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In this document, we present an approach of doing perturbation theory around the atomic limit applicable to non-equilibrium DMFT. We start by noting the local action of the Anderson impurity model (AIM)

$$S_{loc} = -\int_{\mathcal{C}} dt \sum_{p} H_{loc}[\hat{d}_p^\dagger(t), \hat{d}_p(t), t] \tag{1}$$

and the hybridization

$$S_{hyb} = -\int_{\mathcal{C}}\int_{\mathcal{C}} dtdt' \sum_{p,p'} \hat{d}_p^\dagger(t)\Delta(t,t')\hat{d}_p(t') \tag{2}$$

In the local basis, we may write the local hamiltonian as

$$H_{loc}(t) = \sum_{mm'} |m\rangle\, h_{mm'}(t)\, \langle m'| = \sum_{mm'} \hat{a}_m^\dagger(t) h_{mm'}(t) \hat{a}_{m'}(t) \tag{3}$$

where we have defined the creation operators corresponding to the local states as $\hat{a}_m^\dagger$ which will be referred to as the ***pseudoparticle*** (pp) operators. The indices m will be referred to as flavor indices. To be concrete, these will in the single AIM correspond to $|0\rangle$ - empty site, $|\sigma\rangle$ - a single electron with spin σ and $|\uparrow,\downarrow\rangle$ - doubly occupied site. We furthermore define an operator counting the number of pseudoparticles on the impurity as

$$\hat{Q} = \sum_{m} \hat{a}_m^\dagger \hat{a}_m \tag{4}$$

where m runs over all flavor indices in the problem. With the considerations above, it should be clear that any physical state of the impurity should obey $\hat{Q}\,|\Psi\rangle = 1\,|\Psi\rangle$.

A crucial point to note about fermionic creation and annihilation operators in this context is that they can represent different processes. For instance, inserting an electron onto an impurity site can either correspond to creating a singly occupied site or creating a doubly occupied site. Generally, we may therefore write

$$\hat{d}_p^\dagger(t) = \sum_{mn} (F_p)_{mn} \hat{a}_m^\dagger(t) \hat{a}_n(t) \tag{5}$$

where $(F_p)_{mn} = \langle m| \hat{d}_p^\dagger |n\rangle$. It is easy to calculate this explicitly for the AIM: Defining $|\uparrow,\downarrow\rangle = \hat{d}_\downarrow^\dagger \hat{d}_\uparrow^\dagger$ we observe that $\langle\sigma| \hat{d}_\sigma |0\rangle$ and $\langle\uparrow\downarrow| \hat{d}_\sigma^\dagger |\overline{\sigma}\rangle = \pm 1$, where $+(-)$ corresponds to $\sigma = \downarrow$ ($\sigma = \uparrow$). Thus,

$$\begin{aligned} \hat{d}_\uparrow^\dagger &= \hat{a}_\uparrow^\dagger \hat{a}_0 - \hat{a}_{\uparrow\downarrow}^\dagger \hat{a}_\downarrow \\ \hat{d}_\downarrow^\dagger &= \hat{a}_\downarrow^\dagger \hat{a}_0 + \hat{a}_{\uparrow\downarrow}^\dagger \hat{a}_\uparrow \end{aligned} \tag{6}$$

In any case, we will make use of this representation for the action of the AIM

$$S_{loc} = -\int_{\mathcal{C}} dt \sum_p h_{mn}(t) \hat{a}_m^\dagger(t) \hat{a}_n(t) \tag{7}$$

and upon inserting equation (5) into equation (2) we get

$$S_{hyb} = -\int_{\mathcal{C}} \int_{\mathcal{C}} dt dt' \sum_{mnm'n'} \sum_{p,p'} \hat{a}_m^\dagger(t) \hat{a}_n(t) F_{mn}^p \Delta(t,t') (F_{m'n'}^p)^* \hat{a}_{m'}^\dagger(t') \hat{a}_n'(t') \tag{8}$$

