

# I EG-X Model with interactions

## I.1 BdG Hamiltonian and free energy

### I.1.1 BdG Hamiltonian

Define sublattice index

$$\alpha = 1, 2, 3 \quad (\text{I.1})$$

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

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

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\text{Gr}} & 0 \\ t_{\text{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\text{X}} \end{pmatrix} \quad (\text{I.3})$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \quad (\text{I.4})$$

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

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

Fourier transformation:

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

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

$$H_{int} = - \sum_{\alpha, \mathbf{k}, \mathbf{k}'} U_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \quad (\text{I.7})$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha, \mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^{*} c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{I.8})$$

with

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

$$\Delta_{\alpha}^{*} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\alpha\uparrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow}^{\dagger} \rangle \quad (\text{I.10})$$

This gives the BCS mean field Hamiltonian:

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

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c_{1,-\mathbf{k}\downarrow}^{\dagger} \\ c_{2,-\mathbf{k}\downarrow}^{\dagger} \\ c_{3,-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \quad (\text{I.12})$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \quad (\text{I.13})$$

with

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

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

### I.1.2 BdG Hamiltonian in band basis

Use transformation

$$c_{\mathbf{k}\alpha\sigma}^\dagger = \sum_n [\mathbf{G}]_{\alpha n}^* d_{n\mathbf{k}\sigma}^\dagger \quad (\text{I.15})$$

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

$$\mathbf{G} = (\mathbf{G}_1 \quad \mathbf{G}_2 \quad \mathbf{G}_3) \quad (\text{I.16})$$

with that:

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

So the kinetic part of the BdG Hamiltonian becomes:

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

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

$$= \sum_{mn\mathbf{k}\sigma} d_{n\mathbf{k}\sigma}^\dagger d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \quad (\text{I.20})$$

$$= \sum_{n\mathbf{k}\sigma} \epsilon_n d_{n\mathbf{k}\sigma}^\dagger d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \quad (\text{I.21})$$

$$=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d_{n\mathbf{k}\sigma}^\dagger d_{n\mathbf{k}\sigma} \quad (\text{I.22})$$

with  $\xi_{\mathbf{k}} := \epsilon_{\mathbf{k}} - \mu$ . The pairing terms become:

$$\sum_{\mathbf{k}\alpha} \Delta_\alpha c_{\mathbf{k}\alpha\uparrow}^\dagger c_{-\mathbf{k}\alpha\downarrow}^\dagger = \sum_{\mathbf{k}\alpha} \Delta_\alpha \sum_n [\mathbf{G}_\uparrow(\mathbf{k})]_{\alpha n}^* d_{n\mathbf{k}\uparrow}^\dagger \sum_m [\mathbf{G}_\downarrow(-\mathbf{k})]_{\beta m}^* d_{m-\mathbf{k}\downarrow}^\dagger \quad (\text{I.23})$$

$$= \quad (\text{I.24})$$

So that:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & G^\dagger \Delta G \\ G^\dagger \Delta^\dagger G & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix} \quad (\text{I.25})$$

with

$$\epsilon_{\mathbf{k}} = \begin{pmatrix} \epsilon_1(\mathbf{k}) & 0 & 0 \\ 0 & \epsilon_2(\mathbf{k}) & 0 \\ 0 & 0 & \epsilon_3(\mathbf{k}) \end{pmatrix} \quad (\text{I.26})$$

Concrete example for transformation of gaps from orbital to band basis at  $\mathbf{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ . There, the non-interacting part becomes simply:

$$\mathcal{H}_0 = \begin{pmatrix} 0 & 0 & V \\ 0 & 0 & 0 \\ V & 0 & 3t_X \end{pmatrix} \quad (\text{I.27})$$

The eigenvalue problem can be solved e.g. via sympy:

$$G = \begin{pmatrix} \frac{-3t_X - \sqrt{4V^2 + 9t_X^2}}{\sqrt{4V^2 + (3t_X + \sqrt{4V^2 + 9t_X^2})^2}} & 0 & \frac{-3t_X + \sqrt{4V^2 + 9t_X^2}}{\sqrt{4V^2 + (3t_X - \sqrt{4V^2 + 9t_X^2})^2}} \\ 0 & 1 & 0 \\ \frac{2V}{\sqrt{4V^2 + (3t_X + \sqrt{4V^2 + 9t_X^2})^2}} & 0 & \frac{2V}{\sqrt{4V^2 + (3t_X - \sqrt{4V^2 + 9t_X^2})^2}} \end{pmatrix} \quad (\text{I.28})$$

So for  $V \rightarrow 0$ :

$$G = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{I.29})$$

but for  $V > 0$ , there are off-diagonal elements, e.g.  $V = 0.1$ :

$$G = \begin{pmatrix} -0.7578 & 0 & 0.6526 \\ 0 & 1 & 0 \\ 0.6526 & 0 & 0.7578 \end{pmatrix} \quad (\text{I.30})$$

So the transformation of the gap from orbital to band space reads:

$$G^\dagger \Delta G = \begin{pmatrix} \frac{3\Delta_1 t_X - 3\Delta_3 t_X + (\Delta_1 + \Delta_3)\sqrt{4V^2 + 9t_X^2}}{2\sqrt{4V^2 + 9t_X^2}} & 0 & \frac{V(-\Delta_1 + \Delta_3)}{\sqrt{4V^2 + 9t_X^2}} \\ 0 & \Delta_2 & 0 \\ \frac{V(-\Delta_1 + \Delta_3)}{\sqrt{4V^2 + 9t_X^2}} & 0 & \frac{-3\Delta_1 t_X + 3\Delta_3 t_X + (\Delta_1 + \Delta_3)\sqrt{4V^2 + 9t_X^2}}{2\sqrt{4V^2 + 9t_X^2}} \end{pmatrix} \quad (\text{I.31})$$

So in particular there is no interband pairing for  $V \rightarrow 0$ :

$$G^\dagger \Delta G = \begin{pmatrix} \Delta_1 & 0 & 0 \\ 0 & \Delta_2 & 0 \\ 0 & 0 & \Delta_3 \end{pmatrix} \quad (\text{I.32})$$

But for  $V > 0$ , there is interband pairing (e.g.  $V = 0.1$ ):

$$G^\dagger \Delta G = \begin{pmatrix} 0.5742\Delta_1 + 0.4258\Delta_3 & 0 & -0.4945\Delta_1 + 0.4945\Delta_3 \\ 0 & \Delta_2 & 0 \\ -0.4945\Delta_1 + 0.4945\Delta_3 & 0 & 0.4258\Delta_1 + 0.5742\Delta_3 \end{pmatrix} \quad (\text{I.33})$$