Contents

I Green's Function Formalism **1**
I.1 Nambu-Gorkov GF 2

II Superconductivity **3**
II.0.1 Extracting T_C 3

III d-wave Superconductivity **5**
III.1 BCS theory with momentum dependent coupling 5
III.2 Anisotropic pairing 6
III.2.1 Hubbard interaction 6
III.2.2 Magnetic interaction 9
III.3 d-wave superconductivity in two dimensions - cuprates 9

IV Coherence length and penetration depth in strongly correlated superconductors **15**
IV.1 Ginzburg-Landau description 15

V Dynamical Mean-Field Theory **17**

VI Hubbard model **19**

VII EG-X Model **21**
VII.1 Lattice Structure of Graphene 21
VII.2 EG-X Model 24
VII.2.1 Review: Hubbard model on the honeycomb lattice . . 25
VII.2.2 Band structure of the non-interacting EG-X model . . 25
VII.3 BCS Theory on the EG-X Model 28
VII.3.1 BdG Hamiltonian 28
VII.3.2 BdG Hamiltonian in band basis 30
VII.3.3 Self-consistent calculation of the superconducting gaps 31

VII.3.4 Computational Implementation 36

Bibliography **39**

List of Symbols **41**

I Green's Function Formalism

Following [1]

Green's functions: method to encode influence of many-body effects on propagation of particles in a system.

Have different kinds of Green's functions, for example the retarded Green's function:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -\mathrm{i}\Theta(t-t')\left\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(t')\}\right\rangle \tag{I.1}$$

They give the amplitude of a particle inserted at point $\mathbf{r}'$ at time t' to propagate to position $\mathbf{r}$ at time t. In a translation invariant system: can use $\mathbf{k}$ as a natural basis set:

$$G^R(\mathbf{k}, \sigma t, \sigma' t') = -\mathrm{i}\Theta(t-t')\left\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma}(t')\}\right\rangle \tag{I.2}$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma, \omega) = -2\Im G^R(\mathbf{k}\sigma, \omega) \tag{I.3}$$

Mathematical technique to calculate retarded GFs involves defining GFs on imaginary times τ:

$$t \to -\mathrm{i}\tau \tag{I.4}$$

where τ is real and has the dimension time. This enables the simultaneous expansion of exponential $e^{-\beta H}$ coming from the thermodynamic average and $e^{-\mathrm{i}Ht}$ coming from the time evolution of operators.

Define imaginary time/Matsubara GF $\mathcal{C}_{AB}(\tau, 0)$:

$$\mathcal{C}_{AB}(\tau, 0) = -\left\langle T_\tau(A(\tau)B(0))\right\rangle \tag{I.5}$$

with time-ordering operator in imaginary time:

Can prove from properties of Matsubara GF, that they are only defined for

$$-\beta < \tau < \beta \tag{I.6}$$

Due to this, the Fourier transform of the Matsubara GF is defined on discrete values:

$$\mathcal{C}_{AB}(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{I.7}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{I.8}$$

Extrapolation of the Matsubara GF to zero is proportional to the density of states at the chemical potential. Gapped: density is zero (Matsubara GF goes to 0), metal: density is finite (Matsubara GF goes to finite value) [1, p. 8.3.4].

I.1 Nambu-Gorkov GF

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{I.9}$$

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{I.10}$$

that can be calculated from the anomalous self-energy Σ^{AN} and quasiparticle weight Z

II Superconductivity

II.0.1 Extracting T_C

From Niklas

Übrigens: Typische Varianten, um 'sauber(er)' Tc zu bestimmen, ist $|OP|^2$ gegen T aufzutragen, da das (als Phasenübergang 2. Ordnung) proportional zu T-Tc ist. Heißt, man kann Tc dann mittels linearem Fit finden - ist leider auch nicht immer der einfachste Weg, weil der Bereich, in dem diese lineare Näherung prinzipiell sehr klein um Tc herum sein kann. Aber pi-mal-Daumen Abschätzungen gehen damit ganz gut. Oder man macht es wie unten beschrieben mit einer daraus abgeleiteten Formel.

in the superconducting region in Fig. 2A. To estimate T_c, we assume that the order parameter as a function of temperature behaves like $P_{SC}(T) \propto \sqrt{T_c - T}$ for $T \lesssim T_c$. We pick the highest and the second highest temperatures (T_1 and T_2, respectively), which give stable superconducting solutions ($P_{SC} \gtrsim 0.01$). Then, T_c is determined by

$$T_c = T_1 + (T_1 - T_2)\frac{P_{SC}^2(T_1)}{P_{SC}^2(T_2) - P_{SC}^2(T_1)}. \qquad \text{(S4)}$$

