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I Green's Function Formalism

Source: [1]

For doing calculations for finite temperatures: introduce imaginary time τ .

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \quad (\text{I.1})$$

with lattice coordinates i, j and spin σ .

From TRIQS tutorial: As you can see, the behavior of the imaginary part is very different for the two values of U . When U is small, the system is a metal and the imaginary part extrapolated to zero goes to a finite value. Instead, for large U , the system is a Mott insulator and the imaginary part goes to zero. The reason is that the extrapolation to zero is directly proportional to the density of states at the chemical potential. If the system is gapped, the density is zero; if the system is a metal, there is spectral weight and the density is finite. Therefore, even on the Matsubara axis, one has a way to decide if the system is metallic or not.

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

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)} \quad (\text{I.2})$$

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

The Dyson equation

$$G(\mathbf{k}, i\omega_n) = (G_0(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n))^{-1} \quad (\text{I.3})$$

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

Definitions of GFs

Imaginary time and frequency

Show how Green's functions can be used to describe many-body effects -> Spectral function, self-energy

Source for that connection between self energy and DOS

I.1 Nambu-Gorkov GF

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\text{loc}}(\tau = 0^-) \quad (\text{I.4})$$

or the superconducting gap

$$\Delta = Z\Sigma^{\text{AN}} \quad (\text{I.5})$$

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

Sources for these?

How to get quasiparticle weight?

II Superconductivity

II.0.1 Extracting T_C

From Niklas

Übrigens: Typische Varianten, um ‘sauber(er)’ T_c zu bestimmen, ist $|OP|^2$ gegen T aufzutragen, da das (als Phasenübergang 2. Ordnung) proportional zu $T - T_c$ ist. Heißt, man kann T_c 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 T_c herum sein kann. Aber pi-mal-Daumen Abschätzungen gehen damit ganz gut. Oder man macht es wie unten beschrieben mit einer daraus abgeleiteten Formel.

Find a source for that! Phase transitions

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

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

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 $V_{\mathbf{k},\mathbf{k}'}$:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \quad (\text{III.1})$$

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

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -\frac{g_0}{V}, & |\epsilon_{\mathbf{k}}| < \omega_D \\ 0 & \text{otherwise} \end{cases} \quad (\text{III.2})$$

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:

Point out specific difference to BCS theory!

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

or at $T = 0$:

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \quad (\text{III.4})$$

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 particular stemming from the Coulomb interaction), so the gap function cannot be

What is the E_k ?

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

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

So for an attractive interaction we have:

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

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 .

Why large gap?

Connection from gap to transition temperature?

Are there more?

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

$$V_{\mathbf{k},\mathbf{k}'} \Psi_{\mathbf{k}}^{\dagger} \Psi_{\mathbf{k}'} \quad (\text{III.7})$$

We start from a Hubbard-like interaction term

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

Proper implementation of normal-ordering

Hubbard-like would be $V_{\mathbf{q}} = U$?

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

$$\mathbf{k}_1 + \mathbf{k}_2 = 0 \implies \mathbf{k}_1 = -\mathbf{k}_2 \text{ :- } \mathbf{k}' \quad (\text{III.9})$$

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

and we can split up the interaction term

Show why the third line works!

$$V_{\text{BCS}} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma'} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}\sigma}^\dagger c_{-\mathbf{k}\sigma'}^\dagger c_{-\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma} \quad (\text{III.11})$$

$$= \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \quad \left(= \frac{1}{2} V_{\text{BCS}}^{\uparrow\downarrow} \right) \quad (\text{III.12})$$

$$+ \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}'\uparrow} c_{\mathbf{k}'\downarrow} \quad \left(= \frac{1}{2} V_{\text{BCS}}^{\downarrow\uparrow} = \frac{1}{2} V_{\text{BCS}}^{\uparrow\downarrow} \right) \quad (\text{III.13})$$

$$+ \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}'\uparrow} c_{\mathbf{k}'\uparrow} \quad \left(= V_{\text{BCS}}^{\uparrow\uparrow} \right) \quad (\text{III.14})$$

$$+ \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\downarrow} \quad \left(= V_{\text{BCS}}^{\downarrow\downarrow} \right) \quad (\text{III.15})$$

$$= V_{\text{BCS}}^{\uparrow\downarrow} + V_{\text{BCS}}^{\uparrow\uparrow} + V_{\text{BCS}}^{\downarrow\downarrow} \quad (\text{III.16})$$

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

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

We define spatial parity of this wavefunction:

$$F(-\mathbf{k})_{\alpha\beta} = P F(\mathbf{k})_{\alpha\beta} \quad (\text{III.18})$$

as well as the spin parity:

$$F(\mathbf{k})_{\beta\alpha} = X F(\mathbf{k})_{\alpha\beta}, \quad (\text{III.19})$$

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

Why do we define spatial parity? Only symmetrised wavefunctions physical?

