DMFT

Hu Haoyu

1 Impurity model

A general impurity model is

$$
\begin{aligned}
S_{imp} = &\sum d_\alpha^\dagger(-i\omega + \epsilon_d + \Delta_{\alpha\gamma}(i\omega))d_\gamma \\
&+ \sum n_l(-i\Omega)(U_l - \Lambda_l(i\Omega))n_l(i\Omega) \\
&+ \sum_l L_l^\dagger(i\Omega)(J_l - \Gamma_l(i\Omega))L_l(i\Omega)
\end{aligned}
$$

where each n_l field denotes the superposition of the density field, and L_l denotes the superposition of $d_\alpha^\dagger d_\gamma$ fields.

We first introduce the fermionic bath,

$$
\begin{aligned}
&\exp(-\sum d_\alpha^\dagger(-i\omega + \Delta_{\alpha\gamma}(i\omega))d_\gamma) \\
=&\int D[c, c^\dagger]\exp(-\sum c^\dagger(-i\omega + \epsilon)c - \sum(V_{p,\alpha}^l c_{p,l}^\dagger d_\alpha + h.c.))
\end{aligned}
$$

where

$$
\Delta = \sum_p V^\dagger[i\omega - \epsilon]^{-1}V
$$

Then we define the bosonic bath for the density density interaction part

$$
\begin{aligned}
&\exp(\sum n_l(-i\Omega)\Lambda_l(i\Omega)n_l(i\Omega)) \\
=&\int D[b, b^\dagger]\exp\left[-\sum b_{l,q}^\dagger(-i\Omega + \omega_{l,q}^b)b_{l,q} - \sum g_l \sum_q (b_{l,q} + b_{l,q}^\dagger)n_l\right]
\end{aligned}
$$

where

$$\Lambda_l(i\Omega) = \sum_q \frac{g_l^2 \omega_{l,q}^b}{\Omega^2 + (\omega_{l,q}^b)^2}$$

It's worth to mention that we only need to consider a odd DOS of ω^b. We assume $n_l = \sum v_\alpha^l n_\alpha$, the coupling with bosonic bath can be written as

$$\sum g_l \sum_q (b_{l,q} + b_{l,q}^\dagger) n_l = \sum n_\alpha(i\Omega) B_\alpha(-i\Omega)$$
$$B_\alpha(i\Omega) = \sum_l g_l v_\alpha^l (b_{l,q}^\dagger(-i\Omega) + b_{l,q}(i\Omega))$$

Finally, we consider the L_l part

$$\begin{aligned}&\exp(\sum L_l^\dagger(i\Omega)\Gamma_l(i\Omega)L_\gamma^l(i\Omega))\\ =&\int D[\phi_l^\dagger, \phi_l] \exp(-\sum(\phi_{l,q}^\dagger(-i\Omega + \omega_{l,q}^\phi)\phi_{l,q} + L_l^\dagger h_l^\dagger \phi_{l,q} + \phi_{l,q}^\dagger h_l L_l))\end{aligned}$$

where

$$\Gamma_l(i\Omega) = \sum_q \frac{h_l^\dagger h_l}{-i\Omega + \omega_{l,q}^\phi}$$

The action is hermitian which requires $\Gamma_l(i\Omega)^\dagger = \Gamma_l(i\Omega)$. Consequently, we have $\sum_q \frac{1}{\Omega^2 + (\omega_{l,q}^\phi)^2} = 0$, and the density of state corresponding to the $\omega_{l,q}^\phi$ is odd. Then we have

$$\Gamma_l(i\Omega) = \sum_{q, \omega_{l,q}^\phi > 0} \frac{h_l^\dagger h_l 2\omega_{l,q}^\phi}{\Omega^2 + (\omega_{l,q}^\phi)^2}$$

We assume $L^l = \sum_{\alpha,\gamma} u_{\alpha\gamma}^l d_\alpha^\dagger d_\gamma$. The coupling between impurity and bosonic bath takes the form of

$$\sum \left[h_l u_{\alpha\gamma}^l \phi_{l,q}^\dagger d_\alpha^\dagger d_\gamma + h.c. \right]$$

At this step, we write down the Hamiltonian of BF model as following

$$\begin{aligned}H =& \sum d^\dagger \epsilon_d d + \sum_l n_l U_l n_l + \sum_l L_l^\dagger J_l L_l\\ &+ \sum_{\alpha,p} V_{p\alpha} \left[c_{p,\alpha}^\dagger d_\alpha + h.c. \right] + \sum_\alpha d_\alpha^\dagger d_\alpha \left(\sum_{l,q} g_l v_\alpha^l (b_{l,q}^\dagger + b_{l,q}) \right) + \sum_{\alpha,\gamma} \left[d_\alpha^\dagger d_\gamma \left(\sum_{l,q} h_l u_{\alpha\gamma}^l \phi_{l,q}^\dagger \right) + h.c. \right]\\ &+ \sum \epsilon_{\alpha\gamma,p} c_{\alpha,p}^\dagger c_{\gamma,p} + \sum_{l,q} \omega_{l,q}^b b_{l,q}^\dagger b_{l,q} + \sum_{l,q} \omega_{l,q}^\phi \phi_{l,q}^\dagger \phi_{l,q}\end{aligned}$$

Here, we consider a orbital diagronalized ϵ_d.