Figure II.1: *Formula for extracting T_C*

III d-wave Superconductivity

Source: Coleman - *Introduction to Many-Body Physics* [2, ch. 15]

III.1 BCS theory with momentum dependent coupling

Starting point is a BCS-Hamiltonian with momentum-dependent coupling term $V_{\mathbf{k},\mathbf{k}'}$:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{III.1}$$

The original idea by Bardeen, Cooper and Schrieffer uses the coupling

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -\frac{g_0}{V} \ , \ |\epsilon_{\mathbf{k}}| < \omega_D \\ 0 \end{cases} \tag{III.2}$$

Then similar process as for BCS theory without the momentum-dependent term (Hubbard-Stratonovich decoupling, minimization of mean-field free energy). Gives self-consistent equation for the gap function:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{III.3}$$

or at $T = 0$:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tag{III.4}$$

Important note: there is a minus sign in the front! If $V_{\mathbf{k},\mathbf{k}'} < 0$ (a uniformly attractive interaction), the equation is fulfilled by a uniformly positive gap function. In general $V_{\mathbf{k},\mathbf{k}'}$ contains repulsive (positive) terms (in particual stemming from the Coulomb interaction), so the gap function cannot be

uniformly positive, it acquires nodes in momentum space. Most satisfying solutions fulfill:

$$\operatorname{sign}(\Delta_{\mathbf{k}}) = -\operatorname{sign}(V_{\mathbf{k},\mathbf{k}'})\operatorname{sign}(\Delta_{\mathbf{k}'}) \tag{III.5}$$

So for an attractive interaction we have:

$$\operatorname{sign}(\Delta_{\mathbf{k}}) = -(-1)\operatorname{sign}(\Delta_{\mathbf{k}'}) \tag{III.6}$$

So areas in phase space linked by an attractive interaction have the same sign (and areas linked by repulsive interaction have opposite signs)! Solutions like this have the largest gaps and thus the largest mean-field transition temperature .

Two cases :

- Electron-phonon superconductors: interaction is repulsive at high energies, $\Delta_{\mathbf{k}}$ is largely isotropic in momentum space, but changes sign at $\approx$ Debye frequency
- Anisotropic superconductors: $\Delta_{\mathbf{k}}$ is strongly momentum-dependent, acquires nodes in momentum space

The last mechanism is at work in heavy-fermion, high-temperature cuprate and iron-based superconductors.

III.2 Anisotropic pairing

III.2.1 Hubbard interaction

The goal in this section is to derive a BCS-like Hamiltonian with a term

$$V_{\mathbf{k},\mathbf{k}'}\Psi^{\dagger}_{\mathbf{k}}\Psi_{\mathbf{k}'} \tag{III.7}$$

We start from a Hubbard-like interaction term

$$V = \sum_{\mathbf{q}} V_{\mathbf{q}} : \rho_{-\mathbf{q}}\rho_{\mathbf{q}} := \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q},\sigma,\sigma'} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k}_1+\mathbf{q}\sigma} c^{\dagger}_{\mathbf{k}_2-\mathbf{q}\sigma'} c_{\mathbf{k}_2\sigma'} c_{\mathbf{k}_1\sigma} \tag{III.8}$$

Cooper pairs have zero total momentum and the pairing potential is determined by the interaction on them, so we have

$$\mathbf{k}_1 + \mathbf{k}_2 = 0 \implies \mathbf{k}_1 = -\mathbf{k}_2 -: \mathbf{k}' \tag{III.9}$$

$$\mathbf{k}_1 + \mathbf{q} = -(\mathbf{k}_2 - \mathbf{q}) -: \mathbf{k} \implies \mathbf{k}' + \mathbf{q} = \mathbf{k} \implies \mathbf{q} = \mathbf{k} - \mathbf{k}' \tag{III.10}$$

and we can split up the interaction term

$$V_{\mathrm{BCS}} = \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} V_{\mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}\sigma} c^\dagger_{-\mathbf{k}\sigma'} c_{-\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma} \tag{III.11}$$

