

I MEAN FIELD TREATMENT, MULTI-BAND BCS THEORY

Introduced BCS theory in ??, but EG-X has multiple band, this is the important factor for having quantum geometry.

I.1 BdG HAMILTONIAN

Test

Define sublattice index

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

with $1 \cong \text{Gr}_1, 2 \cong \text{Gr}_2, 3 \cong \text{X}$. 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 α (with changed signs compared to Niklas, to keep in line with papers about the attractive Hubbard model):

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

Fourier transformation:

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

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.1.1 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:

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

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

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

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

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

with $\tilde{\epsilon}_{\mathbf{k}} := \epsilon_{\mathbf{k}} - \mu$. 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 $K = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. 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. $V = 0.1$):

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

I.2 GRAND POTENTIAL

See [peottaSuperfluidityTopologicallyNontrivial2015], especially supplementary material, notes 1 and 3.

Mean-Field Hamiltonian (with the last two terms due to exchange of anticommuting fermion operators and the term quadratic in the expectation value from the mean-field decoupling respectively):

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \text{Tr}(H_{\mathbf{k}}^\dagger) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} \quad (\text{I.34})$$

The second term is the trace of the non-interacting Hamiltonian.

Thermodynamic grand potential (which at zero temperature is equivalent to the mean-field energy):

$$\Omega(T, \Delta) = -\frac{1}{\beta} \ln Z_\Omega = -\frac{1}{\beta} \ln \text{Tr}(e^{-\beta H_{MF}}) \quad (\text{I.35})$$

$$= \sum_{\mathbf{k}} \text{Tr}(H_{\mathbf{k}}^\dagger) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{\beta} \ln \text{Tr}(e^{-\beta \Psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}}) \quad (\text{I.36})$$

Zero temperature limit:

$$\Omega(\Delta) = \sum_{\mathbf{k}} \text{Tr}(H_{\mathbf{k}}^\dagger) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{2} \sum_{\mathbf{k}} \text{Tr}([|\mathcal{H}_{\mathbf{k}}|]) \quad (\text{I.37})$$

where a function of a matrix H (such as taking the absolute value of the BdG Hamiltonian $\mathcal{H}_{\mathbf{k}}$) is defined for the diagonal matrix of eigenvalues D and the unitary matrix U that diagonalizes H :

$$f(H) = U f(D) U^\dagger \quad (\text{I.38})$$

The route to finding the value of the order parameter for a fixed interaction U is minimizing the grand potential with respect to Δ .