1 Pseudoparticle Green's functions

In this section a useful construction dubbed the pseudoparticle Green's function (ppGF) will be given. We will now work in a grand canonical ensemble with respect to $\hat{Q}$ and will let $\hat{Q}$ take on any values. (whatever that means!) However, we will work with a chemical potential, λ. In the end, we will let its limit go to infinity. Evaluating any expectation value in this grand canonical ensemble will be understood as follows

$$\left\langle \hat{O} \right\rangle_{\tilde{\mathcal{S}}} = \sum_{Q=0}^{\infty} \mathrm{Tr}_Q[e^{\tilde{\mathcal{S}}} \hat{O}] \tag{9}$$

with $\tilde{\mathcal{S}} = \tilde{\mathcal{S}}_{imp} + \tilde{\mathcal{S}}_{hyb}$. We begin by defining the expectation value of an operator in this ensemble as

$$\left\langle \hat{O}(t) \right\rangle_\lambda = \frac{\left\langle e^{-\beta\lambda\hat{Q}} \hat{O}(t) \right\rangle_{\tilde{\mathcal{S}}}}{\left\langle e^{-\beta\lambda\hat{Q}} \right\rangle_{\tilde{\mathcal{S}}}} = (1-\xi) \left\langle e^{-\beta\lambda\hat{Q}} \hat{O}(t) \right\rangle_{\tilde{\mathcal{S}}} \tag{10}$$

where we used

$$\left\langle e^{-\beta\lambda\hat{Q}}\right\rangle_{\tilde{\mathcal{S}}} = \sum_{n=0}^{\infty}\xi^n = \frac{1}{1-\xi} \tag{11}$$

with $\xi \equiv \left\langle e^{-\beta\lambda}\right\rangle$ The ppGF is given as

$$\begin{aligned}\mathcal{G}^{\lambda}_{mm'}(t,t') &= \left\langle \hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')\right\rangle_{\lambda} \\ &= -i\Theta_c(t,t')\left\langle \hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')\right\rangle_{\lambda} - i\Theta_c(t',t)\left\langle \hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')\right\rangle_{\lambda}\end{aligned} \tag{12}$$

where $\hat{T}_c$ is the time ordering operator on the contour. It is obvious that the above simplifies to

$$\begin{aligned}\mathcal{G}^{\lambda}_{mm'}(t,t') = &-i\Theta_c(t,t')\{(1-\xi)Tr_{Q=0}[\hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]\} \\ &- i\Theta_c(t',t)\{(1-\xi)\xi Tr_{Q=1}[\hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]\} + \mathcal{O}(\xi)\end{aligned} \tag{13}$$

Collecting only the lowest order terms in ξ here leaves us with

$$\begin{aligned}\mathcal{G}^{\lambda}_{mm'}(t,t') = &-i\Theta_c(t,t')\{Tr_{Q=0}[\hat{T}_c e^{\tilde{\mathcal{S}}}\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]\} \\ &- i\Theta_c(t',t)\{\xi Tr_{Q=1}[\hat{T}_c e^{\tilde{\mathcal{S}}}\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]\} + \mathcal{O}(\xi)\end{aligned} \tag{14}$$

which can be compared to equation (4) in the supplementary material of [1]. Now, to aid us with constructing the physical Green's function, we will have to give some interpretation of the quantities $Tr_{Q=0}[\hat{T}_c e^{\tilde{\mathcal{S}}}\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]$ and $Tr_{Q=1}[\hat{T}_c e^{\tilde{\mathcal{S}}}\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]$. By the time ordering, one must for $t > t'$ consider $Tr_{Q=0}[\hat{T}_c\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]$. Here, unitary time evolution is performed in the $Q = 0$ subspace in the time interval $[0^+, t']$ before $\hat{a}^{\dagger}_{m'}(t')$ creates a particle in the physical subspace of $Q = 1$. After the action of $\hat{a}_m(t)$ we are back in $Q = 0$ at time t and the system is propagated in this subspace in the contour time interval $[t, -i\beta]$. For the opposite contour time ordering, $t < t'$, we must consider $Tr_{Q=1}[\hat{T}_c e^{\tilde{\mathcal{S}}}\hat{a}_m(t)\hat{a}^{\dagger}_{m'}(t')]$. By the same arguments, it is shown that the propagation in the $Q = 1$ subspace happens for $t_c \in [0^+, t]$ and $t_c \in [t', -i\beta]$ and in $Q = 0$ for $t_c \in [t, t']$. An illustration is given in figure 1