$$= \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \qquad \left(= \frac{1}{2} V^{\uparrow\downarrow}_{\mathrm{BCS}}\right) \tag{III.12}$$

$$+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\uparrow} c_{-\mathbf{k}'\uparrow} c_{\mathbf{k}'\downarrow} \qquad \left(= \frac{1}{2} V^{\downarrow\uparrow}_{\mathrm{BCS}} = \frac{1}{2} V^{\uparrow\downarrow}_{\mathrm{BCS}}\right) \tag{III.13}$$

$$+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\uparrow} c_{-\mathbf{k}'\uparrow} c_{\mathbf{k}'\uparrow} \qquad \left(= V^{\uparrow\uparrow}_{\mathrm{BCS}}\right) \tag{III.14}$$

$$+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\downarrow} \qquad \left(= V^{\downarrow\downarrow}_{\mathrm{BCS}}\right) \tag{III.15}$$

$$= V^{\uparrow\downarrow}_{\mathrm{BCS}} + V^{\uparrow\uparrow}_{\mathrm{BCS}} + V^{\downarrow\downarrow}_{\mathrm{BCS}} \tag{III.16}$$

First we treat $V^{\uparrow\downarrow}_{\mathrm{BCS}}$. Pair of opposite spins are neither single nor triplet, because they are not appropiately symmetrised. If we have the pair wavefunction

$$F(\mathbf{k})_{\alpha\beta} = \langle \mathbf{k}\alpha, -\mathbf{k}\beta | \, |\mathbf{k}\rho\rangle \tag{III.17}$$

We define spatial parity of this wavefunction:

$$F(-\mathbf{k})_{\alpha\beta} = PF(\mathbf{k})_{\alpha\beta} \tag{III.18}$$

as well as the spin parity:

$$F(\mathbf{k})_{\beta\alpha} = XF(\mathbf{k})_{\alpha\beta} \, , \tag{III.19}$$

where we define singlets ($X = +1$) and triplets ($X = -1$). The join application of XP is an exchange of fermions, so it should have an eigenvalue -1. So we have

- even-parity pairs, $P = +1 \implies X = -1$, spin singlets, $(X, P) = (+, -)$
- odd-parity pairs, $P = -1 \implies X = +1$, spin triplets, $(X, P) = (-, +)$

We split up the interaction into the symmetric and asymmetric parts :

$$V_{\rm BCS} = \sum_{\mathbf{k},\mathbf{k'}} \left(\frac{V_{\mathbf{k}-\mathbf{k'}} + V_{\mathbf{k}+\mathbf{k'}}}{2} + \frac{V_{\mathbf{k}-\mathbf{k'}} - V_{\mathbf{k}+\mathbf{k'}}}{2} \right) \Psi^\dagger_{\mathbf{k}} \Psi_{\mathbf{k'}} \tag{III.20}$$

$$:- \left(V^S_{\mathbf{k},\mathbf{k'}} + V^T_{\mathbf{k},\mathbf{k'}} \right) \Psi^\dagger_{\mathbf{k}} \Psi_{\mathbf{k'}} \ , \tag{III.21}$$

where we have defined the BCS pairing interaction in the singlet and triplet channel:

$$V^{S,T}_{\mathbf{k},\mathbf{k'}} = \frac{1}{2} \left(V_{\mathbf{k}-\mathbf{k'}} \pm V_{\mathbf{k}+\mathbf{k'}} \right) \tag{III.22}$$

The singlet channel is even in $\mathbf{k}, \mathbf{k'}$:

$$V^S_{-\mathbf{k},-\mathbf{k'}} = \frac{1}{2} \left(V_{-\mathbf{k}+\mathbf{k'}} \pm V_{-\mathbf{k}-\mathbf{k'}} \right) = \frac{1}{2} \left(V_{-(\mathbf{k}-\mathbf{k'})} \pm V_{-(\mathbf{k}+\mathbf{k'})} \right) = \frac{1}{2} \left(V_{\mathbf{k}-\mathbf{k'}} \pm V_{\mathbf{k}+\mathbf{k'}} \right) \ , \tag{III.23}$$

while the triplet channel is odd in $\mathbf{k}, \mathbf{k'}$. In the sum:

With everything we write the unequal spin pairing as:

$$V^{\uparrow\downarrow}_{\rm BCS} = \frac{1}{4} \sum_{\mathbf{k}\mathbf{k'}} \left[V^S_{\mathbf{k},\mathbf{k'}} \Psi^{S\dagger}_{\mathbf{k}} \Psi^S_{\mathbf{k'}} + V^T_{\mathbf{k},\mathbf{k'}} \Psi^{T\dagger}_{\mathbf{k}} \Psi^T_{\mathbf{k'}} \right] \tag{III.24}$$

$$= \sum_{\mathbf{k}\mathbf{k'} \in \frac{1}{2}\rm BZ} \left[V^S_{\mathbf{k},\mathbf{k'}} \Psi^{S\dagger}_{\mathbf{k}} \Psi^S_{\mathbf{k'}} + V^T_{\mathbf{k},\mathbf{k'}} \Psi^{T\dagger}_{\mathbf{k}} \Psi^T_{\mathbf{k'}} \right] \tag{III.25}$$

The equal spin pairing also includes triplet pairing (these are wrapped up in the vectors) and all in all the BCS pairing potential is:

$$V_{\rm BCS} = \sum_{\mathbf{k}\mathbf{k'} \in \frac{1}{2}\rm BZ} \left[V^S_{\mathbf{k},\mathbf{k'}} \Psi^{S\dagger}_{\mathbf{k}} \Psi^S_{\mathbf{k'}} + V^T_{\mathbf{k},\mathbf{k'}} * \Psi^{T\dagger}_{\mathbf{k}} \cdot * \Psi^T_{\mathbf{k'}} \right] \tag{III.26}$$

In real materials we mostly see singlet pairing , in this case we can just write:

$$V_{\rm BCS} = \sum_{\mathbf{k}\mathbf{k'} \in \frac{1}{2}\rm BZ} V^S_{\mathbf{k},\mathbf{k'}} (c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})(c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow}) \tag{III.27}$$

III.2.2 Magnetic interaction

Starting point here is a magnetic interaction:

$$V_{\text{mag}} = \frac{1}{2}\sum_{\mathbf{q}} J_{\mathbf{q}} \left[\mathbf{S}_{-\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}}\right] \tag{III.28}$$

$$= \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} J_{\mathbf{q}} c^{\dagger}_{\mathbf{k}_1+\mathbf{q}\alpha} c^{\dagger}_{\mathbf{k}_2-\mathbf{q}\gamma} \left(\frac{\boldsymbol{\sigma}}{2}\right)_{\alpha\beta} \left(\frac{\boldsymbol{\sigma}}{2}\right)_{\gamma\delta} c_{\mathbf{k}_2\delta} c_{\mathbf{k}_1\beta} \tag{III.29}$$

Important point: eigenvalues of $\mathbf{S}_1 \cdot \mathbf{S}_2$ are different for singlet and triplet states:

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \begin{cases} +\frac{1}{4} & \text{(triplet)} \\ -\frac{3}{4} & \text{(singlet)} \end{cases} \tag{III.30}$$

These eigenvalues enter as prefactors into the pairing potentials:

$$V^S_{\mathbf{k},\mathbf{k}'} = -\frac{3}{4}\left(\frac{J_{\mathbf{k}-\mathbf{k}'} + J_{\mathbf{k}+\mathbf{k}'}}{2}\right) \tag{III.31}$$

$$V^T_{\mathbf{k},\mathbf{k}'} = \frac{1}{4}\left(\frac{J_{\mathbf{k}-\mathbf{k}'} - J_{\mathbf{k}+\mathbf{k}'}}{2}\right) \tag{III.32}$$

So antiferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} > 0 \implies V^S_{\mathbf{k},\mathbf{k}'} < 0$) attract in the singlet channel, while ferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} < 0 \implies V^T_{\mathbf{k},\mathbf{k}'} < 0$) attracts in the triplet channel.

III.3 d-wave superconductivity in two dimensions - cuprates

Cuprate superconductors cannot be understood in Fermi liquid theory.

