I EG-X Model

I.1 Lattice Structure of Graphene

Structure of honeycomb lattice following [**Yang_Li_Lee_Ng_2018**].
Monolayer graphene forms a hexagonal lattice.
Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \tag{I.1}$$

$$\mathbf{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \tag{I.2}$$

with lattice constant $a \approx 2.46\,\text{Å}$ (distance between unit cells). Have

$$a = \sqrt{3}a_0 \tag{I.3}$$

with the nearest-neighbour distance a_0.
Vectors to the nearest-neighbor B_i $(i = 1, 2, 3,)$ atoms from atom A:

$$\boldsymbol{\delta}_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \tag{I.4}$$

Vectors to the nearest-neighbor A_i $(i = 1, 2, 3,)$ atoms from atom B:

$$\boldsymbol{\delta}_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix} \tag{I.5}$$

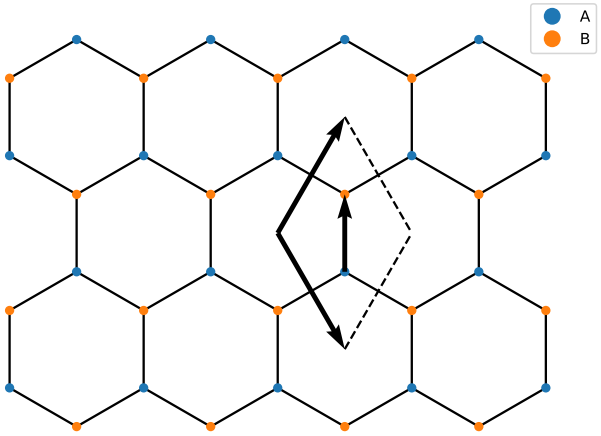

Figure I.1: *Graphene lattice structure*

The vectors between the Graphene A atom and the six neighbours on the same sub lattice can be found by rotating $\mathbf{a}_1$ six times by $1/6 * 2\pi = \pi/3$:

$$\boldsymbol{\delta}_{AA,1} = \mathbf{a}_1 = \frac{a}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} = a\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} = a\begin{pmatrix}\sin\left(\frac{\pi}{6}\right)\\ \cos\left(\frac{\pi}{6}\right)\end{pmatrix} \tag{I.6}$$

$$\boldsymbol{\delta}_{AA,2} = a\begin{pmatrix}\sin\left(\frac{3\pi}{6}\right)\\ \cos\left(\frac{3\pi}{6}\right)\end{pmatrix} = a\begin{pmatrix}1\\ 0\end{pmatrix} \tag{I.7}$$

$$\boldsymbol{\delta}_{AA,3} = a\begin{pmatrix}\sin\left(\frac{5\pi}{6}\right)\\ \cos\left(\frac{5\pi}{6}\right)\end{pmatrix} = a\begin{pmatrix}\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} \tag{I.8}$$

$$\boldsymbol{\delta}_{AA,4} = a\begin{pmatrix}\sin\left(\frac{7\pi}{6}\right)\\ \cos\left(\frac{7\pi}{6}\right)\end{pmatrix} = a\begin{pmatrix}-\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} \tag{I.9}$$

$$\boldsymbol{\delta}_{AA,5} = a\begin{pmatrix}\sin\left(\frac{9\pi}{6}\right)\\ \cos\left(\frac{9\pi}{6}\right)\end{pmatrix} = a\begin{pmatrix}-1\\ 0\end{pmatrix} \tag{I.10}$$

$$\boldsymbol{\delta}_{AA,6} = a\begin{pmatrix}\sin\left(\frac{11\pi}{6}\right)\\ \cos\left(\frac{11\pi}{6}\right)\end{pmatrix} = a\begin{pmatrix}-\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} \tag{I.11}$$

