How to compute the gap with Δ in orbital space

I. REFRESH ON NAMBU FORMALISM

Nambu-Gorkov spinor is

$$\Psi^\dagger_{\mathbf{k},i} = (c^\dagger_{\mathbf{k}i\uparrow}, c_{-\mathbf{k}i\downarrow}) \tag{1}$$

and the Nambu Green's function is

$$G_{\mathbf{k},ij}(\tau) = -\langle T_\tau \begin{pmatrix} c_{\mathbf{k}i\uparrow}(\tau) \\ c^\dagger_{-\mathbf{k}i\downarrow}(\tau) \end{pmatrix} \begin{pmatrix} c^\dagger_{\mathbf{k}j\uparrow} & c_{-\mathbf{k}j\downarrow} \end{pmatrix} \rangle = -\begin{pmatrix} \langle T_\tau c_{\mathbf{k}i\uparrow}(\tau) c^\dagger_{\mathbf{k}j\uparrow}\rangle & \langle T_\tau c_{\mathbf{k}i\uparrow}(\tau) c_{-\mathbf{k}j\downarrow}\rangle \\ \langle T_\tau c^\dagger_{-\mathbf{k}i\downarrow}(\tau) c^\dagger_{\mathbf{k}j\uparrow}\rangle & \langle T_\tau c^\dagger_{-\mathbf{k}i\downarrow}(\tau) c_{-\mathbf{k}j\downarrow}\rangle \end{pmatrix} \tag{2}$$

We define

$$\mathcal{G}_{\mathbf{k},ij}(\tau) = -\langle T_\tau c_{\mathbf{k}i\uparrow}(\tau) c^\dagger_{\mathbf{k}j\uparrow}\rangle \tag{3}$$

$$\mathcal{F}_{\mathbf{k},ij}(\tau) = -\langle T_\tau c_{\mathbf{k}i\uparrow}(\tau) c_{-\mathbf{k}j\downarrow}\rangle \tag{4}$$

and see that

$$\begin{aligned} G_{22} &= -\langle T_\tau c^\dagger_{-\mathbf{k}i\downarrow}(\tau) c_{-\mathbf{k}j\downarrow}\rangle = \langle T_\tau c_{-\mathbf{k}j\downarrow}(-\tau) c^\dagger_{-\mathbf{k}i\downarrow}\rangle = \\ &= -\mathcal{G}_{-\mathbf{k},ji}(-\tau) \\ G_{12} &= -\langle T_\tau c^\dagger_{-\mathbf{k}i\downarrow}(\tau) c^\dagger_{\mathbf{k}j\uparrow}\rangle = \mathcal{F}^*_{\mathbf{k},ji}(\tau) \end{aligned} \tag{5}$$

To prove the last identity, we check $\tau > 0$ case, and write

$$\begin{aligned} \mathcal{F}^*_{\mathbf{k},ij}(\tau) &= -\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H^*} e^{\tau H^*} c^*_{\mathbf{k}i\uparrow} e^{-\tau H^*} c^*_{-\mathbf{k}j\downarrow}\right) = \\ -\frac{1}{Z}&\mathrm{Tr}\left(\left(e^{-\beta H+\tau H}\right)^T (c^\dagger_{\mathbf{k}i\uparrow})^T \left(e^{-\tau H}\right)^T (c^\dagger_{-\mathbf{k}j\downarrow})^T\right) = \\ &-\frac{1}{Z}\mathrm{Tr}\left(\left(c^\dagger_{-\mathbf{k}j\downarrow} e^{-\tau H} c^\dagger_{\mathbf{k}i\uparrow} e^{-\beta H+\tau H}\right)^T\right) = \\ &-\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H+\tau H} c^\dagger_{-\mathbf{k}j\downarrow} e^{-\tau H} c^\dagger_{\mathbf{k}i\uparrow}\right) = \\ &-\langle T_\tau c^\dagger_{-\mathbf{k}j\downarrow}(\tau) c^\dagger_{\mathbf{k}i\uparrow}\rangle \end{aligned} \tag{6}$$