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

How exactly?

studied superconductors are mostly singlet, pure triplet not found? That's why we split it up! Paper for that?

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

$$V_{\text{BCS}} = \sum_{\mathbf{k}, \mathbf{k}'} \left(\frac{V_{\mathbf{k}-\mathbf{k}'} + V_{\mathbf{k}+\mathbf{k}'}}{2} + \frac{V_{\mathbf{k}-\mathbf{k}'} - V_{\mathbf{k}+\mathbf{k}'}}{2} \right) \Psi_{\mathbf{k}}^{\dagger} \Psi_{\mathbf{k}'} \quad (\text{III.20})$$

$$:- \left(V_{\mathbf{k}, \mathbf{k}'}^S + V_{\mathbf{k}, \mathbf{k}'}^T \right) \Psi_{\mathbf{k}}^{\dagger} \Psi_{\mathbf{k}'} , \quad (\text{III.21})$$

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

$$V_{\mathbf{k}, \mathbf{k}'}^{S,T} = \frac{1}{2} (V_{\mathbf{k}-\mathbf{k}'} \pm V_{\mathbf{k}+\mathbf{k}'}) \quad (\text{III.22})$$

explain last step here

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

$$V_{-\mathbf{k}, -\mathbf{k}'}^S = \frac{1}{2} (V_{-\mathbf{k}+\mathbf{k}'} \pm V_{-\mathbf{k}-\mathbf{k}'}) = \frac{1}{2} (V_{-(\mathbf{k}-\mathbf{k}')} \pm V_{-(\mathbf{k}+\mathbf{k}')}) = \frac{1}{2} (V_{\mathbf{k}-\mathbf{k}'} \pm V_{\mathbf{k}+\mathbf{k}'}) , \quad (\text{III.23})$$

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

With everything we write the unequal spin pairing as:

$$V_{\text{BCS}}^{\uparrow\downarrow} = \frac{1}{4} \sum_{\mathbf{k}, \mathbf{k}'} \left[V_{\mathbf{k}, \mathbf{k}'}^S \Psi_{\mathbf{k}}^{S\dagger} \Psi_{\mathbf{k}'}^S + V_{\mathbf{k}, \mathbf{k}'}^T \Psi_{\mathbf{k}}^{T\dagger} \Psi_{\mathbf{k}'}^T \right] \quad (\text{III.24})$$

$$= \sum_{\mathbf{k}, \mathbf{k}' \in \frac{1}{2}\text{BZ}} \left[V_{\mathbf{k}, \mathbf{k}'}^S \Psi_{\mathbf{k}}^{S\dagger} \Psi_{\mathbf{k}'}^S + V_{\mathbf{k}, \mathbf{k}'}^T \Psi_{\mathbf{k}}^{T\dagger} \Psi_{\mathbf{k}'}^T \right] \quad (\text{III.25})$$

vector arrows over the psi (or bold)

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

$$V_{\text{BCS}} = \sum_{\mathbf{k}, \mathbf{k}' \in \frac{1}{2}\text{BZ}} \left[V_{\mathbf{k}, \mathbf{k}'}^S \Psi_{\mathbf{k}}^{S\dagger} \Psi_{\mathbf{k}'}^S + V_{\mathbf{k}, \mathbf{k}'}^T \Psi_{\mathbf{k}}^{T\dagger} \cdot \Psi_{\mathbf{k}'}^T \right] \quad (\text{III.26})$$

How can we access that information in experiment?

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

$$V_{\text{BCS}} = \sum_{\mathbf{k}, \mathbf{k}' \in \frac{1}{2}\text{BZ}} V_{\mathbf{k}, \mathbf{k}'}^S (c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}) (c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}) \quad (\text{III.27})$$

Source for that?

III.2.2 Magnetic interaction

Starting point here is a magnetic interaction:

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

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

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

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

These eigenvalues enter as prefactors into the pairing potentials:

$$V_{\mathbf{k}, \mathbf{k}'}^S = -\frac{3}{4} \left(\frac{J_{\mathbf{k}-\mathbf{k}'} + J_{\mathbf{k}+\mathbf{k}'}}{2} \right) \quad (\text{III.31})$$

$$V_{\mathbf{k}, \mathbf{k}'}^T = \frac{1}{4} \left(\frac{J_{\mathbf{k}-\mathbf{k}'} - J_{\mathbf{k}+\mathbf{k}'}}{2} \right) \quad (\text{III.32})$$

So antiferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} > 0 \implies V_{\mathbf{k}, \mathbf{k}'}^S < 0$) attract in the singlet channel, while ferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} < 0 \implies V_{\mathbf{k}, \mathbf{k}'}^T < 0$) 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

A bit more information on history, structure etc.