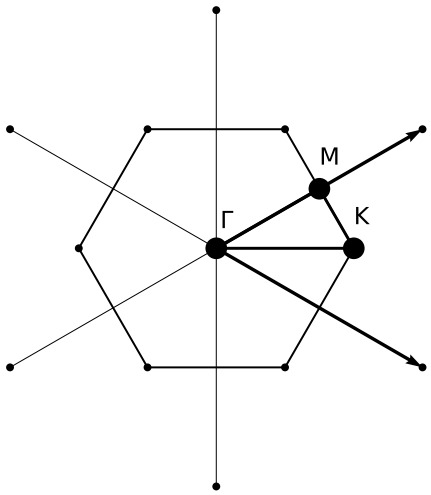

Figure I.2: *Graphene Brillouin Zone*

The primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$ fulfill

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{I.12}$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\ , \tag{I.13}$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.14}$$

$$\mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.15}$$

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{I.16}$$

$$\mathrm{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.17}$$

$$\mathrm{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{I.18}$$

I.2 EG-X Model

Graphene lattice and a site X. Real-life motivation: layer of graphene on top

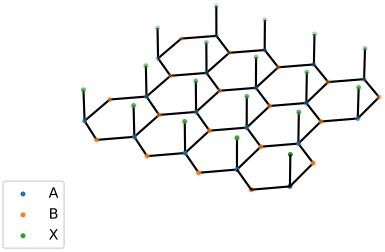

Figure I.3: *EG-X model*

of a substrate of another material (which provides the additional X atoms). There is no spin-orbit coupling considered in the model (but when according to Niklas: when mapping to substrates Sn or Pb, it could be necessary (but does not the qualitative result?)).

Without interaction :

$$H_0 = -t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma\sigma'} d^\dagger_{i,\sigma} d_{j,\sigma'} + \mathrm{h.c.} - t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma\sigma'} \left(c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} + c^{(B),\dagger}_{j,\sigma'} c^{(A)}_{i,\sigma} + \mathrm{h.c.} \right) \tag{I.19}$$

$$+ V \sum_{i,\sigma\sigma'} \left(d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma'} + c^{(A),\dagger}_{i,\sigma} d_{i,\sigma'} \right) \tag{I.20}$$

with:

- d operators on the X atom
- $c^{(\epsilon)}$ operators on the graphene site ($\epsilon = A, B$)
- t_X NN hopping for X
- t_{Gr} NN hopping of Gr
- V hybridization between X and Graphene B sites

We can also introduce an onsite Hubbard interaction:

$$H_{\mathrm{int}} = U_{\mathrm{X}} \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{\mathrm{Gr}} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{I.21}$$

I.2.1 Review: Hubbard model on the honeycomb lattice

I.2.2 Band structure of the non-interacting EG-X model

To treat eq. I.19, we first write out the sums over nearest neighbours $\langle i, j\rangle$ explicitly, writing $\boldsymbol{\delta}_{\mathrm{X}}, \boldsymbol{\delta}_\epsilon$ ($\epsilon = A, B$) for the connections to the nearest neighbours of the X atoms and Graphene A, B sites. Doing the calculation for the example of the X atoms:

$$- t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma\sigma'} (d^\dagger_{i,\sigma} d_{j,\sigma'} + d^\dagger_{j,\sigma} d_{i,\sigma'}) \tag{I.22}$$

$$= -\frac{t_X}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma'} - \frac{t_X}{2} \sum_{j,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{j,\sigma} d_{j+\delta_{\mathrm{X}},\sigma'} \tag{I.23}$$

$$= -t_X \sum_{i,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma'} \tag{I.24}$$

(The factor $1/2$ is to account for double counting when going to the sum over all lattice sites i)

Now we can input the discrete Fourier transform (for both graphene and X operators) into eq. I.21

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}} \tag{I.25}$$

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \tag{I.26}$$

with the completeness relation:

$$\sum_i e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} \ . \tag{I.27}$$

We get:

$$-t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} d_{i,\sigma}^\dagger d_{i+\boldsymbol{\delta}_\mathrm{X},\sigma'} = -t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} \sum_{\mathbf{k},\mathbf{k}'} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} \tag{I.28}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \tag{I.29}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} N\delta_{\mathbf{k},\mathbf{k}'} \tag{I.30}$$

$$= -t_X \sum_{\mathbf{k},\sigma,\sigma'} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_\mathrm{X}} \tag{I.31}$$

