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Master thesis

Title

Title Deutsch

vorgelegt von
Tjark Sievers

Fakultät: Mathematik, Informatik und Naturwissenschaften
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Studiengang: Physik
Matrikelnummer: 7147558
Erstgutachter: Prof. Dr. Annica Black-Schaffer (Uppsala University)
Zweitgutachterin: Prof. Dr. Tim Wehling

Kurzzusammenfassung

Abstract

Contents

Motivation

Test

Test source

Conventions

Throughout the text of this thesis scalars are written in italic s, vectors in bold italic $*s$ and matrices in bold $\mathbf{M}$ fonts. A matrix element is denoted as $[\mathbf{M}]_{\alpha,\beta}$. The summation/multiplication over nearest neighbour sites i and j is $\langle ij \rangle$ as a subscript to $\sum/\prod$. Furthermore, Hartree atomic units are used in general and only in selected instances it is deviated from this: $\hbar = m_\mathrm{e} = \mathrm{e} = {}^{4\pi}/_{\varepsilon_0} = 1$.

I Green's Function Formalism

Following [**Bruus__Flensberg__2004**]

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. For time-independent Hamiltonians and systems in equilibrium, the GFs only depend on time differences:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t-t') \tag{I.2}$$

So we can take $t' = 0$ and consider t as the only free variable:

$$G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) = -\mathrm{i}\Theta(t)\left\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(0)\}\right\rangle \tag{I.3}$$

In a translation invariant system: can use $\mathbf{k}$ as a natural basis set:

$$G^R(\mathbf{k}, \sigma, \sigma' t) = -\mathrm{i}\Theta(t-t')\left\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma'}(0)\}\right\rangle \tag{I.4}$$

Define Fourier-transform:

$$G^R(\mathbf{k}, \sigma, \sigma', \omega) = \int_{-\infty}^{\infty} \mathrm{d}t G^R(\mathbf{k}, \sigma, \sigma' t) \tag{I.5}$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma, \omega) = -2\Im G^R(\mathbf{k}\sigma, \omega) \tag{I.6}$$

Looking at the diagonal elements of G^R here. The spectral function can be thought of as the energy resolution of a particle with energy ω. This mean,

for non-interacting systems, the spectral function is a delta-function around the single-particle energies:

$$A_0(\mathbf{k}\sigma, \omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}\sigma}) \tag{I.7}$$

Show GFs can be related to observables

For interacting systems this is not true, but A can still be peaked.

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

$$t \to -\mathrm{i}\tau \tag{I.8}$$

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 $\mathcal{C}_{AB}(\tau, 0)$:

$$\mathcal{C}_{AB}(\tau, 0) = -\langle T_\tau(A(\tau)B(0))\rangle \tag{I.9}$$

with time-ordering operator in imaginary time:

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau - \tau')A(\tau)B(\tau') \pm \Theta(\tau' - \tau)B(\tau')A(\tau) \tag{I.10}$$

so that operators with later 'times' go to the left.

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

$$-\beta < \tau < \beta \tag{I.11}$$

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

$$\mathcal{C}_{AB}(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{I.12}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{I.13}$$

How to resolve ambiguity at borders of integral

It turns out that Matsubara GFs and retarded GFs can be generated from a common function $\mathcal{C}_{AB}(z)$ that is defined on the entire complex plane except for the real axis. So we can get the retarded GF $\mathcal{C}^R_{AB}(\omega)$ by analytic continuation:

$$\mathcal{C}^R_{AB}(\omega) = \mathcal{C}_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{I.14}$$

So in particular the 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) [**Bruus_Flensberg_2004**].

single-particle Matsubara GF

equations of motion for Matsubara GF

Short introduction to diagrams

Self energy

Dyson equation

I.1 Perturbation theory, Dyson equation

Dyson equation:

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}-\Sigma_\sigma(\mathbf{k},\mathrm{i}\omega_n)}} \tag{I.15}$$

I.2 Nambu-Gorkov GF

More general introduction into NG GFs, how they look like, what they describe etc.