2 Canonical transformation

We consider the following canonical transformation

$$
\begin{aligned}
S &= \exp\left[\sum_{\alpha\sigma}\sum_{l} g_l v_\alpha^l n_\alpha \sum_q \frac{1}{\omega_{l,q}^b}(b_{l,q}^\dagger - b_{l,q})\right] \\
\tilde{H} &= e^S H e^{-S}
\end{aligned}
$$

it seems that, we can make the gauge transformation $d(\tau) = e^{A(\tau)} f(\tau)$ with $\partial_\tau A(\tau) = B(\tau)$ to do the same thing??

We notice that

$$
\begin{aligned}
\widetilde{d}_\alpha &= e^S d_{\alpha,\sigma} e^{-S} \\
&= d_\alpha e^{-\sum_l g_l v_l^\alpha \sum_q \frac{1}{\omega_{l,q}^b}(b_{l,q}^\dagger - b_{l,q}))} \\
\widetilde{b}_l &= e^S b_l e^{-S} \\
&= b_{l,q} - \sum_\alpha g_l v_\alpha^l n_\alpha \frac{1}{\omega_{l,q}^b}
\end{aligned}
$$

Then we have

$$
\begin{aligned}
H =& \sum d^\dagger \widetilde{\epsilon}_d d + \sum_{\alpha\neq\gamma} n_\alpha \widetilde{U}_{\alpha\gamma} n_\gamma + \sum_l \widetilde{L}_l^\dagger J_l \widetilde{L}_l \\
&+ \sum_{\alpha,p} V_{p\alpha}\left[c_{p,\alpha}^\dagger \widetilde{d}_\alpha + h.c.\right] + \sum_{l,q}\left[\widetilde{L}_l \phi_{l,q}^\dagger + h.c.\right] \\
&+ \sum \epsilon_{\alpha\gamma,p} c_{\alpha,p}^\dagger c_{\gamma,p} + \sum_{l,q} \omega_{l,q}^b b_{l,q}^\dagger b_{l,q} + \sum_{l,q} \omega_{l,q}^\phi \phi_{l,q}^\dagger \phi_{l,q}
\end{aligned}
$$

where

$$
\begin{aligned}
\widetilde{U}_{\alpha\gamma} &= U_{\alpha\gamma} - \sum_l g_l^2 v_\alpha^l v_\gamma^l (\sum_q \frac{1}{\omega_{l,q}^b}) \\
(\widetilde{\epsilon}_d)_\alpha &= (\epsilon_d)_\alpha - \sum_l g_l^2 (v_\alpha^l)^2 \sum_q \frac{1}{\omega_{l,q}^b}
\end{aligned}
$$

Can we do the same thing for L ?

3 Expansion scheme

To derive a expansion scheme, we reformulate the Hamiltonian as following

$$
\begin{aligned}
H =& \sum d^\dagger \epsilon_d d + \sum_l n_l \widetilde{U}_l n_l \\
&+ \sum_{\alpha,\gamma} \widetilde{L}^\dagger_{\alpha\gamma} J_{\alpha\gamma,\delta\sigma} \widetilde{L}_{\delta\sigma} \\
&+ \sum_\alpha \left[C^\dagger_\alpha \widetilde{d}_\alpha + h.c. \right] + \sum_{\alpha,\gamma} \left[\widetilde{L}_{\alpha\gamma} \phi^\dagger_{\alpha\gamma} + h.c. \right] \\
&+ \sum \epsilon_{\alpha\gamma,p} c^\dagger_{\alpha,p} c_{\gamma,p} + \sum_{l,q} \omega^b_{l,q} b^\dagger_{l,q} b_{l,q} + \sum_{l,q} \omega^\phi_{l,q} \phi^\dagger_{l,q} \phi_{l,q}
\end{aligned}
$$

where $C_\alpha = \sum_p V_{p,\alpha} c_{p,\alpha}$,$L_{\alpha\gamma} = \widetilde{d}^\dagger_\alpha \widetilde{d}_\gamma$ and $\phi_{\alpha\gamma} = \sum_{q,l} u^l_{\alpha\gamma} \phi_{l,q}$ We do a triple expansion to expand the following three terms

$$
\begin{aligned}
&\sum_{\alpha,p} V_{p\alpha} \left[c^\dagger_{p,\alpha} \widetilde{d}_\alpha + h.c. \right] \\
&\sum_{\alpha,\gamma} \widetilde{L}^\dagger_{\alpha\gamma} J_{\alpha\gamma,\delta\sigma} \widetilde{L}_{\delta\sigma} \\
&\sum_{\alpha,\gamma} \left[\widetilde{L}_{\alpha\gamma} \phi^\dagger_{\alpha\gamma} + h.c. \right]
\end{aligned}
$$