Three regimes :

- Undoped: antiferromagnetic Mott insulators
- Doped: d-wave superconductors
- Over-doped: Fermi liquid behaviours reoccurs, BCS treatment is applicable

Approximate by 2D tight-binding lattice (with nearest-neighbour hopping strength t) with

$$\epsilon_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a)) - \mu \tag{III.33}$$

interacting via onsite Coulomb repulsion and nearest-neighbour antiferromagnetic interaction:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_j U n_{j\uparrow} n_{j\downarrow} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{III.34}$$

In momentum space:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{q}} U \rho_{-\mathbf{q}} \rho_{\mathbf{q}} + J \sum_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}} \tag{III.35}$$

with $J_{\mathbf{q}} = 2J(\cos(q_x a) + \cos(q_y a))$. From the treatment of the Hubbard and magnetic interaction earlier we can get the singlet interaction

$$V_{\mathbf{k},\mathbf{k}'} = U - \frac{3J}{2}\left(c_x c_{x'} + c_y c_{y'}\right) \tag{III.36}$$

where we use the abbreviation $c_x = \cos(k_x a)$. So the mean-field BCS Hamiltonian is

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} \left(U - \frac{3J}{2}\left(c_x c_{x'} + c_y c_{y'}\right)\right) \tag{III.37}$$

Looking at the gap equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right), \tag{III.38}$$

we see that the interaction preserves the symmetries of the pair ($\hat{=}$ symmetries of $\Delta_{\mathbf{k}}$). We divide the interaction into two parts:

$$V^S_{\mathbf{k},\mathbf{k}'} = U - \frac{3J}{4}(c_x + c_y)(c_{x'} + c_{y'}) \tag{III.39}$$

$$V^D_{\mathbf{k},\mathbf{k}'} = -\frac{3J}{2}(c_x - c_y)(c_{x'} - c_{y'}) \tag{III.40}$$

$$V^S_{\mathbf{k},\mathbf{k}'} + V^D_{\mathbf{k},\mathbf{k}'} = U - \frac{3J}{4}(c_x c_{x'} + c_x c_{y'} + c_{x'} c_y + c_y c_{y'}) \tag{III.41}$$

$$- \frac{3J}{4}(c_x c_{x'} - c_x c_{y'} - c_{x'} c_y + c_y c_{y'}) \tag{III.42}$$

$$= U - \frac{3J}{2}(c_x c_{x'} + c_y c_{y'}) = V_{\mathbf{k},\mathbf{k}'} \tag{III.43}$$

We call $\frac{3J}{4}(c_x + c_y)(c_{x'} + c_{y'})$ the extended s-wave term. The s-wave term is invariant under 90° rotations of $\mathbf{k}$ or $\mathbf{k}'$, whereas the d-wave term changes sign :

$$V^S_{\mathbf{k},\mathbf{k}'} = V^S_{\mathbf{k}R\mathbf{k}'} \tag{III.44}$$

$$V^D_{\mathbf{k},\mathbf{k}'} = -V^D_{\mathbf{k}R\mathbf{k}'} \tag{III.45}$$

with $R\mathbf{k} = (-k_y, k_x)$. Another point to note is that in the d-wave term, there is no onsite Coulomb interaction. So a condensate with d-wave symmetry ,

$$\Delta^D_{\mathbf{k}} = \Delta_D(c_x - c_y) \tag{III.46}$$

$$\Delta^D_{R\mathbf{k}} = -\Delta^D_{\mathbf{k}} \tag{III.47}$$

couples to cooper pairs via d-wave interaction , because

$$\sum_{\mathbf{k}'} V^S_{\mathbf{k},\mathbf{k}'} \Delta^D_{\mathbf{k}'}(\ldots) = 0 \tag{III.48}$$

(see gap equation, it preserves the symmetry of the pair). A condensate with extended s-wave symmetry

$$\Delta^S_{\mathbf{k}} = \Delta_1 + \Delta_2(c_x + c_y) \tag{III.49}$$

vanishes when integrated with the d-wave part of the interaction. This means the two types of pairing are symmetry decoupled and moreover, the symmetry of the d-wave pair decouples against the local Coulomb pseudopotential.

The quasiparticle energy for the d-wave condensate is:

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2 (c_y - c_x)^2} \tag{III.50}$$

It vanishes at intersections of nodes (where $\Delta_{\mathbf{k}} = 0$) and the Fermi surface