Introduction following [1, ch. 14.7]

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{I.16}$$

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{I.17}$$

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

Find a source for that! Phase transitions

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_2015 - Coleman_2015** [**Coleman_2015**]

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

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

Point out specific difference to BCS theory!

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 $T = 0$:

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

What is the E_k?

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 .

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

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

We start from a Hubbard-like interaction term

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

Proper implementation of normal-ordering

Hubbard-like would be $V_q = U$?

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

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

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

and we can split up the interaction term

Show why the third line works!

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

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

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

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

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

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

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

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

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

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, $(X, P) = (-, +)$

How exactly?

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

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

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

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

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

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

explain last step here

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:

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

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

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:

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

How can we access that information in experiment?

Source for that?

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

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

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.

A bit more information on history, structure etc.

Three regimes :

How doped?

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

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

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

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

$V_q^{singlet}$ as well?

Put table here as well?

Calculate that fully

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

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:

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

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

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

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

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

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

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 :

Calculate that

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

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

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 ,

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

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

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

couples to cooper pairs via d-wave interaction , because

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

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

(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:

What quasiparticle?

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

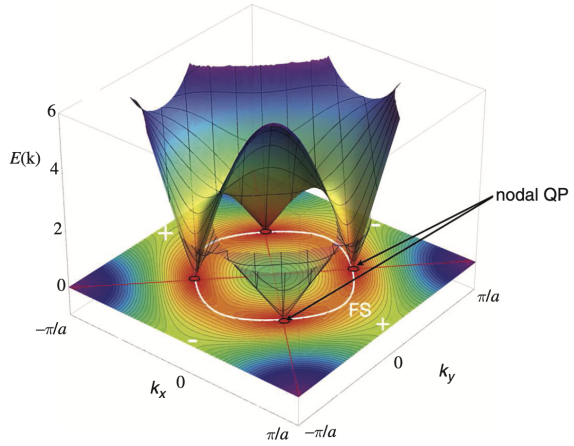

Figure III.1

What exactly is shown in the fig

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

What is the exact dispersion?

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

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?

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

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.

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

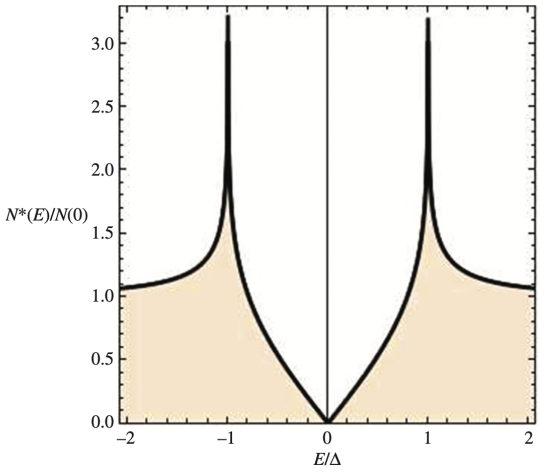

Figure III.2

IV Ginzburg-Landau theory of superconductivity

IV.1 Coherence length and penetration depth in strongly correlated superconductors

[2]

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.

What does that mean? More details on FFLO theory

IV.2 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

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

Fill in equation

More details on GL theory in general

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.

Fill in equation

IV.3 Phase transitions and broken symmetry

Following [1, ch. 11].

IV.3.1 Order parameter concept

Landau theory: phase transitions (e.g. iron becomes magnetic, water freezes, superfluidity/superconductivity) are associated with the development of an order parameter when the temperature drops below the transition temperature T_C

This works also for phase transitions not dependent of temperatures, so e.g. in pressures?

$$|\psi| = \begin{cases} 0\ ,\ T > T_C \\ |\psi_0| > 0\ ,\ T < T_C \end{cases} \tag{IV.4}$$

Landau theory does not need microscopic expression for order parameter, it provides corse-grained description of the properties of matter. The order parameter description is good at length scales above ξ_0, the coherence length (e.g. size of Cooper pairs for SC).