Then we have

$$
\begin{aligned}
Z =& Z_0 \sum_{\langle\sigma\rangle,n} \int_0^\beta d\tau_1^{\sigma_1} \int_{\tau_1^{i_1}}^\beta d\tau_1^{\sigma_2} ... d\tau_n^{\sigma_n} (-J)^{n_J} \\
& Tr[e^{-\beta H_C} \langle C^\dagger, C \rangle] \\
& Tr[e^{-\beta H_\phi} \langle \phi^\dagger, \phi \rangle] \\
& Tr[e^{-\beta H_{loc} - \beta H_b} \langle \widetilde{d}, \widetilde{d}^\dagger, \widetilde{L}, \widetilde{L}^\dagger \rangle]
\end{aligned}
$$

where $\sigma_i \in \{C^-_\alpha, C^+_\alpha, \phi^+_{\alpha\gamma}, \phi^-_{\alpha\gamma}, L^+_{\alpha\gamma}, L^-_{\alpha\gamma}\}$. Each symbol denotes the corresponding expansion term. n_J represents the order of $\widetilde{L}^\dagger J \widetilde{L}$ term

3.1 Fermionic bath

We first consider trace term of $C, C^\dagger$. Consider the following sequence

$$
Tr[e^{-\beta H_C} \Pi_{i=1}^{2n} C^{p_i}_{\alpha_i}(\tau_i)]
$$

with $p_i \in \{null, \dagger\}$ and $\tau_1 \le \tau_2 \le, ..., \le \tau_{2n}$. We reformulate $\{\tau_i\}$, into two sets, with $\{\tau_j^{s,\alpha_j}\}$ corresponds to C_{α_j} and $\{\tau_j^{e,\alpha_i}\}$ corresponds to $C^\dagger_{\alpha_j}$. So

$$\begin{aligned}
&Tr[e^{-\beta H_C} \langle C_{\alpha_i^s}(\tau_i^{s,\alpha_i^s}), C^\dagger_{\alpha_i^e}(\tau_i^{e,\alpha_i^e})\rangle]\\
=&Tr[T_\tau e^{-\beta H_C} \Pi_i C^\dagger_{\alpha_i^e}(\tau_i^{s,\alpha_i^e}) C_{\alpha_i^s}(\tau_i^{s,\alpha_i^s})](-1)^{P_C}\\
=&\det(M_{ij}^{-1})(-1)^{P_C}
\end{aligned}$$

where

$$\begin{aligned}
M_{ij}^{-1} &= \Delta_{\alpha_i^s,\alpha_j^e}(\tau_j^{s,\alpha_i^s} - \tau_i^{e,\alpha_j^e})\\
\Delta_{\alpha\gamma}(i\omega) &= \sum_p V^\dagger_{p,\alpha}[i\omega - \epsilon_p]^{-1} V_{p,\gamma}
\end{aligned}$$

and P_C denotes the permutation from time order to $\Pi C^\dagger C$ configuration.

3.2 density bosonic bath

For the density bosonic bath, we need to evaluate the following trace

$$\begin{aligned}
&Tr[T_\tau e^{-H_b\beta} \exp(\sum_i s_i B_{\alpha_i}(\tau_i))]\\
&B_{\alpha_i} = \sum_l g_l v_l^\alpha \sum_q \frac{1}{\omega^b_{l,q}}(b^\dagger_{l,q} - b_{l,q})
\end{aligned}$$

Note that each phase factor is attached to a d operator. $s_i = +/-$ if the corresponding d operator is creation/annihilation operator. To evaluate the trace, we consider the following path integral form

$$\begin{aligned}
&\int D[b,b^\dagger]\exp(-\sum b^\dagger(-i\Omega + \omega^b)b + \int d\tau J_{l,q}(\tau)(b^\dagger_{l,q}(\tau) - b_{l,q}(\tau))\\
=&\int D[b,b^\dagger]\exp(-\sum b^\dagger(-i\Omega + \omega^b)b + \sum J_{l,q}(\Omega)b^\dagger_{l,q}(\Omega) - \sum J_{l,q}(-\Omega)b_{l,q}(\Omega))\\
=&Z_0\exp(J_{l,q}(-i\Omega)\frac{1}{i\Omega - \omega_b}J_{l,q}(i\Omega))\\
=&Z_0\exp(-\int J_{l,q}(\tau_1)F_{l,q}(\tau_1 - \tau_2)J_{l,q}(\tau_2))
\end{aligned}$$

where

$$F_{l,q}(\tau) = \sum_\Omega \frac{e^{-i\Omega\tau}}{-i\Omega + \omega^b} = \frac{e^{\omega^b_{l,q}(\beta-\tau)}}{e^{\beta\omega^b_{l,q}} - 1}$$

