I Trash

Collection of some notes that could maybe be relevant, but really arent right now.

I.1 Dressed Graphene model

I.1.1 BdG Hamiltonian in band basis

Use transformation

$$c^\dagger_{\mathbf{k}\alpha\sigma} = \sum_n [\mathbf{G}]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \tag{I.1}$$

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

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 & \mathbf{G}_3 \end{pmatrix} \tag{I.2}$$

with that:

$$\mathbf{G}^\dagger_\sigma(\mathbf{k})\mathbf{H}_{0,\sigma}(\mathbf{k})\mathbf{G}_\sigma(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \tag{I.3}$$

So the kinetic part of the BdG Hamiltonian becomes:

$$\begin{aligned}
&\sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} \sum_n [\mathbf{G}(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \sum_m [\mathbf{G}(\mathbf{k})]_{\beta m} d_{m\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} && \text{(I.4)}\\
&= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \sum_{\alpha\beta} [\mathbf{G}(\mathbf{k})]^*_{\alpha n} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} [\mathbf{G}(\mathbf{k})]_{\beta m} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} && \text{(I.5)}\\
&= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} && \text{(I.6)}\\
&= \sum_{n\mathbf{k}\sigma} \epsilon_n d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} && \text{(I.7)}\\
&=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} && \text{(I.8)}
\end{aligned}$$

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

$$\sum_{\mathbf{k}\alpha} \Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} = \sum_{\mathbf{k}\alpha} \Delta_\alpha \sum_n [\mathbf{G}_\uparrow(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\uparrow} \sum_m [\mathbf{G}_\downarrow(-\mathbf{k})]^*_{\beta m} d^\dagger_{m-\mathbf{k}\downarrow} \tag{I.9}$$

$$= \tag{I.10}$$

So that:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & G^\dagger \Delta G \\ G^\dagger \Delta^\dagger G & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix} \tag{I.11}$$

with

$$\epsilon_{\mathbf{k}} = \begin{pmatrix} \epsilon_1(\mathbf{k}) & 0 & 0 \\ 0 & \epsilon_2(\mathbf{k}) & 0 \\ 0 & 0 & \epsilon_3(\mathbf{k}) \end{pmatrix} \tag{I.12}$$

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:

$$\mathcal{H}_0 = \begin{pmatrix} 0 & 0 & V \\ 0 & 0 & 0 \\ V & 0 & 3t_X \end{pmatrix} \tag{I.13}$$

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

$$G = \begin{pmatrix} \frac{-3t_X - \sqrt{4V^2+9t_X^2}}{\sqrt{4V^2+\left(3t_X+\sqrt{4V^2+9t_X^2}\right)^2}} & 0 & \frac{-3t_X + \sqrt{4V^2+9t_X^2}}{\sqrt{4V^2+\left(3t_X-\sqrt{4V^2+9t_X^2}\right)^2}} \\ 0 & 1 & 0 \\ \frac{2V}{\sqrt{4V^2+\left(3t_X+\sqrt{4V^2+9t_X^2}\right)^2}} & 0 & \frac{2V}{\sqrt{4V^2+\left(3t_X-\sqrt{4V^2+9t_X^2}\right)^2}} \end{pmatrix} \tag{I.14}$$

So for $V \to 0$:

$$G = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{I.15}$$

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

$$G = \begin{pmatrix} -0.7578 & 0 & 0.6526 \\ 0 & 1 & 0 \\ 0.6526 & 0 & 0.7578 \end{pmatrix} \tag{I.16}$$

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

$$G^{\dagger}\Delta G = \begin{pmatrix} \frac{3\Delta_1 t_X - 3\Delta_3 t_X + (\Delta_1+\Delta_3)\sqrt{4V^2+9t_X^2}}{2\sqrt{4V^2+9t_X^2}} & 0 & \frac{V(-\Delta_1+\Delta_3)}{\sqrt{4V^2+9t_X^2}} \\ 0 & \Delta_2 & 0 \\ \frac{V(-\Delta_1+\Delta_3)}{\sqrt{4V^2+9t_X^2}} & 0 & \frac{-3\Delta_1 t_X + 3\Delta_3 t_X + (\Delta_1+\Delta_3)\sqrt{4V^2+9t_X^2}}{2\sqrt{4V^2+9t_X^2}} \end{pmatrix} \tag{I.17}$$

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

$$G^{\dagger}\Delta G = \begin{pmatrix} \Delta_1 & 0 & 0 \\ 0 & \Delta_2 & 0 \\ 0 & 0 & \Delta_3 \end{pmatrix} \tag{I.18}$$

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

$$G^{\dagger}\Delta G = \begin{pmatrix} 0.5742\Delta_1 + 0.4258\Delta_3 & 0 & -0.4945\Delta_1 + 0.4945\Delta_3 \\ 0 & \Delta_2 & 0 \\ -0.4945\Delta_1 + 0.4945\Delta_3 & 0 & 0.4258\Delta_1 + 0.5742\Delta_3 \end{pmatrix} \tag{I.19}$$

I.1.2 Grand potential

See [1], 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):

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \mathrm{Tr}(H_{\mathbf{k}}^{\downarrow}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} \tag{I.20}$$

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):

$$\Omega(T,\Delta) = -\frac{1}{\beta}\ln Z_{\Omega} = -\frac{1}{\beta}\ln \mathrm{Tr}(e^{-\beta H_{MF}}) \tag{I.21}$$

$$= \sum_{\mathbf{k}} \mathrm{Tr}(H_{\mathbf{k}}^{\downarrow}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{\beta}\ln \mathrm{Tr}(e^{-\beta \Psi_{\mathbf{k}}^{\dagger}\mathcal{H}(\mathbf{k})\Psi_{\mathbf{k}}}) \tag{I.22}$$

Zero temperature limit:

$$\Omega(\Delta) = \sum_{\mathbf{k}} \mathrm{Tr}(H^{\downarrow}_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{2} \sum_{\mathbf{k}} \mathrm{Tr}([|\mathcal{H}_{\mathbf{k}}|]) \tag{I.23}$$

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:

$$f(H) = Uf(D)U^{\dagger} \tag{I.24}$$

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