The nearest neighbours for X atoms are the vectors $\boldsymbol{\delta}_{AA,i}$ from section I.1. With that, we can calculate:

$$f_{\mathrm{X}}(\mathbf{k}) = -t_X \sum_{\boldsymbol{\delta}_{\mathrm{X}}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{\mathrm{X}}} \tag{I.32}$$

$$= -t_X \left(e^{\mathrm{i}a(\frac{k_x}{2}+\frac{\sqrt{3}k_y}{2})} + e^{\mathrm{i}ak_x} + e^{\mathrm{i}a(\frac{k_x}{2}-\frac{\sqrt{3}k_y}{2})} \right. \tag{I.33}$$

$$\left. + e^{\mathrm{i}a(-\frac{k_x}{2}-\frac{\sqrt{3}k_y}{2})} + e^{-\mathrm{i}ak_x} + e^{\mathrm{i}a(-\frac{k_x}{2}+\frac{\sqrt{3}k_y}{2})} \right) \tag{I.34}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{\mathrm{i}a\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-\mathrm{i}a\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \tag{I.35}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x)\cos(\sqrt{3}\frac{a}{2}k_y) \right) \tag{I.36}$$

We can do the same for the hopping between Graphene sites, for example :

$$-t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_{\mathrm{Gr}} \sum_{i,\sigma\sigma'} \sum_{\boldsymbol{\delta}_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\boldsymbol{\delta}_{AB},\sigma'} \tag{I.37}$$

$$= -t_{\mathrm{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} \tag{I.38}$$

We note

$$\sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} = \left(\sum_{\boldsymbol{\delta}_{BA}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}} \right)^* = \sum_{\boldsymbol{\delta}_{BA}} e^{-\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}} \tag{I.39}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} \tag{I.40}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{I.41}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x} \right) \right) \tag{I.42}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \cos(\frac{a}{2}k_x) \right) \tag{I.43}$$

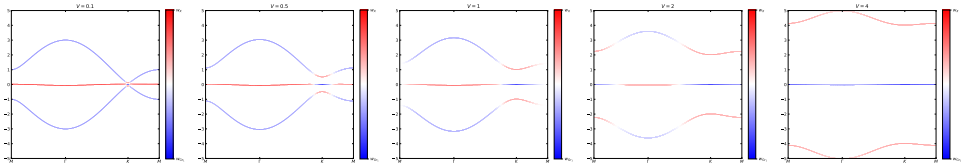

Figure I.4: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^{*}_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{I.44}$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. I.43. This was done in fig. I.4.

Values used for calculation:

- $a_0 = 1$
- $t_{\mathrm{Gr}} = 1$
- $t_{\mathrm{X}} = 0.01$

V is the control parameter. (According to Niklas), a range from $V = 0.1$ to $V = 2$ can be mapped onto materials in experiment.

I.3 BCS Theory on the EG-X Model

I.3.1 BdG Hamiltonian

Define sublattice index

$$\alpha = 1, 2, 3 \tag{I.45}$$

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

$$H_0 = -\sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^{\dagger}_{i\alpha} c_{j\beta} \tag{I.46}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{I.47}$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{I.48}$$

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

$$H_{int} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{I.49}$$

Fourier transformation:

$$H_{int} = -\frac{1}{N^2} \sum_{\alpha,\mathbf{k}_{1,2,3,4}} U_\alpha e^{\mathrm{i}(\mathbf{k}_1+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_3)r_{i\alpha}} c^\dagger_{\mathbf{k}_1\alpha\uparrow} c^\dagger_{\mathbf{k}_3\alpha\downarrow} c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \tag{I.50}$$