We let $J_{l,q}(\tau) = \sum_i s_i g_l v_l^{\alpha_i} \frac{1}{\omega_{l,q}^b}\delta(\tau - \tau_i)$. Then we have

$$
\begin{aligned}
&Tr[T_\tau e^{-H_b\beta} \exp(\sum_i s_i B_{\alpha_i}(\tau_i))] \\
\propto &\exp\Big[-\sum_{i,j} s_i s_j \sum_l v_l^{\alpha_i} v_l^{\alpha_j} \sum_q (\frac{1}{\omega_{l,q}^b})^2 F_{l,q}(\tau_i - \tau_j)\Big] \\
= &\exp\Big[-\sum_l (\sum_i s_i v_l^{\alpha_i})^2 B_{l,q}(0) - 2\sum_{i>j} s_i s_j \sum_l v_l^{\alpha_i} v_l^{\alpha_j} (B_l(\tau_i - \tau_j) - B_l(0))\Big]
\end{aligned}
$$

Where

$$
\begin{aligned}
F_l(i\Omega) &= \sum_q \frac{\omega_{l,q}^b}{\Omega^2 + (\omega_{l,q}^b)^2} \\
&= \int_0^\infty d\omega \frac{2\omega\rho_l^b(\omega)}{\Omega^2 + \omega^2} \\
F_l(\tau) &= \frac{1}{\beta} F(i\Omega = 0) + \frac{1}{\beta}\sum_{\Omega\neq 0} F(i\Omega)\cos(\Omega\tau) \\
B_l(\tau) &= \sum_q (\frac{1}{\omega_{l,q}^b})^2 F_{l,q}(\tau_i - \tau_j)
\end{aligned}
$$

Then we found $B_l(\tau)$ and $F_l(\tau)$ satisfy

$$
\begin{aligned}
&\frac{d^2}{d\tau^2} X(\tau) = F_l(\tau) \\
&X(\tau \to 0^+) = X(\tau \to \beta - 0^+) = 0 \\
&X(\tau) = B(\tau) - B(0)
\end{aligned}
$$

We found

$$
B(\tau) - B(0) = \frac{F_l(0)}{2\beta}\tau(\tau - \beta) + \frac{1}{\beta}\sum_{\Omega\neq 0} F_l(i\Omega)\frac{1 - \cos(\Omega\tau)}{\Omega^2}
$$

If we maintain segment picture, i.e. the local Hamiltonian only involves density-density interaction and local potential is diagonal, then each $d_\alpha^\dagger$ operator matches a corresponding d_α operator. Consequently. $\sum_i s_i v_l^{\alpha_i} = 0$

3.3 Flipped bosonic bath

We need to evaluate:

$$
\begin{aligned}
&\phi_{\alpha_i\gamma_i} = \sum_{l,q} h_l^*(u_{\alpha\gamma}^l)^*\phi_{l,q} \\
&\langle T_\tau e^{-\beta H_\phi}\Pi_i \phi_{\alpha_i\gamma_i}(\tau_i^s)\phi^\dagger_{\alpha_i\gamma_i}(\tau_i^e)\rangle \\
\propto &\prod_{i,j} D_{\alpha_i\gamma_i,\alpha_j\gamma_j}(\tau_i^s-\tau_j^e) \\
&D_{\alpha_i\gamma_i,\alpha_j\gamma_j}(\tau_i^s-\tau_j^e) \\
= &\sum_l h_l^*(u_{\alpha_i\gamma_i}^l)^* h_l u_{\alpha_j\gamma_j}^l \Gamma_l(\tau) \\
&\Gamma_l(\tau) = \frac{1}{\beta}\sum F_l(i\Omega)e^{-i\Omega\tau}
\end{aligned}
$$

3.4 Summary

We summarize the expansion as following First, the original Hamiltonian is

$$
\begin{aligned}
H = &\sum d^\dagger \epsilon_d d + \sum n_\alpha U_{\alpha\gamma} n_\gamma + \sum (L_{\alpha\gamma})^\dagger J_{\alpha\gamma,\delta\sigma} L_{\sigma\delta} \\
&+ \sum_{l,\alpha,p}\left[V_{p,\alpha}^l c_{p,\alpha}^\dagger d_\alpha + h.c.\right] + \sum_\alpha d_\alpha^\dagger d_\alpha\left(\sum_{l,q} g_l v_\alpha^l(b_{l,q}^\dagger + b_{l,q})\right) + \sum_{\alpha>\gamma}\left[d_\alpha^\dagger d_\gamma\left(\sum_{l,q} h_l u_{\alpha\gamma}^l \phi_{l,q}^\dagger\right) + h.c.\right] \\
&+ \sum \epsilon_{l,p} c_{l,p}^\dagger c_{l,p} + \sum_{l,q}\omega_{l,q}^b b_{l,q}^\dagger b_{l,q} + \sum_{l,q}\omega_{l,q}^\phi \phi_{l,q}^\dagger \phi_{l,q}
\end{aligned}
$$