How doped?

Why can we only treat BCS when we also have Fermi liquid?

Do we just treat this case in the following?

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

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

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

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

In momentum space:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{q}} U \rho_{-\mathbf{q}} \rho_{\mathbf{q}} + J \sum_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}} \quad (\text{III.35})$$

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

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

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

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

Looking at the gap equation

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

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

$V_q^{singlet}$ as well?

Put table here as well?

Calculate that fully

Why is the symmetry preserved? And why are the symmetries of the pair conserved? Are these the same as of Δ_k ?

$$V_{\mathbf{k},\mathbf{k}'}^S = U - \frac{3J}{4}(c_x + c_y)(c_{x'} + c_{y'}) \quad (\text{III.39})$$

$$V_{\mathbf{k},\mathbf{k}'}^D = -\frac{3J}{2}(c_x - c_y)(c_{x'} - c_{y'}) \quad (\text{III.40})$$

$$V_{\mathbf{k},\mathbf{k}'}^S + V_{\mathbf{k},\mathbf{k}'}^D = U - \frac{3J}{4}(c_x c_{x'} + c_x c_{y'} + c_{x'} c_y + c_y c_{y'}) \quad (\text{III.41})$$

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

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

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 :

Calculate that

$$V_{\mathbf{k},\mathbf{k}'}^S = V_{\mathbf{k}R\mathbf{k}'}^S \quad (\text{III.44})$$

$$V_{\mathbf{k},\mathbf{k}'}^D = -V_{\mathbf{k}R\mathbf{k}'}^D \quad (\text{III.45})$$

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 ,

$$\Delta_{\mathbf{k}}^D = \Delta_D(c_x - c_y) \quad (\text{III.46})$$

$$\Delta_{R\mathbf{k}}^D = -\Delta_{\mathbf{k}}^D \quad (\text{III.47})$$

Can an s-wave condensate also appear? How is it decided what symmetry the condensate has?

couples to cooper pairs via d-wave interaction , because

$$\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^S \Delta_{\mathbf{k}'}^D (\dots) = 0 \quad (\text{III.48})$$

What is the relationship between gap and interaction? aka where does this equation come from?

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

$$\Delta_{\mathbf{k}}^S = \Delta_1 + \Delta_2(c_x + c_y) \quad (\text{III.49})$$

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:

What quasiparticle?

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

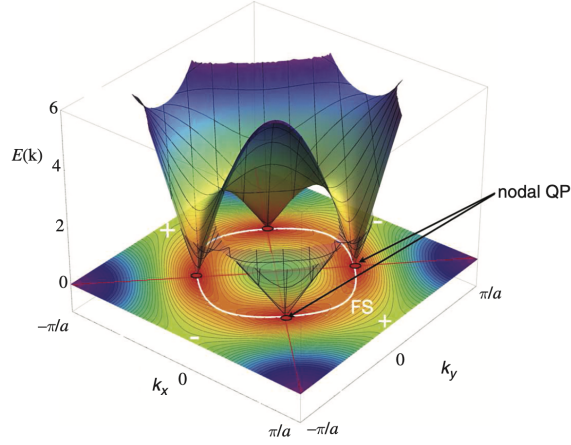


Figure III.1

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

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

What is the exact dispersion?

What exactly is shown in the figure?

How exactly typical? $l = 2$?

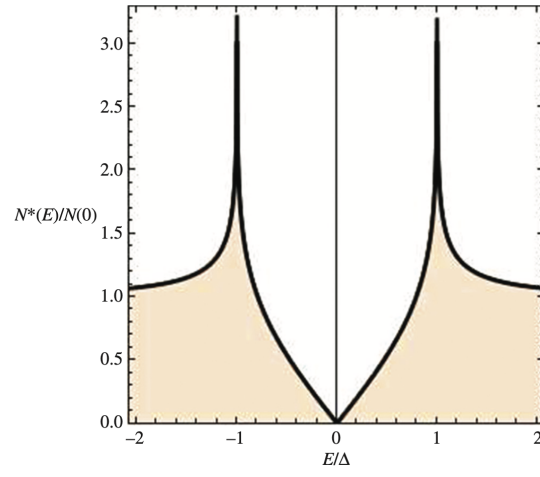
The dependence $\Delta \propto \cos(2\theta)$ is typical for an $l = 2$ Cooper pair. The quasiparticle energy is then

Visualise that somehow?

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

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.

How does the DOS compare with real materials? Do we have the V-shaped structure?

**Figure III.2**

IV Coherence length and penetration depth in strongly correlated superconductors

Put in source

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

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

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.