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

$$H_{int} = -\sum_{\alpha,\mathbf{k},\mathbf{k}'} U_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \tag{I.51}$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{I.52}$$

with

$$\Delta_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \tag{I.53}$$

$$\Delta^*_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\alpha\uparrow} c^\dagger_{-\mathbf{k}'\alpha\downarrow} \rangle \tag{I.54}$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{I.55}$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c^{\dagger}_{1,-\mathbf{k}\downarrow} \\ c^{\dagger}_{2,-\mathbf{k}\downarrow} \\ c^{\dagger}_{3,-\mathbf{k}\downarrow} \end{pmatrix} \tag{I.56}$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \tag{I.57}$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^{\dagger} & -H^{*}_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{I.58}$$

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

I.3.2 BdG Hamiltonian in band basis

Use transformation

$$c^{\dagger}_{\mathbf{k}\alpha\sigma} = \sum_{n} [\mathbf{G}]^{*}_{\alpha n} d^{\dagger}_{n\mathbf{k}\sigma} \tag{I.59}$$

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

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 & \mathbf{G}_3 \end{pmatrix} \tag{I.60}$$

with that:

$$\mathbf{G}^{\dagger}_{\sigma}(\mathbf{k}) \mathbf{H}_{0,\sigma}(\mathbf{k}) \mathbf{G}_{\sigma}(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \tag{I.61}$$

So the kinetic part of the BdG Hamiltonian becomes:

$$\sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} \sum_n [\mathbf{G}(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \sum_m [\mathbf{G}(\mathbf{k})]_{\beta m} d_{m\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.62}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \sum_{\alpha\beta} [\mathbf{G}(\mathbf{k})]^*_{\alpha n} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} [\mathbf{G}(\mathbf{k})]_{\beta m} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.63}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.64}$$

$$= \sum_{n\mathbf{k}\sigma} \epsilon_n d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{I.65}$$

$$=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} \tag{I.66}$$

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

$$\sum_{\mathbf{k}\alpha} \Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} = \sum_{\mathbf{k}\alpha} \Delta_\alpha \sum_n [\mathbf{G}_\uparrow(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\uparrow} \sum_m [\mathbf{G}_\downarrow(-\mathbf{k})]^*_{\beta m} d^\dagger_{m-\mathbf{k}\downarrow} \tag{I.67}$$

$$= -\sum_{n\mathbf{k}} \Delta_n d^\dagger_{n\mathbf{k}\uparrow} d^\dagger_{n-\mathbf{k}\downarrow} \tag{I.68}$$

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.

$$\sum_{\mathbf{k}\alpha} \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow} = -\sum_{n\mathbf{k}} \Delta^*_n d_{n-\mathbf{k}\downarrow} d_{n\mathbf{k}\uparrow} \tag{I.69}$$

So the BdG Hamiltonian is:

$$H_{BdG} = \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \sum_{n\mathbf{k}} (\Delta^*_n d_{n-\mathbf{k}\downarrow} d_{n\mathbf{k}\uparrow} + \Delta_n d^\dagger_{n\mathbf{k}\uparrow} d^\dagger_{n-\mathbf{k}\downarrow}) \tag{I.70}$$

I.3.3 Self-consistent calculation of the superconducting gaps

Compare [**Bruus_Flensberg_2004**]. Notable here: Multiple bands, and the gaps in each band depend in a complicated manner on the parameters U_α and the orbital Green's functions.

Define normal Green's function:

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) = -\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0) \rangle \tag{I.71}$$

Anomalous Green's function:

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = -\left\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.72}$$

Equations of motion (Heisenberg equation), follow [**Bruus_Flensberg_2004**]:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \left\langle T_\tau \left[d_{n\mathbf{k}\uparrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.73}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \left\langle T_\tau \left[d_{n-\mathbf{k}\downarrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.74}$$