After integrating out fermionic and bosonic bath

$$
\begin{aligned}
S = &\sum d^\dagger(-i\omega + \epsilon_d)d + \sum n_\alpha U_{\alpha\gamma} n_\gamma + \sum (L_{\alpha\gamma})^\dagger J_{\alpha\gamma,\delta\sigma} L_{\sigma\delta} \\
&+ \sum d_\alpha^\dagger \Delta_{\alpha\gamma} d_\gamma \\
&- \sum n(-i\Omega)_\alpha \Lambda_{\alpha,\gamma}(i\Omega) n_\gamma(i\Omega) \\
&- \sum (L_{\alpha\gamma})^\dagger(i\Omega)\Gamma_{\alpha\gamma,\delta\sigma}(i\Omega) L_{\delta\sigma}(i\Omega)
\end{aligned}
$$

with $n_\alpha = d_\alpha^\dagger d_\alpha$, $L_{\alpha\gamma} = d_\alpha^\dagger d_\gamma$.

$$\Delta(i\omega)_{\alpha\gamma} = \sum_{p,l} \frac{(V^l_{\alpha,p})^\dagger V^l_{\gamma,p}}{i\omega - \epsilon_{l,p}}$$

$$\Lambda_{\alpha,\gamma}(i\Omega) = \sum_{q,l} g_l^2 \frac{(v^l_\alpha) v^l_\gamma}{-i\Omega + \omega^b_{l,q}} = \sum_{q,l} g_l^2 \frac{(v^l_\alpha)^\dagger v^l_\gamma \omega^b_{l,q}}{\Omega^2 + (\omega^b_{l,q})^2}$$

$$\Gamma_{\alpha\gamma,\delta\sigma}(i\Omega) = \sum_{q,l} h_l^\dagger h_l \frac{(u^l_{\alpha\gamma})^\dagger u^l_{\delta\sigma}}{-i\Omega + \omega^\phi_{l,q}} = \sum_{q,l} h_l^\dagger h_l \frac{(u^l_{\alpha\gamma})^\dagger u^l_{\delta\sigma} \omega^\phi_{l,q}}{\Omega^2 + (\omega^\phi_{l,q})^2}$$

We perform canonical transformation and let

$$\widetilde{d}_\alpha = d_\alpha e^{-\sum_l g_l v^\alpha_l \sum_q \frac{1}{\omega^b_{l,q}} (b^\dagger_{l,q} - b_{l,q})}$$

We then have

$$\begin{aligned}
H &= H_{loc} + H_c + H_b + H_\phi + H_{dc} + H_{L\phi} + H_{LL} \\
H_{loc} &= \sum \epsilon^\alpha_d n_\alpha + \sum_l n_\alpha \widetilde{U}_{\alpha\gamma} n_\gamma \\
H_c &= \sum_{l,p} \epsilon_{l,p} c^\dagger_{l,p} c_{l,p} \\
H_b &= \sum_{l,q} \omega^b_{l,p} b^\dagger_{l,p} b_{l,p} \\
H_\phi &= \sum_{l,q} \omega^\phi_{l,p} \phi^\dagger_{l,p} \phi_{l,p} \\
H_{dc} &= \sum_{\alpha,l,p} V^l_{\alpha,p} c^\dagger_{l,p} \widetilde{d}_{\alpha,p} + h.c. \\
H_{L\phi} &= \sum_{l,\alpha\gamma,q} h_l u^l_{\alpha\gamma} \phi^\dagger_{l,q} \widetilde{L}_{\alpha\gamma} + h.c. \\
H_{LL} &= \sum_{\alpha\gamma,\delta\sigma} (\widetilde{L}_{\alpha\gamma})^\dagger J_{\alpha\gamma,\delta\sigma} \widetilde{L}_{\sigma\delta}
\end{aligned}$$