What does that mean? More details on FFLO theory

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

$$1 \quad (\text{IV.2})$$

Fill in equation

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

More details on GL theory in general

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

with the zero temperature value ξ_0 being the coherence length.

Fill in equation

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.

VI EG-X Model

VI.1 Lattice Structure of Graphene

Following [6].

Monolayer graphene forms a hexagonal lattice. This is formed by two triangular sub lattices. So in the unit cell of the hexagonal actually has two atoms.

Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \quad (\text{VI.1})$$

$$\mathbf{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \quad (\text{VI.2})$$

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

$$a = \sqrt{3}a_0 \quad (\text{VI.3})$$

with the nearest-neighbour distance a_0 .

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

$$\boldsymbol{\delta}_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \quad (\text{VI.4})$$

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

$$\boldsymbol{\delta}_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \boldsymbol{\delta}_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix} \quad (\text{VI.5})$$

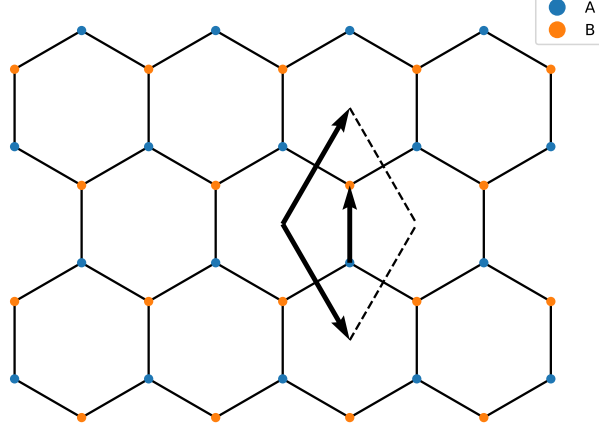


Figure VI.1: Graphene lattice structure

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

$$\delta_{AA,1} = \mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = a \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = a \begin{pmatrix} \sin(\frac{\pi}{6}) \\ \cos(\frac{\pi}{6}) \end{pmatrix} \quad (\text{VI.6})$$

$$\delta_{AA,2} = a \begin{pmatrix} \sin(\frac{3\pi}{6}) \\ \cos(\frac{3\pi}{6}) \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{VI.7})$$

$$\delta_{AA,3} = a \begin{pmatrix} \sin(\frac{5\pi}{6}) \\ \cos(\frac{5\pi}{6}) \end{pmatrix} = a \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{VI.8})$$

$$\delta_{AA,4} = a \begin{pmatrix} \sin(\frac{7\pi}{6}) \\ \cos(\frac{7\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{VI.9})$$

$$\delta_{AA,5} = a \begin{pmatrix} \sin(\frac{9\pi}{6}) \\ \cos(\frac{9\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -1 \\ 0 \end{pmatrix} \quad (\text{VI.10})$$

$$\delta_{AA,6} = a \begin{pmatrix} \sin(\frac{11\pi}{6}) \\ \cos(\frac{11\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{VI.11})$$

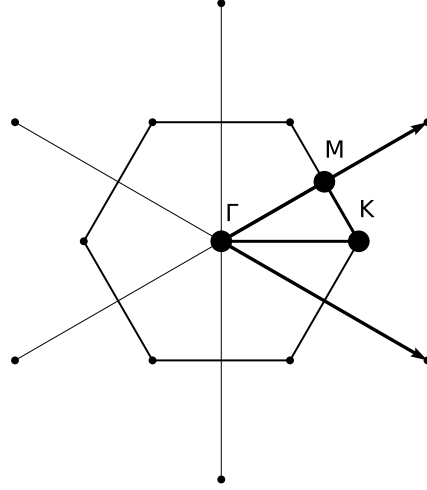


Figure VI.2: Graphene Brillouin Zone

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

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \quad (\text{VI.12})$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0, \quad (\text{VI.13})$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{VI.14})$$

$$\mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{VI.15})$$

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (\text{VI.16})$$

$$\text{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{VI.17})$$

$$\text{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{VI.18})$$

VI.2 EG-X Model

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

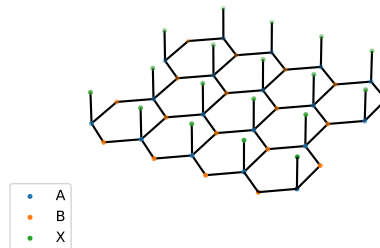


Figure VI.3: *EG-X model*

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

Spin-orbit coupling,
drop second spin
index?

