I EG-X Model with interactions

I.1 BdG Hamiltonian and free energy

I.1.1 BdG Hamiltonian

Define sublattice index

$$\alpha = 1, 2, 3 \tag{I.1}$$

with $1 \mathrel{\widehat{=}} \mathrm{Gr}_1, 2 \mathrel{\widehat{=}} \mathrm{Gr}_2, 3 \mathrel{\widehat{=}} \mathrm{X}$. Then we can write the non-interacting term as

$$H_0 = - \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta} \, c_{i\alpha}^{\dagger} c_{j\beta} \tag{I.2}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{I.3}$$

Does that make sense?

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{I.4}$$

Also write the interaction part with α (with changed signs compared to Niklas, to keep in line with papers about the attractive Hubbard model):

$$H_{int} = - \sum_{i\alpha} U_\alpha c_{i\alpha\uparrow}^{\dagger} c_{i\alpha\downarrow}^{\dagger} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{I.5}$$

Fourier transformation:

$$H_{int} = -\frac{1}{N^2} \sum_{\alpha, \mathbf{k}_{1,2,3,4}} U_\alpha e^{i(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_3) r_{i\alpha}} c_{\mathbf{k}_1\alpha\uparrow}^{\dagger} c_{\mathbf{k}_3\alpha\downarrow}^{\dagger} c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \tag{I.6}$$

Impose zero-momentum pairing: $\mathbf{k}_1 + \mathbf{k}_3 = 0$ and $\mathbf{k}_2 + \mathbf{k}_4 = 0$:

$$H_{int} = -\sum_{\alpha,\mathbf{k},\mathbf{k}'} U_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \tag{I.7}$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{I.8}$$

with

$$\Delta_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \tag{I.9}$$

$$\Delta^*_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\alpha\uparrow} c^\dagger_{-\mathbf{k}'\alpha\downarrow} \rangle \tag{I.10}$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{I.11}$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c^\dagger_{1,-\mathbf{k}\downarrow} \\ c^\dagger_{2,-\mathbf{k}\downarrow} \\ c^\dagger_{3,-\mathbf{k}\downarrow} \end{pmatrix} \tag{I.12}$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \tag{I.13}$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H^*_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{I.14}$$

with $H_{0,\sigma}$ being the F.T. of the kinetic term and $\Delta = diag(\Delta_1, \Delta_2, \Delta_3)$.

I.1.2 BdG Hamiltonian in band basis

Use transformation

$$c^\dagger_{\mathbf{k}\alpha\sigma} = \sum_n [\mathbf{G}]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \tag{I.15}$$

where the columns are made up of the eigenvectors of $\mathbf{H}_{0,\sigma}$ for a given $\mathbf{k}$:

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 & \mathbf{G}_3 \end{pmatrix} \tag{I.16}$$

with that:

$$\mathbf{G}^\dagger_\sigma(\mathbf{k})\mathbf{H}_{0,\sigma}(\mathbf{k})\mathbf{G}_\sigma(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \tag{I.17}$$

So the kinetic part of the BdG Hamiltonian becomes:

$$\sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} \sum_n [\mathbf{G}(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \sum_m [\mathbf{G}(\mathbf{k})]_{\beta m} d_{m\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.18}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \sum_{\alpha\beta} [\mathbf{G}(\mathbf{k})]^*_{\alpha n} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} [\mathbf{G}(\mathbf{k})]_{\beta m} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.19}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.20}$$

$$= \sum_{n\mathbf{k}\sigma} \epsilon_n d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.21}$$

$$=: \sum_{n\mathbf{k}\sigma} \xi_\mathbf{k} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} \tag{I.22}$$

with $\xi_\mathbf{k} := \epsilon_\mathbf{k} - \mu$. The pairing terms become (I set $n = m$ here, which seems only sensible, but I dont have a real reason why?):

$$\sum_{\mathbf{k}\alpha} \Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} = \sum_{\mathbf{k}\alpha} \Delta_\alpha \sum_n [\mathbf{G}_\uparrow(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\uparrow} \sum_m [\mathbf{G}_\downarrow(-\mathbf{k})]^*_{\beta m} d^\dagger_{m-\mathbf{k}\downarrow} \tag{I.23}$$

$$= -\sum_{n\mathbf{k}} \Delta_n d^\dagger_{n\mathbf{k}\uparrow} d^\dagger_{n-\mathbf{k}\downarrow} \tag{I.24}$$

with gap $\Delta_n(\mathbf{k}) = -\sum_\alpha [\mathbf{G}_\uparrow(\mathbf{k})]^*_{\alpha n} \Delta_\alpha [\mathbf{G}_\downarrow(-\mathbf{k})]^*_{\alpha n}$ for band n.

$$\sum_{\mathbf{k}\alpha} \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow} = -\sum_{n\mathbf{k}} \Delta^*_n d_{n-\mathbf{k}\downarrow} d_{n\mathbf{k}\uparrow} \tag{I.25}$$

So the BdG Hamiltonian is:

$$H_{BdG} = \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d_{n\mathbf{k}\sigma}^{\dagger} d_{n\mathbf{k}\sigma} - \sum_{n\mathbf{k}} (\Delta_n^* d_{n-\mathbf{k}\downarrow} d_{n\mathbf{k}\uparrow} + \Delta_n d_{n\mathbf{k}\uparrow}^{\dagger} d_{n-\mathbf{k}\downarrow}^{\dagger}) \qquad \text{(I.26)}$$