We only need to expand $H_{dc}, H_{L\phi}, H_{LL}$ terms. We reach the following configuration

$$\begin{aligned}
&\prod_i C^\dagger_{\alpha_i^{c,e}}(\tau_i^{c,e}) C_{\alpha_i^{c,s}}(\tau_i^{c,s}) \prod_i \widetilde{d}_{\alpha_i^{c,e}}(\tau_i^{c,e}) \widetilde{d}^\dagger_{\alpha_i^{c,s}}(\tau_i^{s,e}) \\
&\prod_i \Phi_{\alpha_i^{\phi,s}\gamma_i^{\phi,s}}(\tau_i^{\phi,s}) \Phi^\dagger_{\alpha_i^{\phi,e}\gamma_i^{\phi,e}}(\tau_i^{\phi,e}) \prod_i \widetilde{L}^\dagger_{\alpha_i^{\phi,s}\gamma_i^{\phi,s}}(\tau_i^{\phi,s}) \widetilde{L}_{\alpha_i^{\phi,e}\gamma_i^{\phi,e}}(\tau_i^{\phi,e}) \\
&\prod_i \Big(- J_{\alpha_i^L \gamma_i^L, \delta_i^L \sigma_i^L} \Big) (\widetilde{L}_{\alpha_i^L \gamma_i^L})^\dagger (\tau_i^L) \widetilde{L}_{\sigma_i^L \delta_i^L}(\tau_i^L)
\end{aligned}$$

Let us calculate the weight term by term

$$
\begin{aligned}
&\langle T_\tau \prod\nolimits_i C^\dagger_{\alpha_i^{c,e}}(\tau_i^{c,e}) C_{\alpha_i^{c,s}}(\tau_i^{c,s})\rangle = \det(M_{ij}^{-1})\\
&M_{ij}^{-1} = \Delta_{\alpha_i^{c,s},\alpha_j^{c,e}}(\tau_i^{c,s}-\tau_j^{c,e})\\
&\Delta_{\alpha,\gamma}(i\omega) = \sum_{p,l} \frac{(V^l_{\alpha,p})^\dagger V^l_{\gamma,p}}{i\omega-\epsilon_p}\\
&\Delta_{\alpha,\gamma}(\tau) = (V^l_\alpha)^\dagger V^l_\gamma \int_{-D}^{D} d\epsilon \frac{\rho_l^C(\epsilon)e^{\tau\epsilon}}{e^{\beta\epsilon}+1} \quad , \quad \beta>\tau>0
\end{aligned}
$$

$$
\begin{aligned}
&\langle T_\tau \prod_i \Phi_{\alpha_i^{\phi,s}\gamma_i^{\phi,s}}(\tau_i^{\phi,s})\Phi^\dagger_{\alpha_i^{\phi,e}\gamma_i^{\phi,e}}(\tau_i^{\phi,e})\rangle = \sum_{i,j} \Gamma_{\alpha_i^{\phi,s}\gamma_i^{\phi,s},\alpha_j^{\phi,e}\gamma_j^{\phi,e}}(\tau_i^{\phi,s}-\tau_j^{\phi,e})\\
&\Gamma_{\alpha_i\gamma_i,\alpha_j\gamma_j} = \sum_l h_l^*(u^l_{\alpha_i\gamma_i})^* h_l u^l_{\alpha_j\gamma_j}\Gamma_l(\tau)\\
&\Gamma_l(\tau) = \Gamma_l(i\Omega_n=0) + \frac{2}{\beta}\sum_{n>0}\Gamma_l(i\Omega_n)\cos(\Omega_n\tau)\\
&\Gamma_l(i\Omega_n) = \int_0^\infty d\omega \frac{\rho_l^\phi(\omega)2\omega}{\Omega^2+\omega^2}
\end{aligned}
$$

$$
\begin{aligned}
&\langle \prod_i \widetilde{d}_{\alpha_i^{c,e}}(\tau_i^{c,e})\widetilde{d}^\dagger_{\alpha_i^{c,s}}(\tau_i^{s,e}) \prod_i \widetilde{L}^\dagger_{\alpha_i^{\phi,s}\gamma_i^{\phi,s}}(\tau_i^{\phi,s})\widetilde{L}_{\alpha_i^{\phi,e}\gamma_i^{\phi,e}}(\tau_i^{\phi,e}) \prod_i (\widetilde{L}_{\alpha_i^L\gamma_i^L})^\dagger(\tau_i^L)\widetilde{L}_{\sigma_i^L\delta_i^L}(\tau_i^L)\rangle\\
=&(-1)^p \exp(-2\sum_{i>j} s_i s_j \sum_l X_{\alpha_i,\alpha_j}(\tau_i-\tau_j))\langle \text{Time order}\{d,d^\dagger\}\rangle\\
&X_{\alpha\gamma}(\tau) = \sum_l g_l^2 v_l^{\alpha_i} v_l^{\alpha_j}\left(\frac{1}{2\beta}\Lambda(0)\tau(\tau-\beta) + \frac{2}{\beta}\sum_{n>0}\Lambda(i\Omega_n)\frac{1-\cos(\Omega\tau)}{\Omega^2}\right)\\
&\Lambda_l(i\Omega) = \int_0^\infty d\omega \frac{\rho_l^b(\omega)2\omega}{\Omega^2+\omega^2}
\end{aligned}
$$