Without interaction :

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma \sigma'} d_{i,\sigma}^\dagger d_{j,\sigma'} - t_{Gr} \sum_{\langle ij \rangle, \sigma \sigma'} \left(c_{i,\sigma}^{(A)\dagger} c_{j,\sigma'}^{(B)} + c_{j,\sigma'}^{(B)\dagger} c_{i,\sigma}^{(A)} \right) + V \sum_{i,\sigma \sigma'} \left(d_{i,\sigma}^\dagger c_{i,\sigma'}^{(A)} + c_{i,\sigma}^{(A)\dagger} d_{i,\sigma'} \right) \quad (\text{VI.19})$$

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:

$$H_{\text{int}} = U_X \sum_i d_{i,\uparrow}^\dagger d_{i,\downarrow}^\dagger d_{i,\downarrow} d_{i,\uparrow} + U_{Gr} \sum_{i,\epsilon=A,B} c_{i,\uparrow}^{(\epsilon)\dagger} c_{i,\downarrow}^{(\epsilon)\dagger} c_{i,\downarrow}^\epsilon c_{i,\uparrow}^\epsilon \quad (\text{VI.20})$$

VI.2.1 Band structure of the non-interacting EG-X model

To treat eq. VI.19, we first write out the sums over nearest neighbours $\langle i, j \rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) 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:

$$-t_X \sum_{\langle ij \rangle, \sigma \sigma'} d_{i,\sigma}^\dagger d_{j,\sigma'} = -\frac{t_X}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} \quad (\text{VI.21})$$

$$(\text{VI.22})$$

(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. VI.21

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}} \quad (\text{VI.23})$$

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \quad (\text{VI.24})$$

with the completeness relation:

$$\sum_i e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} . \quad (\text{VI.25})$$

We get:

$$-\frac{t_X}{2} \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} = -\frac{t_X}{2} \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} \sum_{\mathbf{k},\mathbf{k}'} e^{-i\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \quad (\text{VI.26})$$

$$= -\frac{t_X}{2} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \quad (\text{VI.27})$$

$$= -\frac{t_X}{2} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} N\delta_{\mathbf{k},\mathbf{k}'} \quad (\text{VI.28})$$

$$= -\frac{t_X}{2} \sum_{\mathbf{k},\sigma,\sigma'} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma'} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad (\text{VI.29})$$

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

$$f_X(\mathbf{k}) = -\frac{t_X}{2} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad (\text{VI.30})$$

$$= -\frac{t_X}{2} \left(e^{ia(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right) \quad (\text{VI.31})$$

$$+ e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \quad (\text{VI.32})$$

$$= -\frac{t_X}{2} \left(2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \quad (\text{VI.33})$$

$$= -t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x) \cos(\sqrt{3}\frac{a}{2}k_y) \right) \quad (\text{VI.34})$$

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

$$-t_{\text{Gr}} \sum_{\langle ij \rangle, \sigma \sigma'} c_{i, \sigma}^{(A), \dagger} c_{j, \sigma'}^{(B)} = -\frac{t_{\text{Gr}}}{2} \sum_{i, \sigma \sigma'} \sum_{\delta_{AB}} c_{i, \sigma}^{(A), \dagger} c_{i+\delta_{AB}, \sigma'}^{(B)} \quad (\text{VI.35})$$

$$= -\frac{t_{\text{Gr}}}{2} \sum_{\mathbf{k}, \sigma, \sigma'} c_{\mathbf{k}, \sigma}^{(A), \dagger} c_{\mathbf{k}, \sigma'}^{(B)} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{VI.36})$$

We note

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \quad (\text{VI.37})$$

and calculate

$$f_{Gr} = -\frac{t_{Gr}}{2} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{VI.38})$$

$$= -\frac{t_{Gr}}{2} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{i\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{i\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \quad (\text{VI.39})$$

$$= -\frac{t_{Gr}}{2} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{-i\frac{a}{2\sqrt{3}}k_y} \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x} \right) \right) \quad (\text{VI.40})$$

$$= -\frac{t_{Gr}}{2} \left(e^{i\frac{a}{\sqrt{3}}k_y} + 2e^{-i\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) \quad (\text{VI.41})$$

All together, we get:

$$H_0 = \sum_{\mathbf{k}, \sigma, \sigma'} \quad (\text{VI.42})$$

$$= \sum_{\mathbf{k}, \sigma, \sigma'} \begin{pmatrix} c_{\mathbf{k}, \sigma}^{A, \dagger} & c_{\mathbf{k}, \sigma}^{B, \dagger} & d_{\mathbf{k}, \sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}, \sigma}^A \\ c_{\mathbf{k}, \sigma}^B \\ d_{\mathbf{k}, \sigma} \end{pmatrix} \quad (\text{VI.43})$$

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

Values used for calculation:

- $a_0 = 1$
- $t_{\text{Gr}} = 1$
- $t_X = 0.01$

V is the control parameter. (According to Niklas), a range from $V = 0.1$ to $V = 2$ can be crudely onto real experimental materials.