Hence, Bogolubov Green's function is

$$G_{\mathbf{k},ij}(\tau) = \begin{pmatrix} \mathcal{G}_{\mathbf{k},ij}(\tau) & \mathcal{F}_{\mathbf{k},ij}(\tau) \\ \mathcal{F}^*_{\mathbf{k},ji}(\tau) & -\mathcal{G}_{-\mathbf{k},ji}(-\tau) \end{pmatrix} \tag{7}$$

or in matrix notation

$$G_{\mathbf{k}}(\tau) = \begin{pmatrix} \mathcal{G}_{\mathbf{k}}(\tau) & \mathcal{F}_{\mathbf{k}}(\tau) \\ \mathcal{F}^\dagger_{\mathbf{k}}(\tau) & -\mathcal{G}^T_{-\mathbf{k}}(-\tau) \end{pmatrix} \tag{8}$$

and in frequency

$$G_{\mathbf{k}}(i\omega) = \begin{pmatrix} \mathcal{G}_{\mathbf{k}}(i\omega) & \mathcal{F}_{\mathbf{k}}(i\omega) \\ \mathcal{F}^\dagger_{\mathbf{k}}(-i\omega) & -\mathcal{G}^T_{-\mathbf{k}}(-i\omega) \end{pmatrix} \tag{9}$$

II. AB-INITIO DMFT AND SC GAP

We first write LDA+DMFT solution in eigenbasis, which is frequency dependent

$$\mathcal{G}_{\mathbf{k}}(i\omega, \mathbf{r}\mathbf{r}') = \psi^R_{\mathbf{k}l}(i\omega, \mathbf{r}) \frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}l,i\omega}} \psi^L_{\mathbf{k}l}(i\omega, \mathbf{r}') \tag{10}$$

or

$$\int d\mathbf{r}d\mathbf{r}' \psi^L_{\mathbf{k}l}(i\omega, \mathbf{r}) \mathcal{G}^{-1}_{\mathbf{k}}(i\omega, \mathbf{r}\mathbf{r}') \psi^R_{\mathbf{k}l}(i\omega, \mathbf{r}') = i\omega + \mu - \varepsilon_{\mathbf{k}l,i\omega}$$

The DMFT projector $U_{\mathbf{r}\alpha}$, which is used to embed the self-energy, can embed gap and give its real space representation as

$$\Delta^{\mathbf{k}}(\mathbf{r}\mathbf{r}') = U_{\mathbf{r}\alpha} \Delta^{\mathbf{k}}_{\alpha\beta} U^\dagger_{\beta\mathbf{r}'} \tag{11}$$

being non-local in band index or real space. We can transform it to DMFT eigenbasis by

$$\bar{\Delta}^{\mathbf{k}}_{ll'}(i\omega) = \int d\mathbf{r}d\mathbf{r}' \psi^L_{\mathbf{k}l}(i\omega, \mathbf{r}) U_{\mathbf{r}\alpha} \Delta^{\mathbf{k}}_{\alpha\beta} U^\dagger_{\beta\mathbf{r}'} \psi^R_{\mathbf{k}l}(i\omega, \mathbf{r}') \tag{12}$$

These projectors are computed by "dmftgk" in "e" mode, and they are printed to file "UL.dat " as $UAl = \psi^L_{\mathbf{k}l}(i\omega, \mathbf{r}) U_{\mathbf{r}\alpha}$ and "UR.dat" as $UAr = U^\dagger_{\beta\mathbf{r}'} \psi^R_{\mathbf{k}l}(i\omega, \mathbf{r}')$.

Finally, we need to solve for Bogolubov quasiparticles by diagonalizing the following Hamiltonian

$$H_{BG} = \begin{pmatrix} \varepsilon_{\mathbf{k},i\omega} - \mu & \bar{\Delta}^{\mathbf{k}}(i\omega) \\ \bar{\Delta}^{\mathbf{k}\dagger}(-i\omega) & -\varepsilon^T_{-\mathbf{k},-i\omega} + \mu \end{pmatrix} \tag{13}$$

It turns out that $\varepsilon_{\mathbf{k},i\omega}$ and $\bar{\Delta}(i\omega)$ do not have a branch-cut at $i\omega = 0$ hence we can safely take the zero frequency limit. We will also assume that the lattice has inversion symmetry, hence $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$. We hence diagonalize

$$H_{BG} = \begin{pmatrix} \varepsilon_{\mathbf{k},0} - \mu & \bar{\Delta}_{\mathbf{k}} \\ \bar{\Delta}^\dagger_{\mathbf{k}} & -\varepsilon^T_{\mathbf{k},0} + \mu \end{pmatrix} \tag{14}$$

The difference between the smallest positive eigenvalue λ^- and the largest negative eigenvalue λ^+ is equal twice the gap $2\Delta = \lambda^+ - \lambda^-$.