4 Update

4.1 Transformation between diagonal flip boson bath and fermion bath

Fermion bath to diagonal flip boson bath

1. Randomly pick $d_\alpha(t_{st}^\alpha)$ from orbital α. (n_α fermion-bath segments)

2. Find $d^\dagger_\gamma(t^\gamma_{st})$ in orbital γ with time t^γ_{st} the latest time before time t^α_{st}.

3. Get $l_1 = \tilde{t}^\alpha_{st} - t^\gamma_{st}$, where $\tilde{t}^\alpha_{st}$ is the time in orbital α right after t^α_{st}

4. Randomly pick $d_\gamma(t^\gamma_{en})$ from orbital γ. (n_γ fermion-bath segments)

5. Find $d^\dagger_\alpha(t^\alpha_{en})$ in orbital α with time t^α_{en} the latest time before time t^α_{en}.

6. Get $l_2 = \tilde{t}^\gamma_{en} - t^\alpha_{en}$, where $\tilde{t}^\gamma_{en}$ is the time in orbital γ right after t^γ_{en}

7. Try to shift $d_\alpha(t^\alpha_{st})$ to $d_\alpha(t^\gamma_{st})$ and shift $d_\gamma(t^\gamma_{en})$ to $d_\gamma(t^\alpha_{en})$. If can't shift, then return false

8. Remove $d_\alpha(t^\alpha_{st})$, $d^\dagger_\gamma(t^\gamma_{st})$, $d_\gamma(t^\gamma_{en})$, $d^\dagger_\alpha(t^\alpha_{en})$. And corresponding $c^\dagger, c$

9. Insert $L^\dagger(t^\gamma_{st})L(t^\alpha_{en})$ and corresponding bosonic operators. $L = d^\dagger_\alpha d_\gamma$. Before insertion, there are n_L links.

10. Accept ratio:

$$
\begin{aligned}
p =& \frac{n_\alpha n_\gamma}{l_1 l_2 (n_L+1)} \cdot \text{ fermion-bath-remove-ratio } \cdot D_{\alpha\gamma,\alpha\gamma}(t^\gamma_{st} - t^\alpha_{en}) \\
& \cdot \text{density-bath-shift-ratio} \cdot \text{ trace-shift-ratio}
\end{aligned}
$$

diagonal flip bath to fermion bath

1. Randomly pick $L^\dagger(t_s)L(t_e)$ pair. $L = d^\dagger_\alpha d_\gamma$. ($n_L$ pairs)

2. At t_e, try to shift d_γ to the $d_\gamma(t^\gamma_e)$ with l_1 the largest shift length.

3. At t_s, try to shift d_α to the $d_\gamma(t^\alpha_s)$ with l_2 the largest shift length.

4. Remove $L^\dagger L$ pair.

5. Insert $d^\dagger_\alpha(t_e), d_\gamma(t^\gamma_e), d^\dagger_\gamma(t_s), d_\alpha(t^\alpha_s)$ and corresponding $c^\dagger, c$. n_α, n_γ number of segments before insertion.

6. Accept ratio:

$$
\begin{aligned}
p =& \frac{l_1 l_2 n_L}{(n_\alpha+1)(n_\gamma+1)} \cdot \text{ fermion-bath-insert-ratio } \cdot \frac{1}{D_{\alpha\gamma,\alpha\gamma}(t_e - t_s)} \\
& \cdot \text{density-bath-shift-ratio} \cdot \text{ trace-shift-ratio}
\end{aligned}
$$

5 Measurement

5.1 Measure one-particle Green's function

Hybridization expansion

$$Z \propto \det M^{-1}$$

where

$$\begin{aligned}
M_{ij}^{-1} &= \Delta_{\alpha_i^s,\alpha_j^e}(\tau_j^{s,\alpha_i^s} - \tau_i^{e,\alpha_j^e}) \\
\Delta_{\alpha\gamma}(i\omega) &= \sum_p V_{p,\alpha}^\dagger [i\omega - \epsilon_p]^{-1} V_{p,\gamma}
\end{aligned}$$

Using

$$\frac{\delta \det[\Delta]}{\delta \Delta_{ij}} = \det(\Delta)[\Delta^{-1}]_{ji}$$

We have

$$\begin{aligned}
& G_{\alpha,\gamma}(\tau^s - \tau^e) \\
=& \langle T_\tau d_\alpha^\dagger(\tau^s) d_\gamma(\tau^e)\rangle \\
=& -\frac{1}{\beta}\langle \sum_{i,j} M_{ji}\delta_{\alpha,\alpha_i^s}\delta_{\gamma,\gamma_j^e}\delta^-\Big((\tau^s - \tau^e) - (\tau_i^s - \tau_j^e)\Big)\rangle
\end{aligned}$$

$$\delta^-(\tau) = \sum_n (-1)^n \delta(\tau - n\beta)$$

5.2 Measure two-particle Green's function

Hybridization expansion

$$Z \propto \det M^{-1}$$

where

$$\begin{aligned}
M_{ij}^{-1} &= \Delta_{\alpha_i^s,\alpha_j^e}(\tau_j^{s,\alpha_i^s} - \tau_i^{e,\alpha_j^e}) \\
\Delta_{\alpha\gamma}(i\omega) &= \sum_p V_{p,\alpha}^\dagger [i\omega - \epsilon_p]^{-1} V_{p,\gamma}
\end{aligned}$$