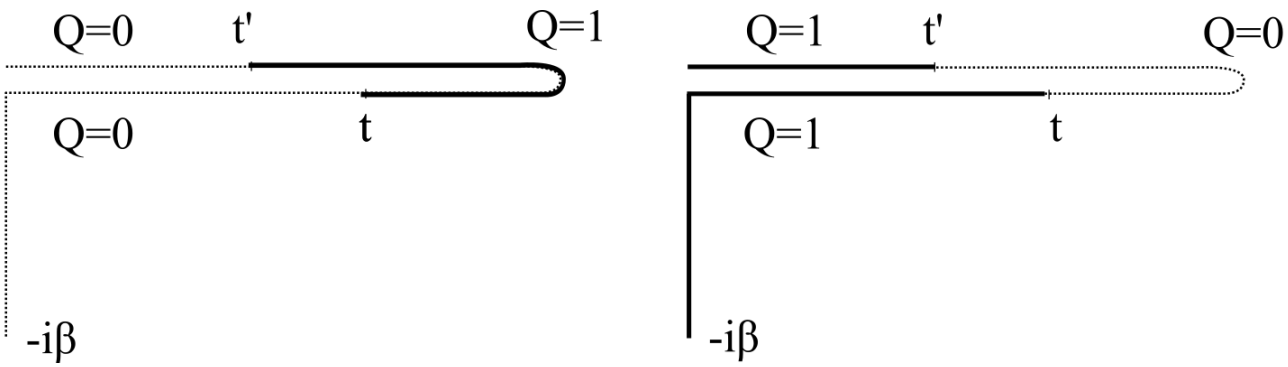

Figure 1: Illustration showing how the greater component of the ppGF, $\mathcal{G}^{\lambda}(t,t')$ on the left and the lesser component, $\mathcal{G}^{\lambda}(t',t)$ on the right.

Still keeping $t > t'$, we can show that the lesser ppGF can be factorized in terms of greater ppGFs.

$$\begin{aligned}
\mathcal{G}^{\lambda}_{m,m}(t',t) &= i\xi Tr_{Q=1}[\hat{T}_{\mathcal{C}} e^{\tilde{S}_{imp}} \hat{a}^{\dagger}_m(t')\hat{a}_m(t)] \\
&= i\xi Tr_{Q=0}[\hat{a}_m(-i\beta)U(-i\beta,t')\hat{a}^{\dagger}_m(t')U(t',t)\hat{a}_m(t)U(t,0)\hat{a}^{\dagger}_m(0)] \\
&= i\xi \sum_{n,l} \langle n|\, \hat{a}_m(-i\beta)U(-i\beta,t')\hat{a}^{\dagger}_m(t')\,|l\rangle \,\langle l|\, U(t',t)\hat{a}_m(t)U(t,0)\hat{a}^{\dagger}_m(0)\,|l\rangle \\
&\propto \mathcal{G}^{\lambda}_{m,m}(-i\beta,t')\mathcal{G}^{\lambda}_{m,m}(t,0)
\end{aligned} \tag{15}$$

where we used the completeness relation, $\sum_{Q,l} |Q,l\rangle \langle Q,l| = 1$ in the third line. In

the last line, we make use of the fact that in the l sum, only the pseudoparticle vacuum will contribute and the fact that this vacuum is unique. I.e., there is only one state in with $Q = 0$.