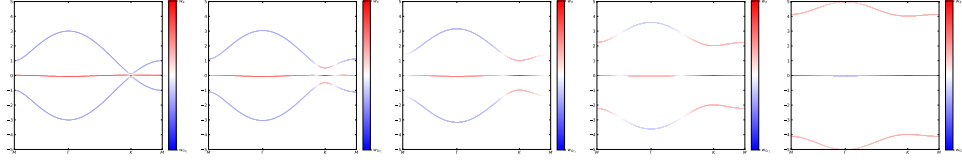


Figure VI.4: Bands of the non-interacting EG-X model. All the bands are spin-degenerate.

VI.3 BCS Theory on the EG-X Model

VI.3.1 BdG Hamiltonian

Define sublattice index

$$\alpha = 1, 2, 3 \quad (\text{VI.44})$$

with $1 \hat{=} \text{Gr}_1, 2 \hat{=} \text{Gr}_2, 3 \hat{=} \text{X}$. Then we can write the non-interacting term as

$$H_0 = - \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta} c_{i\alpha}^\dagger c_{j\beta} \quad (\text{VI.45})$$

Does that make sense?

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\text{Gr}} & 0 \\ t_{\text{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\text{X}} \end{pmatrix} \quad (\text{VI.46})$$

Add chemical potential (to control filling $n = \frac{N_\uparrow + N_\downarrow}{N_{\text{sites}}}$):

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \quad (\text{VI.47})$$

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

$$H_{\text{int}} = - \sum_{i\alpha} U_\alpha c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\alpha\downarrow} c_{i\alpha\uparrow} \quad (\text{VI.48})$$

Fourier transformation:

$$H_{\text{int}} = -\frac{1}{N^2} \sum_{\alpha, \mathbf{k}_1, 2, 3, 4} U_\alpha e^{i(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_3)r_{i\alpha}} c_{\mathbf{k}_1\alpha\uparrow}^\dagger c_{\mathbf{k}_3\alpha\downarrow}^\dagger c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \quad (\text{VI.49})$$

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

$$H_{int} = - \sum_{\alpha, \mathbf{k}, \mathbf{k}'} U_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \quad (\text{VI.50})$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha, \mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^{*} c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{VI.51})$$

with

$$\Delta_{\alpha} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \quad (\text{VI.52})$$

$$\Delta_{\alpha}^{*} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\alpha\uparrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow}^{\dagger} \rangle \quad (\text{VI.53})$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \quad (\text{VI.54})$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c_{1,-\mathbf{k}\downarrow}^{\dagger} \\ c_{2,-\mathbf{k}\downarrow}^{\dagger} \\ c_{3,-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \quad (\text{VI.55})$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \quad (\text{VI.56})$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow} - \mu & \Delta \\ \Delta^{\dagger} & -H_{0,\downarrow}^{*}(-\mathbf{k}) + \mu \end{pmatrix} \quad (\text{VI.57})$$

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

VI.3.2 BdG Hamiltonian in band basis

Use transformation

$$G = \quad (VI.58)$$

where the is made up of the eigenvectors of \mathbf{H}_σ for a given \mathbf{k} :

$$\mathbf{G} = (\mathbf{G}_1 \quad \mathbf{G}_2 \quad \mathbf{G}_3) \quad (VI.59)$$

with that:

$$\mathbf{G}_\sigma^\dagger(\mathbf{k})\mathbf{H}_\sigma(\mathbf{k})\mathbf{G}_\sigma(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \quad (VI.60)$$

So the

VI.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:

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) = -\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d_{n\mathbf{k}\uparrow}^\dagger(0) \rangle \quad (VI.61)$$

Anomalous Green's function:

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) = -\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d_{n\mathbf{k}\uparrow}^\dagger(0) \rangle \quad (VI.62)$$

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

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) = -\delta(\tau) + \langle T_\tau [d_{n\mathbf{k}\uparrow}, H](\tau) d_{n\mathbf{k}\uparrow}^\dagger(0) \rangle \quad (VI.63)$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) = \langle T_\tau [d_{n-\mathbf{k}\downarrow}, H](\tau) d_{n\mathbf{k}\uparrow}^\dagger(0) \rangle \quad (VI.64)$$