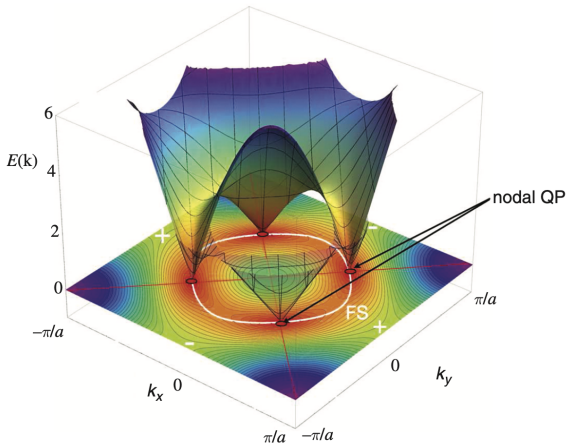

Figure III.1

(where $\epsilon_{\mathbf{k}} = 0$). At these points the dispersion can be linearized, they form Dirac cones of excitations with a relativistic dispersion . We can approximately solve the gap equation and get

$$\Delta_D (c_y - c_x) = \Delta_D (k_x^2 - k_y^2) = \Delta_0 \cos(2\theta) \tag{III.51}$$

The dependence $\Delta \propto \cos(2\theta)$ is typical for an $l = 2$ Cooper pair. The quasiparticle energy is then

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + (\Delta_0 \cos(2\theta))^2} \tag{III.52}$$

The d-wave density of states does not have a clear gap, but instead a V-shaped structure. This linear DOS across the gap is due to the Dirac cones.

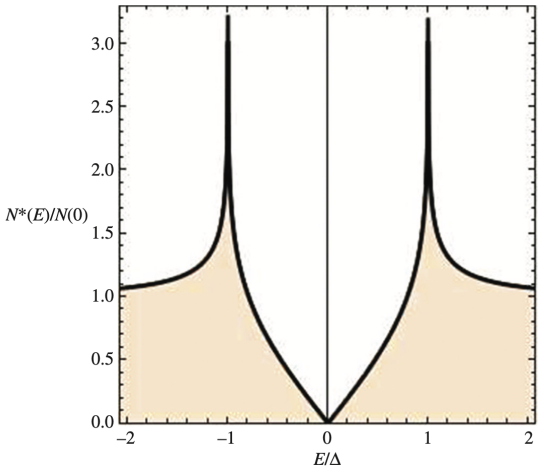

Figure III.2

IV Coherence length and penetration depth in strongly correlated superconductors

Order parameter (OP) of a superconducting condensate with FMP has the form

$$\Psi_{\mathbf{q}}(\mathbf{r}) = |\Psi_{\mathbf{q}}| e^{i\mathbf{q}\mathbf{r}} \tag{IV.1}$$

where $\mathbf{q}$ is the center-of-mass momentum of Cooper pairs.

FMP is well known from Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) theory, where the single-momentum phase used here corresponds to FF-type pairing.

IV.1 Ginzburg-Landau description

First: Motivate how the FMP constraint relates to λ_L and ξ_0.

GL low-order expansion of the free energy density f_{GL} in terms of the FMP-constrained OP reads

$$1 \tag{IV.2}$$

The temperature dependent correlation length ξ appears as the natural length scale of the amplitude mode ($\propto \alpha$) and kinetic energy term

$$\xi(T) = \tag{IV.3}$$

with the zero temperature value ξ_0 being the coherence length.

V Dynamical Mean-Field Theory

Source: Georges et al. - "Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions" [3]

With help from [4] and [5] to make it more concise.

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \tag{V.1}$$

with lattice coordinates i, j and spin σ.

One particle Green's function (many-body object, coming from the Hubbard model):

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)} \tag{V.2}$$

with the self energy $\Sigma(\mathrm{i}\omega_n)$ coming from the solution of the effect on-site problem:

The Dyson equation

$$G(\mathbf{k}, \mathrm{i}\omega_n) = (G_0(\mathbf{k}, \mathrm{i}\omega_n) - \Sigma(\mathbf{k}, \mathrm{i}\omega_n))^{-1} \tag{V.3}$$

relates the non-interacting Greens function $G_0(\mathbf{k}, \mathrm{i}\omega_n)$ and the fully-interacting Greens function $G(\mathbf{k}, \mathrm{i}\omega_n)$ (inversion of a matrix!).