To calculate the commutators, use the relation (for operators A, B, C):

$$[A, BC] = ABC - BCA = (\{A,B\} - BA)C - B(\{C,A\} - AC) \tag{I.75}$$

$$\left[d^\dagger_{n-\mathbf{k}\downarrow}, H_0\right] = \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] \tag{I.76}$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(\{d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'}\} - d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow}\right) d_{n'\mathbf{k}'\sigma'} \tag{I.77}$$

$$- d^\dagger_{n'\mathbf{k}'\sigma'} \left(\{d_{n'\mathbf{k}'\sigma'}, d^\dagger_{n-\mathbf{k}\downarrow}\} - d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) \tag{I.78}$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(-d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'} - d^\dagger_{n'\mathbf{k}'\sigma'} \delta_{n'\mathbf{k}'\sigma',n-\mathbf{k}\uparrow} + d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) \tag{I.79}$$

$$= -\xi_{n\mathbf{k}} d^\dagger_{n\mathbf{k}\uparrow} \tag{I.80}$$

$$\left[d_{n-\mathbf{k}\downarrow}, -\sum_{m\mathbf{k}'} \Delta^*_m d_{m-\mathbf{k}'\downarrow} d_{m\mathbf{k}'\uparrow}\right] \tag{I.81}$$

$$= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\{d_{n-\mathbf{k}\downarrow}, d_{m-\mathbf{k}'\downarrow}\} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} \tag{I.82}$$

$$- d_{m-\mathbf{k}'\downarrow} \left(\{d_{m\mathbf{k}'\uparrow}, d_{n-\mathbf{k}\downarrow}\} - d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow}\right) \tag{I.83}$$

$$= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\delta_{n-\mathbf{k}\downarrow,m-\mathbf{k}'\downarrow} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} + d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow} \tag{I.84}$$

$$= -\Delta^*_n d_{n\mathbf{k}\uparrow} \tag{I.85}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = -\xi_{n\mathbf{k}} \left\langle T_\tau (d^\dagger_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)) \right\rangle - \Delta_n^* \left\langle T_\tau (d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)) \right\rangle \tag{I.86}$$

$$= \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) + \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) \tag{I.87}$$

Similarly:

$$\left[d_{n-\mathbf{k}\uparrow}, H_0\right] = \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] \tag{I.88}$$

$$= \xi_n d^\dagger_{n\mathbf{k}\uparrow} \tag{I.89}$$

$$\left[d_{n-\mathbf{k}\uparrow}, -\sum_{m\mathbf{k}'} \Delta_m d^\dagger_{m-\mathbf{k}'\uparrow} d^\dagger_{m-\mathbf{k}'\downarrow}\right] \tag{I.90}$$

$$= -\Delta_n d^\dagger_{n-\mathbf{k}\downarrow} \tag{I.91}$$

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \xi_{n\mathbf{k}} \left\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow} \right\rangle - \Delta_n \left\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0) \right\rangle \tag{I.92}$$

$$= -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{I.93}$$

$$\tag{I.94}$$

All in all:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{I.95}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) + \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) \tag{I.96}$$

Fourier transform:

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = -1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{I.97}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{I.98}$$

This algebraic expression can be easily solved:

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} (-1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n)) \tag{I.99}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}} - \frac{|\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}})\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{I.100}$$

$$(\frac{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}})\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{I.101}$$

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{-\Delta_n^*}{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2} \tag{I.102}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.103}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{I.104}$$

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = -1 + \frac{-|\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.105}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2 + |\Delta_n|^2 - |\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.106}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.107}$$

$$= \frac{(\mathrm{i}\omega_n + \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.108}$$

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.109}$$

$$= \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{I.110}$$

with the energies $E_{n\mathbf{k}} = \pm\sqrt{\xi_{n\mathbf{k}}^2 + |\Delta_n|^2}$.

To calculate the band gap in band n:

$$\Delta_n(\mathbf{k}) = -\sum_{\alpha}[G_{k\uparrow}]^*_{\alpha n}\Delta_\alpha[G_{-k\downarrow}]^*_{\alpha n} \tag{I.111}$$

$$= \sum_{\alpha\mathbf{k}'} U_\alpha[G_{k\uparrow}]^*_{\alpha n}\left\langle c_{-k'\alpha\downarrow}c_{k'\alpha\uparrow}\right\rangle[G_{-k\downarrow}]^*_{\alpha n} \tag{I.112}$$

$$= \sum_{\alpha\mathbf{k}'} U_\alpha[G_{k\uparrow}]^*_{\alpha n}[G_{-k\downarrow}]^*_{\alpha n}\sum_m[G_{-k'\downarrow}]_{\alpha m}[G_{k'\uparrow}]_{\alpha m}\left\langle d_{-k'm\downarrow}d_{k'm\uparrow}\right\rangle \tag{I.113}$$