2 A simple example

If we have the following action

$$\tilde{S} = \mu \int_0^\beta d\tau \hat{n}(\tau) - \int_0^\beta d\tau \int_0^\beta d\tau' \hat{c}^\dagger(\tau)\Delta(\tau - \tau')\hat{c}(\tau') \tag{16}$$

where μ is the chemical potential and Δ is a hybridization function between the impurity system and a bath. Note that there is no reference to spin, and we may for simplicity only consider one spin at the impurity site (say spin up). In this way, there is only one way to create a physical particle on the impurity and there is only one way to remove one. By looking at equation (6), we see that pseudoparticle and physical particles coincide in the present model.

Our goal is to develop $\mathcal{Z}$, defined as

$$\mathcal{Z} = Tr[\hat{T}e^{\tilde{S}}] \tag{17}$$

in terms of an expansion of the hybridization term in $\tilde{S}$. To zeroth order,

$$\begin{aligned} \mathcal{Z}^{(0)} &= Tr[\hat{T}e^{\mu\int_0^\beta d\tau\hat{n}(\tau)}] \\ &= \langle 0| e^{\mu\int_0^\beta d\tau\hat{n}(\tau)} |0\rangle + \langle 1| e^{\mu\int_0^\beta d\tau\hat{n}(\tau)} |1\rangle \\ &= 1 + e^{\mu\beta} \\ &\equiv \mathcal{G}_1^{(0)} + \mathcal{G}_2^{(0)} \end{aligned} \tag{18}$$

In general, we will write

$$\mathcal{Z} = \sum_{n=0}^{\infty} \mathcal{Z}^{(n)} = \mathcal{G}_1 + \mathcal{G}_2 \tag{19}$$

where n counts the order of the hybridization expansion. These zeroth order terms along with higher order diagrams are shown in figure 2.

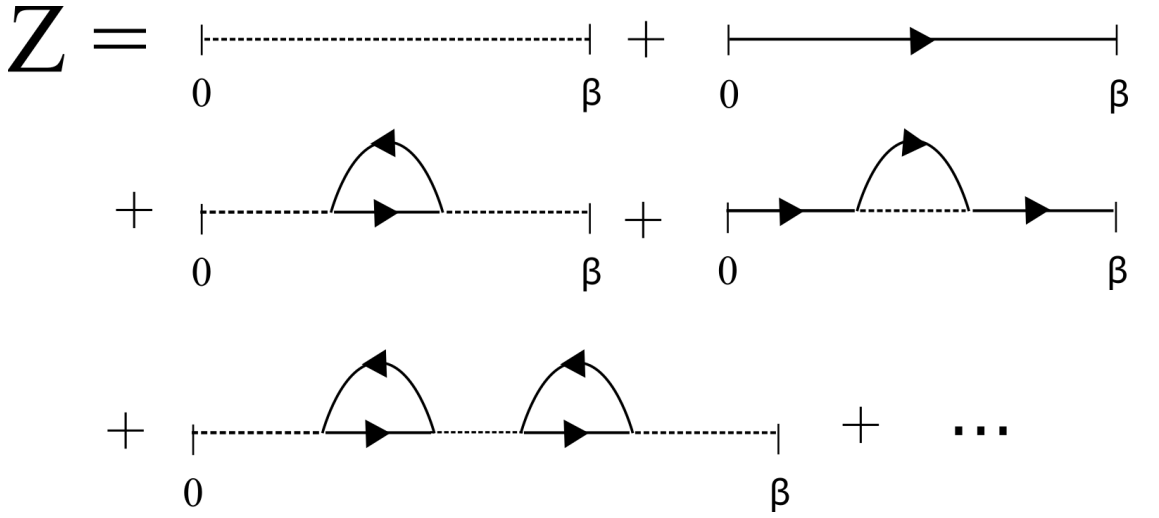

Figure 2: Some of the diagrams arising from the hybridization expansion of the model. Dashed lines indicate the "vacuum propagator" (which is just 1) and the solid lines the propagator $e^{\mu\beta}$