IV.3.2 Landau theory

Rest of Landau theory

Landau theory

Going from a one to a n-component order parameters, we can actually

Particularly important example: complex or two component order parameter in superfluids and superconductors:

$$\psi = \psi_1 + \mathrm{i}\psi_2 = |\psi| e^{\mathrm{i}\phi} \tag{IV.5}$$

The Landau free energy takes the form:

$$f[\psi] = r(\psi^*\psi) + \frac{u}{2}(\psi^*\psi)^2 \tag{IV.6}$$

Figure IV.1 shows the Landau free energy as function of ψ.

In this 'Mexican hat' potential: order parameter can be rotated continuously from one broken-symmetry state to another. If we want the phase to be rigid, we need to introduce an There is a topological argument for the fact that the phase is rigid. This leads to Ginzburg-Landau theory. Will see later: well-defined phase is associated with persistent currents or superflow.

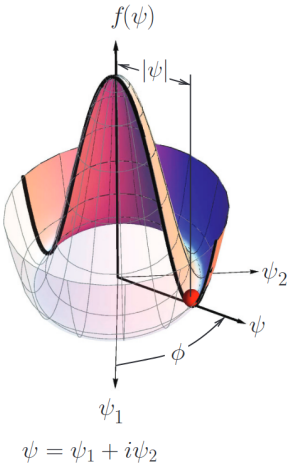

Figure IV.1: *Mexican hat potential*

IV.3.3 Ginzburg-Landau theory I: Ising order

Landau theory: energy cost of a uniform order parameter, more general theory needs to account for inhomogenous order parameters, in which the amplitude varies or direction of order parameter is twisted -> GL theory. First: one-component, 'Ising' order parameter. GL introduces additional energy $\delta f \propto |\Delta\psi|^2$, $f_{GL}[\psi, \Delta\psi] = \frac{s}{2}|\Delta\psi|^2 + f_L[\psi(s)]$, or in full:

$$f_{GL}[\psi, \Delta\psi, h] = \frac{s}{2}(\Delta\psi)^2 + \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 - h\psi \tag{IV.7}$$

GL theory is only valid near critical point, where OP is small enough to permit leading-order expansion.

What is the h here?

length scale/correlation length

IV.3.4 Ginzburg-Landau theory II: complex order and superflow

Now: G-L theory of complex or two-component order parameters, so superfluids and superconductors. Heart of discussion: emergence of a 'macroscopic wavefunction', where the microscopic field operators $\hat{\psi}(x)$ acquire an expectation value:

$$\langle\psi(x)\rangle = \psi(x) = |\psi(x)|e^{i\theta(x)} \tag{IV.8}$$

What exactly are field operators again?

Magnitude determines density of particles in the superfluid:

$$|\psi(x)|^2 = n_s(x) \tag{IV.9}$$

More info on th
Does that come
later in chapter

Twist/gradient of phase determines superfluid velocity:

$$\mathbf{v}_s(x) = \frac{\hbar}{m}\Delta\phi(x) \tag{IV.10}$$

We will derive this later in the chapter. Counterintuitive from quantum mechanics: GL suggested that $\Phi(x)$ is a macroscopic manifestation of a macroscopic number of particles condensed into precisely the same quantum state. Emergent phenomenon, collective properties of mater not a-priori self-evident from microscopic physics.

GL free energy density for superfluid (with one added term in comparison to Landau energy):

$$f_{GL}[\psi, \Delta\psi] = \frac{\hbar^2}{2m}|\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \tag{IV.11}$$

energy density of bosonic field? -> for comparison!