Can now use $\mathcal{F}$ and fourier-transform:

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle = \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \tau = 0^+) \tag{I.114}$$

$$= \frac{1}{\beta} \sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+} \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \mathrm{i}\omega_n) \tag{I.115}$$

The summation over the Matsubara frequencies can be solved via the Residue theorem (the poles z_0 of $\mathcal{F}$ are the energies $\pm E_{m\mathbf{k}}$):

$$\frac{1}{\beta} \sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+} \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \mathrm{i}\omega_n) \tag{I.116}$$

$$= \sum_{z_0 \mathrm{polesof} \mathcal{F}} e^{-z_0 0^+} n_F(z_0) Res_{z_0} \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', z_0) \tag{I.117}$$

$$= e^{-E_{m\mathbf{k}} 0^+} n_F(E_{m\mathbf{k}}) Res_{E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} + e^{E_{m\mathbf{k}} 0^+} n_F(-E_{m\mathbf{k}}) Res_{-E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} \tag{I.118}$$

with residue:

$$Res_{E_{m\mathbf{k}}} \frac{1}{(\mathrm{i}\omega_n)^2 - z_0^2} = \frac{1}{\partial_z|_{z_0 = E_{m\mathbf{k}}} ((\mathrm{i}\omega)^2 - z_0^2)} = \frac{1}{2E_{m\mathbf{k}}} \tag{I.119}$$

So we have

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle = -\Delta_m \left(\frac{n_F(E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} - \frac{n_F(-E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} \right) \tag{I.120}$$

The n_F term can be written as:

$$n_F(E_{m\mathbf{k}'}) - n_F(-E_{m\mathbf{k}'}) = \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \tag{I.121}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \tag{I.122}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}} - e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}} + e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \tag{I.123}$$

$$= -\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right) \tag{I.124}$$

This results in the self-concistency equation for the gap:

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m \mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} [G_{-k\downarrow}]^*_{\alpha n} [G_{-k'\downarrow}]_{\alpha m} [G_{k'\uparrow}]_{\alpha m} \Delta_m(\mathbf{k}') \frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{E_{m\mathbf{k}'}} \tag{I.125}$$

Using time-reversal symmetry $[G_{-\mathbf{k}\downarrow}]^*_{\alpha m} = [G_{\mathbf{k}\uparrow}]_{\alpha m}$ this expression gets a bit simpler:

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m \mathbf{k}'} U_\alpha |[G_{k\uparrow}]_{\alpha n}|^2 |[G_{k'\uparrow}]_{\alpha m}|^2 \Delta_m(\mathbf{k}') \frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{E_{m\mathbf{k}'}} \tag{I.126}$$

I.3.4 Computational Implementation

Use scipys `fixed_point` solver to solve the gap equation self-consistently.

Flatten $\Delta_n(\mathbf{k})$ the following way, to put it into the solver ($\mathbf{k}$ discretized in some way):

$$x = \begin{pmatrix} \Re(\Delta_1(\mathbf{k}_1)) \\ \Re(\Delta_1(\mathbf{k}_2)) \\ \vdots \\ \Re(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Re(\Delta_3(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_1(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_3(\mathbf{k}_1)) \\ \vdots \end{pmatrix} \tag{I.127}$$

so that accessing a certain element takes the form:

$$\Re\Delta_n(\mathbf{k}) = x\left[\text{index}(\mathbf{k}) + \frac{\text{len}(x)\cdot n}{6}\right] \tag{I.128}$$

$$\Im\Delta_n(\mathbf{k}) = x\left[\text{index}(\mathbf{k}) + \frac{\text{len}(x)\cdot n}{6} + \frac{1}{2}\text{len}(x)\right] \tag{I.129}$$