I EG-X Model with interactions

I.1 BdG

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

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

with the matrix

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

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):

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

Fourier transformation:

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

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

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

$$= \tag{I.24}$$

So that:

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

with

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

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

$$\mathcal{H}_0 = \begin{pmatrix} 0 & 0 & V \\ 0 & 0 & 0 \\ V & 0 & 3t_X \end{pmatrix} \tag{I.27}$$

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

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

So for $V \to 0$:

$$G = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{I.29}$$

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

$$G = \begin{pmatrix} -0.7578 & 0 & 0.6526 \\ 0 & 1 & 0 \\ 0.6526 & 0 & 0.7578 \end{pmatrix} \tag{I.30}$$

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

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

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

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

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

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

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):

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \mathrm{Tr}(H^\downarrow_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} \tag{I.34}$$

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):

$$\begin{aligned} \Omega(T, \Delta) &= -\frac{1}{\beta} \ln Z_\Omega = -\frac{1}{\beta} \ln \mathrm{Tr}(e^{-\beta H_{MF}}) && \text{(I.35)} \\ &= \sum_{\mathbf{k}} \mathrm{Tr}(H^\downarrow_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{\beta} \ln \mathrm{Tr}(e^{-\beta \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}}) && \text{(I.36)} \end{aligned}$$

Zero temperature limit:

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

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:

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

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