Interpreted as energy density of a condensate of bosons in which the field operator behaves as a complex order parameter. Gives interpretation of gradient term as kinetic energy:

$$s|\Delta\psi|^2 = \frac{\hbar^2}{2m}\langle\Delta\hat{\psi}^\dagger\Delta\hat{\psi}\rangle \implies s = \frac{\hbar^2}{2m} \tag{IV.12}$$

As in Ising order: correlation length/GL-coherence length governs characteristic range of amplitude fluctuations of the order parameter:

$$\xi = \sqrt{\frac{s}{|r|}} = \sqrt{\frac{\hbar^2}{2m|r|}} = \xi_0(1 - \frac{T}{T_C})^{-\frac{1}{2}} \tag{IV.13}$$

Compare with Ising order, especially dependence on T

where $\xi_0 = \xi(T = 0) = \sqrt{\frac{\hbar^2}{2maT_C}}$ is the coherence length. Beyond this length: only phase fluctuations survive. Freeze out fluctuations in amplitude (no x-dependence in amplitude) $\psi(x) = \sqrt{n_s}e^{i\phi(x)}$, then $\Delta\psi = i\Delta\phi\psi$ and $|\Delta\psi|^2 = n_s(\Delta\phi)^2$, dependency of kinetic energy on the phase twist is (bringing it into the form $\frac{m}{2}v^2$):

Compare with Ising order. Is that derived or postulated?

$$\frac{\hbar^2 n_s}{2m}(\Delta\phi)^2 = \frac{mn_s}{2}(\frac{\hbar}{m}\Delta\phi)^2 \tag{IV.14}$$

So twist of phase results in increase in kinetic energy, associated with a superfluid velocity:

$$\mathbf{v}_s = \frac{\hbar}{m}\Delta\phi \tag{IV.15}$$

Phase rigidity and superflow: in GL theory, energy is sensitive to a twist of the phase. Substitute $\psi = |\psi|e^{i\phi}$ into GL free energy, gradient term is:

$$\Delta\psi = () \tag{IV.16}$$

Coherent states/Interpretation of states/Off-diagonal long-range order

Here: particle-current operator, especially for coherent state, connection with phase twist

Here: Meissner effect, etc

IV.3.5 Ginzburg-Landau theory III: charged fields

V Dynamical Mean-Field Theory

Source: **Georges_Kotliar_Krauth_Rozenberg_1996 - Georges_Kotliar_Krauth_Rozenberg_**

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 Noninteracting EG-X Model and structure

VII.1 Lattice Structure of Graphene

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

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

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

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:

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

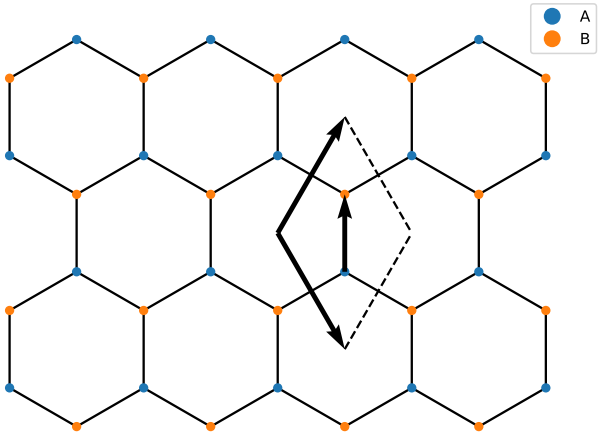

Figure VII.1: *Graphene lattice structure*

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

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

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

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

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

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

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

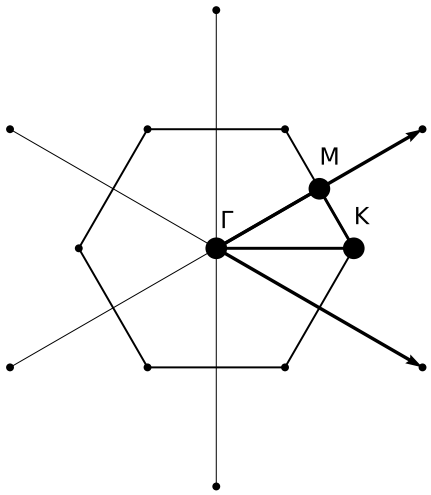

Figure VII.2: *Graphene Brillouin Zone*

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

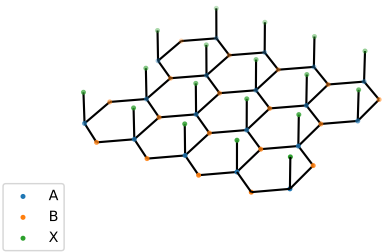

Figure VII.3: *EG-X model*

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?)).

