$G_1(\tau) = g_1(\tau) + \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1\, g_1(\tau)\, \Sigma^1_{NCA}(\tau_2-\tau_1)\, G_1(\tau-\tau_2)$$

Note that the minus sign in the definition of g_0, g_1 (convention) just gives a global minus sign for the diagrams in Z_{NCA}, because $g_\alpha, G_\alpha, \Sigma_\alpha$ are all <0

$\rightarrow$ odd number of negative factors.

$Z_{NCA} = -(G_0(\beta) + G_1(\beta)) > 0$ $\qquad$ $G_0(\beta)$: contribution of $\langle 0| \dots |0\rangle$
$G_1(\beta)$: " " $\langle 1| \dots |1\rangle$

Physical GF:



translational invariance

always particle at 0_+ and T_-

always no particle at T_+ and β_-

$$\overset{\sim}{=} -\frac{1}{Z_{NCA}}\; G_1(T)\; G_0(\beta - T) \quad < 0$$

NCA

(since we have an even # of G_α factors, the sign of G_α does not matter for this formula)

If we define the β-(anti)-periodic boundary conditions

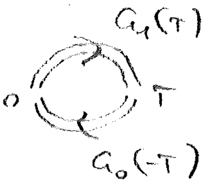
$$G_0(\beta - T) = G_0(-T) \qquad \text{(no fermion)}$$

$$G_1(\beta - T) = -G_1(-T) \qquad \text{(1 fermion)}$$

Note that the pseudoparticle GF are not true bosonic / fermionic GF, ie $G_1(0_+) + G_1(\beta_-) \neq 1$, but they "inherit" the (anti)periodic B.C.

we obtain

$$\tilde{G}_{NCA} = -\underbrace{\frac{1}{Z_{NCA}}}_{>0}$$



< 0

Since this diagram has an even # of GF factors, $\tilde{G}_{NCA}$ will inherit the same sign convention as g_0, g_1, ie $\tilde{G}_{NCA} < 0$.

Sanity check: is $\tilde{G}_{NCA}$ a fermionic GF, ie is $\tilde{G}_{NCA}(0_+) + \tilde{G}_{NCA}(\beta_-) = -1$?

$$\tilde{G}_{NCA}(0_+) + \tilde{G}_{NCA}(\beta_-) = \frac{1}{Z_{NCA}}\Big[-\underbrace{G_1(0_+)}_{-1}\underbrace{G_0(0_-)}_{G_0(\beta_-)} - G_1(\beta_-)\underbrace{G_0(-\beta_+)}_{G_0(0_+) = -1}\Big]$$

$$= +\frac{1}{Z_{NCA}}\big[\underbrace{G_0(\beta_-) + G_1(\beta_-)}_{-Z_{NCA}}\big]$$

$$= -1 \checkmark$$