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

$$[A, BC] = ABC - BCA = (\{A, B\} - BA)C - B(\{C, A\} - AC) \quad (VI.65)$$

$$[d_{n-\mathbf{k}\downarrow}^\dagger, H_0] = \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} [d_{n-\mathbf{k}\downarrow}^\dagger, d_{n'\mathbf{k}'\sigma'}^\dagger d_{n'\mathbf{k}'\sigma'}] \quad (\text{VI.66})$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(\{d_{n-\mathbf{k}\downarrow}^\dagger, d_{n'\mathbf{k}'\sigma'}^\dagger\} - d_{n'\mathbf{k}'\sigma'}^\dagger d_{n-\mathbf{k}\downarrow}^\dagger \right) d_{n'\mathbf{k}'\sigma'} \quad (\text{VI.67})$$

$$- d_{n'\mathbf{k}'\sigma'}^\dagger \left(\{d_{n'\mathbf{k}'\sigma'}, d_{n-\mathbf{k}\downarrow}^\dagger\} - d_{n-\mathbf{k}\downarrow}^\dagger d_{n'\mathbf{k}'\sigma'} \right) \quad (\text{VI.68})$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(-d_{n'\mathbf{k}'\sigma'}^\dagger d_{n-\mathbf{k}\downarrow}^\dagger d_{n'\mathbf{k}'\sigma'} - d_{n'\mathbf{k}'\sigma'}^\dagger \delta_{n'\mathbf{k}'\sigma', n-\mathbf{k}\uparrow} + d_{n'\mathbf{k}'\sigma'}^\dagger d_{n-\mathbf{k}\downarrow}^\dagger d_{n'\mathbf{k}'\sigma'} \right) \quad (\text{VI.69})$$

$$= -\xi_{n\mathbf{k}} d_{n\mathbf{k}\uparrow}^\dagger \quad (\text{VI.70})$$

All in all:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) = -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) \quad (\text{VI.71})$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) = \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) + \Delta_n^* \mathcal{G}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) \quad (\text{VI.72})$$

Fourier transform:

$$(-i\omega_n + \xi_{n\mathbf{k}}) \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, i\omega_n) = -1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) \quad (\text{VI.73})$$

$$(-i\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) = \Delta_n^* \mathcal{G}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) \quad (\text{VI.74})$$

This algebraic expression can be easily solved:

$$(-i\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) = \frac{\Delta_n^*}{-i\omega_n + \xi_{n\mathbf{k}}} (-1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n)) \quad (\text{VI.75})$$

$$(-i\omega_n - \xi_{n\mathbf{k}} - \frac{|\Delta_n|^2}{-i\omega_n + \xi_{n\mathbf{k}}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) = \frac{-\Delta_n^*}{-i\omega_n + \xi_{n\mathbf{k}}} \quad (\text{VI.76})$$

$$\left(\frac{(-i\omega_n - \xi_{n\mathbf{k}})(-i\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2}{-i\omega_n + \xi_{n\mathbf{k}}} \right) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) = \frac{-\Delta_n^*}{-i\omega_n + \xi_{n\mathbf{k}}} \quad (\text{VI.77})$$

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, i\omega_n) = \frac{-\Delta_n^*}{(-i\omega_n - \xi_{n\mathbf{k}})(-i\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2} \quad (\text{VI.78})$$

$$= \frac{-\Delta_n^*}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.79})$$

$$= \frac{-\Delta_n^*}{(i\omega_n)^2 - E_{n\mathbf{k}}} \quad (\text{VI.80})$$

$$(-i\omega_n + \xi_{n\mathbf{k}})\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, i\omega_n) = -1 + \frac{-|\Delta_n|^2}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.81})$$

$$= \frac{-(i\omega_n)^2 + \xi_{n\mathbf{k}}^2 + |\Delta_n|^2 - |\Delta_n|^2}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.82})$$

$$= \frac{-(i\omega_n)^2 + \xi_{n\mathbf{k}}^2}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.83})$$

$$= \frac{(i\omega_n + \xi_{n\mathbf{k}})(-i\omega_n + \xi_{n\mathbf{k}})}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.84})$$

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, i\omega_n) = \frac{i\omega + \xi_{n\mathbf{k}}}{(i\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \quad (\text{VI.85})$$

$$= \frac{i\omega + \xi_{n\mathbf{k}}}{(i\omega_n)^2 - E_{n\mathbf{k}}^2} \quad (\text{VI.86})$$

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 :

$$\Delta_n(\mathbf{k}) = -\sum_{\alpha} [G_{k\uparrow}]_{\alpha n}^* \Delta_{\alpha} [G_{-k\downarrow}]_{\alpha n}^* \quad (\text{VI.87})$$

$$= -\sum_{\alpha\mathbf{k}'} U_{\alpha} [G_{k\uparrow}]_{\alpha n}^* \langle c_{-k'\alpha\downarrow} c_{k'\alpha\uparrow} \rangle [G_{-k\downarrow}]_{\alpha n}^* \quad (\text{VI.88})$$

$$= -\sum_{\alpha\mathbf{k}'} U_{\alpha} [G_{k\uparrow}]_{\alpha n}^* [G_{-k\downarrow}]_{\alpha n}^* \sum_m [G_{-k'\downarrow}]_{\alpha m} [G_{k'\uparrow}]_{\alpha m} \langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle \quad (\text{VI.89})$$