Using

$$\frac{\delta \det[\Delta]}{\delta \Delta_{ij} \delta \Delta_{lm}} = \det(\Delta)\bigg([\Delta^{-1}]_{ji}[\Delta^{-1}]_{ml} - [\Delta^{-1}]_{mi}[\Delta^{-1}]_{jl} \bigg)$$

We have

$$\begin{aligned}
&G_{\alpha,\gamma,\delta,\sigma}(\tau_1,\tau_2,\tau_3,\tau_4) \\
=&\langle T_\tau d^\dagger_\alpha(\tau_1) d_\gamma(\tau_2) d^\dagger_\delta(\tau_3) d_\sigma(\tau_4)\rangle \\
=&\sum_{i,j,l,m} \langle (M_{ji}M_{ml} - M_{jl}M_{mi})\delta^-(\tau_1 - \tau^s_i)\delta^-(\tau_2 - \tau^e_j)\delta^-(\tau_3 - \tau^s_l)\delta^-(\tau_4 - \tau^e_m)\rangle
\end{aligned}$$

For

$$\begin{aligned}
&G_{\alpha,\gamma,\delta,\sigma}(\tau) \\
=&\langle T_\tau d^\dagger_\alpha(\tau) d_\gamma(\tau) d^\dagger_\delta(0) d_\sigma(0)\rangle \\
=&\frac{1}{\beta}\sum_{i,j,l,m} \langle (M_{ji}M_{ml} - M_{jl}M_{mi})\delta^-(\tau - (\tau^s_i - \tau^e_m))\delta^-(\tau - (\tau^s_j - \tau^s_l))\delta^+(\tau - (\tau^s_i - \tau^s_l))\rangle
\end{aligned}$$

$$\delta^-(\tau) = \sum_n (-1)^n \delta(\tau - n\beta)$$

5.3 Measure via diagonalized flip bath

Consider the expansion term with the following form

$$Tr[\Pi_i L^\dagger(\tau^s_i) L(\tau^e_i) J(\tau^s_i - \tau^e_i)]$$

with $L = d^\dagger_{\alpha^1} d_{\alpha^2},\ J = \Gamma_{\alpha^1\alpha^2,\alpha^1\alpha^2}$

Then the measurement

$$\langle L(\tau) L^\dagger(0)\rangle = \frac{1}{\beta}\langle \sum_i \frac{1}{J(\tau^s_i - \tau^e_i)} \delta^+(\tau - \tau^s_i + \tau^e_i)\rangle$$

6 Sign-problem Free

Consider the following configuration appears in ctqmc:

$$\frac{1}{Z}\langle \prod_{i=n}^{i=1} c(\tau^e_i) c^\dagger(\tau^s_i) e^{-\int c^\dagger(\tau) G^{-1}(\tau,\tau') c(\tau')}\rangle = \det\bigg(\Delta^n\bigg)$$

$$\Delta^n_{ij} = [G(\tau^e_i - \tau^s_j)]_{ij}$$

with $\tau_n^e > \tau_n^s > ... > \tau_i^e > \tau_i^s > ... > \tau_1^e > \tau_1^s > 0$.

$$\begin{aligned}
&\langle \prod_{i=n}^{i=1} c(\tau_i^e) c^\dagger(\tau_i^s) e^{-\int c^\dagger(\tau) G^{-1}(\tau,\tau') c(\tau')} \rangle \\
=&\langle 0|\hat{U}(\beta, \tau_i^e)|0\rangle \langle 0|c^\dagger|1\rangle \langle 1|\hat{U}(\tau_i^e, \tau_i^s)|1\rangle \langle 1|... > 0
\end{aligned}$$

7 Appendix

7.1 Fermi Determinant

$$N = \Delta^{-1}$$

Let

$$N_{n+1}^{-1} = \begin{bmatrix} N_n^{-1} & Q \\ R & S \end{bmatrix}$$
$$N_{n+1} = \begin{bmatrix} \tilde{P} & \tilde{Q} \\ \tilde{R} & \tilde{S} \end{bmatrix}$$

with

$$\begin{aligned}
\tilde{S} &= (S - RN_nQ)^{-1} \\
\tilde{Q} &= -N_nQ\tilde{S} \\
\tilde{R} &= -\tilde{S}RN_n \\
\tilde{P} &= N_n + N_nQ\tilde{S}RN_n
\end{aligned}$$

and

$$\frac{\det(N_{n+1}^{-1})}{\det(N_n^{-1})} = \frac{1}{\det(\tilde{S})}$$