Spin-orbit coupling, drop second spin index?

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

Write review for Hubbard model on the honeycomb lattice

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

To treat eq. VII.20, 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.24

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

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

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

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

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

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

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

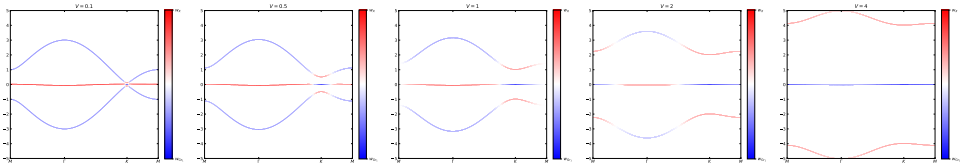

Figure VII.4: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

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.44. 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.

VIII EG-X Model with interactions

VIII.1 BdG Hamiltonian and free energy

VIII.1.1 BdG Hamiltonian

Define sublattice index

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

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

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

with the matrix

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

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{VIII.4}$$

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

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

Fourier transformation:

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

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

$$H_{int} = -\sum_{\alpha,\mathbf{k},\mathbf{k}'} U_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \tag{VIII.7}$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{VIII.8}$$

with

$$\Delta_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \tag{VIII.9}$$

$$\Delta^*_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\alpha\uparrow} c^\dagger_{-\mathbf{k}'\alpha\downarrow} \rangle \tag{VIII.10}$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{VIII.11}$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c^\dagger_{1,-\mathbf{k}\downarrow} \\ c^\dagger_{2,-\mathbf{k}\downarrow} \\ c^\dagger_{3,-\mathbf{k}\downarrow} \end{pmatrix} \tag{VIII.12}$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \tag{VIII.13}$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H^*_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{VIII.14}$$

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

VIII.1.2 BdG Hamiltonian in band basis

Use transformation

$$c^\dagger_{\mathbf{k}\alpha\sigma} = \sum_n [\mathbf{G}]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \tag{VIII.15}$$

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

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 & \mathbf{G}_3 \end{pmatrix} \tag{VIII.16}$$

with that:

$$\mathbf{G}^\dagger_\sigma(\mathbf{k})\mathbf{H}_{0,\sigma}(\mathbf{k})\mathbf{G}_\sigma(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \tag{VIII.17}$$

So the kinetic part of the BdG Hamiltonian becomes:

$$\sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} \sum_n [\mathbf{G}(\mathbf{k})]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \sum_m [\mathbf{G}(\mathbf{k})]_{\beta m} d_{m\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{VIII.18}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \sum_{\alpha\beta} [\mathbf{G}(\mathbf{k})]^*_{\alpha n} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} [\mathbf{G}(\mathbf{k})]_{\beta m} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{VIII.19}$$

$$= \sum_{mn\mathbf{k}\sigma} d^\dagger_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{VIII.20}$$

$$= \sum_{n\mathbf{k}\sigma} \epsilon_n d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{VIII.21}$$

$$=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} \tag{VIII.22}$$

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

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

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

So that:

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

with

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

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

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

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

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

So for $V \to 0$:

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

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

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

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

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

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

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

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

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

IX EG-X Model - Trying BCS theory

IX.1 BCS Theory on the EG-X Model

IX.1.1 Self-consistent calculation of the superconducting gaps

This does not really work! I neglect interband pairing at some point, so i throw away 6 out of 9 gap equations I have, also the GF ansatz works with diagonal Matsubara GFs, so I dont think it works here.