VI Hubbard model

VII EG-X Model

VII.1 Lattice Structure of Graphene

Structure of honeycomb lattice following [6].
Monolayer graphene forms a hexagonal lattice.
Primitive lattice vectors of the hexagonal lattice:

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

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

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

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

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

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

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

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

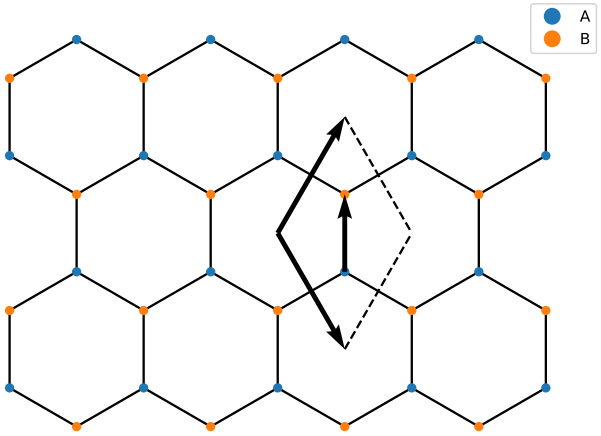

Figure VII.1: *Graphene lattice structure*

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 $1/6 * 2\pi = \pi/3$:

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

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

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

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

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

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

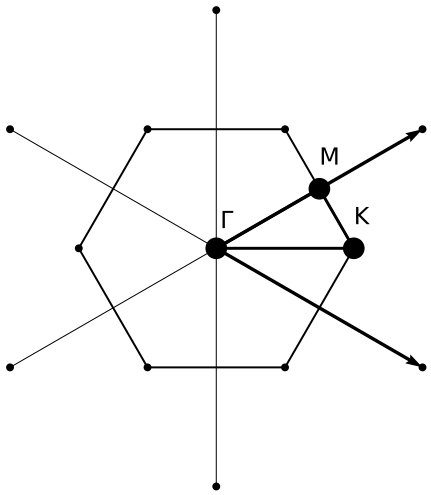

Figure VII.2: *Graphene Brillouin Zone*

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

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{VII.12}$$
$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\ , \tag{VII.13}$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{VII.14}$$
$$\mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{VII.15}$$

Points of high symmetry in the Brillouin zone are:

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

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

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

VII.2 EG-X Model

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

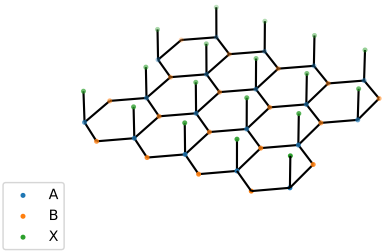

Figure VII.3: *EG-X model*

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 :

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

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

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:

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

VII.2.1 Review: Hubbard model on the honeycomb lattice

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

To treat eq. VII.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:

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

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

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

(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. VII.21

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

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

with the completeness relation:

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

We get:

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

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

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

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

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

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

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

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

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

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

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

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

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

We note

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

and calculate

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

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

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

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

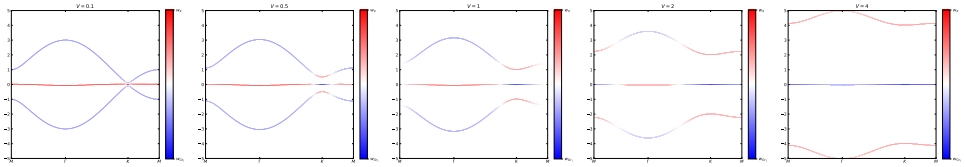

Figure VII.4: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

All together, we get:

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

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

VII.3 BCS Theory on the EG-X Model

VII.3.1 BdG Hamiltonian

Define sublattice index

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

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

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

with the matrix

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

Add chemical potential:

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

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

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

Fourier transformation:

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

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

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

Mean-field approximation:

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

with

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

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

This gives the BCS mean field Hamiltonian:

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

with Nambu spinor

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

we have:

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

with

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

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

VII.3.2 BdG Hamiltonian in band basis

Use transformation

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

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

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

with that:

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

So the kinetic part of the BdG Hamiltonian becomes:

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

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

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

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

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

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?):

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

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

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.

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

So the BdG Hamiltonian is:

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

VII.3.3 Self-consistent calculation of the superconducting gaps

Compare [1, ch. 10]. 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:

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

Anomalous Green's function:

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

Equations of motion (Heisenberg equation), follow [1, ch. 17]:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Similarly:

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

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

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

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

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

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

$$\tag{VII.94}$$

All in all:

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

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

Fourier transform:

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

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

This algebraic expression can be easily solved:

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

with residue:

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

So we have

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

The n_F term can be written as:

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

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

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

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

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

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

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

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

VII.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):

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

so that accessing a certain element takes the form:

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

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

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List of Symbols

Symbol	Meaning	Definition
τ	general imaginary time variable	1
$\mathcal{C}_{AB}(\tau, 0)$	Correlation function in imaginary time	1