From the above figure, we can surmise the general structure of the partition function. This is illustrated in figure 3. In other words, $\mathcal{G}_i$ will satisfy Dyson equations

$$\begin{aligned} \mathcal{G}_0(\tau) &= \mathcal{G}_0^{(0)}(\tau) + [\mathcal{G}_0^{(0)} \star \Sigma_0 \star \mathcal{G}_0](\tau) \\ \mathcal{G}_1(\tau) &= \mathcal{G}_1^{(0)}(\tau) + [\mathcal{G}_1^{(0)} \star \Sigma_1 \star \mathcal{G}_1](\tau) \end{aligned} \tag{20}$$

where

$$[A \star B](\tau) = \int_0^\beta A(\tau - \overline{\tau}) B(\overline{\tau}) \tag{21}$$

It is crucial to note that Σ_0 will depend on $\mathcal{G}_0$ as well as $\mathcal{G}_1$ and Σ_1 will depend on $\mathcal{G}_0$ and $\mathcal{G}_1$. The equations are therefore coupled.

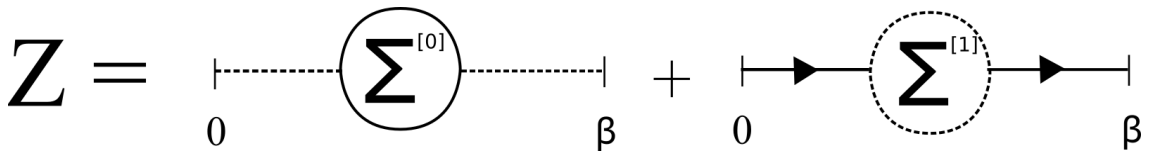

Figure 3: The basic structure of the partition function when expanded in terms of the hybrdization function

3 Physical Green's functions

In the process of solving the partition function through the coupled set of equations above, it turns out that we have the necessary quantities to compute the physical Green's functions. To do this, we simply appeal to the physical interpretation of the physical GF. Note that for $\mathcal{G}(\tau - \tau') = -\left\langle \hat{\mathcal{T}} \hat{c}(\tau)\hat{c}^{\dagger}(\tau') \right\rangle$ the interpretation is that an electron is being added to the impurity at imaginary time τ' and subsequently annihilated at τ. This process is sketched in figure 4. If the time ordering is as shown, the expectation value $\langle ... \rangle = \langle 0| \, .. \, |0\rangle$ where $|0\rangle$ is state of the empty impurity site. By now setting $\tau' = 0$, we get see that

$$\mathcal{G}^{M}(\tau) = \mathcal{G}_1(\tau)\mathcal{G}_0(\beta - \tau) = -\mathcal{G}_1(\tau)\mathcal{G}_0(-\tau) \tag{22}$$

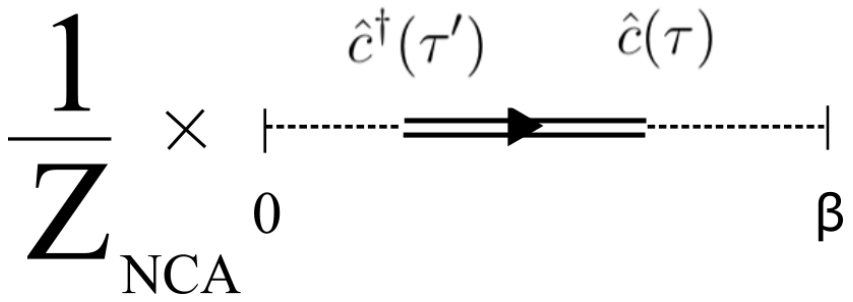

Figure 4: The physical Greens function expressed as a product of ppGFs.

References

[1] Y. Murakami, M. Eckstein, and P. Werner, "High-harmonic generation in mott insulators," *Phys. Rev. Lett.*, vol. 121, p. 057405, Aug 2018. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.121.057405