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

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle = \mathcal{F}_{m\downarrow m\uparrow}^*(\mathbf{k}', \tau = 0^+) \quad (\text{VI.90})$$

$$= \frac{1}{\beta} \sum_{i\omega_n} e^{-i\omega_n 0^+} \mathcal{F}_{m\downarrow m\uparrow}^*(\mathbf{k}', i\omega_n) \quad (\text{VI.91})$$

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

$$\frac{1}{\beta} \sum_{i\omega_n} e^{-i\omega_n 0^+} \mathcal{F}_{m\downarrow m\uparrow}^*(\mathbf{k}', i\omega_n) \quad (\text{VI.92})$$

$$= \sum_{z_0 \text{ poles of } \mathcal{F}} e^{-z_0 0^+} n_F(z_0) \text{Res}_{z_0} \mathcal{F}_{m\downarrow m\uparrow}^*(\mathbf{k}', z_0) \quad (\text{VI.93})$$

$$= e^{-E_{m\mathbf{k}} 0^+} n_F(E_{m\mathbf{k}}) \text{Res}_{E_{m\mathbf{k}}} \frac{-\Delta_m}{(i\omega_n)^2 - E_{m\mathbf{k}}} + e^{E_{m\mathbf{k}} 0^+} n_F(-E_{m\mathbf{k}}) \text{Res}_{-E_{m\mathbf{k}}} \frac{-\Delta_m}{(i\omega_n)^2 - E_{m\mathbf{k}}} \quad (\text{VI.94})$$

with residue:

$$\text{Res}_{E_{m\mathbf{k}}} \frac{1}{(i\omega_n)^2 - z_0^2} = \frac{1}{\partial_z|_{z_0=E_{m\mathbf{k}}} ((i\omega)^2 - z_0^2)} = \frac{1}{2E_{m\mathbf{k}}} \quad (\text{VI.95})$$

So we have

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle = -\Delta_m \left(\frac{n_F(E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} - \frac{n_F(-E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} \right) \quad (\text{VI.96})$$

The n_F term can be written as:

$$n_F(E_{m\mathbf{k}'}) - n_F(-E_{m\mathbf{k}'}) = \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \quad (\text{VI.97})$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}} + 1} \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}} + 1} \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \quad (\text{VI.98})$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}} - e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}} + e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \quad (\text{VI.99})$$

$$= -\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right) \quad (\text{VI.100})$$

VI.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):

$$x = \begin{pmatrix} \Re(\Delta_1(\mathbf{k}_1)) \\ \Re(\Delta_1(\mathbf{k}_2)) \\ \vdots \\ \Re(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Re(\Delta_3(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_1(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_3(\mathbf{k}_1)) \\ \vdots \end{pmatrix} \quad (\text{VI.101})$$

so that accessing a certain element takes the form:

$$\Re \Delta_n(\mathbf{k}) = x \left[\text{index}(\mathbf{k}) + \frac{\text{len}(x) \cdot n}{6} \right] \quad (\text{VI.102})$$

$$\Im \Delta_n(\mathbf{k}) = x \left[\text{index}(\mathbf{k}) + \frac{\text{len}(x) \cdot n}{6} + \frac{1}{2} \text{len}(x) \right] \quad (\text{VI.103})$$

Bibliography

- [1] H. Bruus and K. Flensberg. *Many-Body Quantum Theory in Condensed Matter Physics: An Introduction*. Oxford Graduate Texts. Oxford, New York: Oxford University Press, Nov. 2004. ISBN: 978-0-19-856633-5.
- [2] P. Coleman. *Introduction to Many-Body Physics*. en. Cambridge University Press, Nov. 2015. ISBN: 9780521864886 9781139020916. DOI: 10.1017/CB09781139020916.
- [3] A. Georges et al. “Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions”. In: *Reviews of Modern Physics* 68.1 (Jan. 1996), pp. 13–125. DOI: 10.1103/RevModPhys.68.13.
- [4] M. Schüler. “Theoretical approaches to realistic strongly correlated nanosystems”. PhD thesis.
- [5] P. Werner. “Quantum Monte Carlo Impurity Solvers”. en. In.
- [6] G. Yang et al. “Structure of graphene and its disorders: a review”. In: *Science and Technology of Advanced Materials* 19.1 (Aug. 2018), pp. 613–648. ISSN: 1468-6996. DOI: 10.1080/14686996.2018.1494493.

List of Symbols

Symbol	Meaning	Definition
τ	general imaginary time variable	1