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

Define normal Green's function:

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\rangle \tag{IX.1}$$

Anomalous Green's function:

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = -\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\rangle \tag{IX.2}$$

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

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \langle T_\tau \left[d_{n\mathbf{k}\uparrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\rangle \tag{IX.3}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \langle T_\tau \left[d_{n-\mathbf{k}\downarrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\rangle \tag{IX.4}$$

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

$$[A, BC] = ABC - BCA = (\{A,B\} - BA)C - B(\{C,A\} - AC) \tag{IX.5}$$

$$\left[d^\dagger_{n-\mathbf{k}\downarrow}, H_0\right] = \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] \tag{IX.6}$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(\{d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'}\} - d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow}\right) d_{n'\mathbf{k}'\sigma'} \tag{IX.7}$$

$$- d^\dagger_{n'\mathbf{k}'\sigma'} \left(\{d_{n'\mathbf{k}'\sigma'}, d^\dagger_{n-\mathbf{k}\downarrow}\} - d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) \tag{IX.8}$$

$$= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(-d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'} - d^\dagger_{n'\mathbf{k}'\sigma'} \delta_{n'\mathbf{k}'\sigma',n-\mathbf{k}\uparrow} + d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) \tag{IX.9}$$

$$= -\xi_{n\mathbf{k}} d^\dagger_{n\mathbf{k}\uparrow} \tag{IX.10}$$

$$\left[d_{n-\mathbf{k}\downarrow}, -\sum_{m\mathbf{k}'} \Delta^*_m d_{m-\mathbf{k}'\downarrow} d_{m\mathbf{k}'\uparrow}\right] \tag{IX.11}$$

$$= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\{d_{n-\mathbf{k}\downarrow}, d_{m-\mathbf{k}'\downarrow}\} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} \tag{IX.12}$$

$$- d_{m-\mathbf{k}'\downarrow} \left(\{d_{m\mathbf{k}'\uparrow}, d_{n-\mathbf{k}\downarrow}\} - d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow}\right) \tag{IX.13}$$

$$= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\delta_{n-\mathbf{k}\downarrow,m-\mathbf{k}'\downarrow} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} + d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow} \tag{IX.14}$$

$$= -\Delta^*_n d_{n\mathbf{k}\uparrow} \tag{IX.15}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = -\xi_{n\mathbf{k}} \left\langle T_\tau(d^\dagger_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0))\right\rangle - \Delta^*_n \left\langle T_\tau(d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0))\right\rangle \tag{IX.16}$$

$$= \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) + \Delta^*_n \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) \tag{IX.17}$$

Similarly:

$$[d_{n-\mathbf{k}\uparrow}, H_0] = \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] \tag{IX.18}$$

$$= \xi_n d^\dagger_{n\mathbf{k}\uparrow} \tag{IX.19}$$

$$\left[d_{n-\mathbf{k}\uparrow}, -\sum_{m\mathbf{k}'} \Delta_m d^\dagger_{m-\mathbf{k}'\uparrow} d^\dagger_{m-\mathbf{k}'\downarrow} \right] \tag{IX.20}$$

$$= -\Delta_n d^\dagger_{n-\mathbf{k}\downarrow} \tag{IX.21}$$

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \xi_{n\mathbf{k}} \left\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow} \right\rangle - \Delta_n \left\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0) \right\rangle \tag{IX.22}$$

$$= -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{IX.23}$$

$$\tag{IX.24}$$

All in all:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{IX.25}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) + \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) \tag{IX.26}$$

Fourier transform:

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = -1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{IX.27}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{IX.28}$$

This algebraic expression can be easily solved:

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} (-1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n)) \tag{IX.29}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}} - \frac{|\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{IX.30}$$

$$(\frac{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{IX.31}$$

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2} \tag{IX.32}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.33}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{IX.34}$$

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = -1 + \frac{-|\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.35}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2 + |\Delta_n|^2 - |\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.36}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.37}$$

$$= \frac{(\mathrm{i}\omega_n + \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.38}$$

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{IX.39}$$

$$= \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{IX.40}$$

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:

$$\Delta_n(\mathbf{k}) = -\sum_{\alpha} [G_{k\uparrow}]^*_{\alpha n} \Delta_\alpha [G_{-k\downarrow}]^*_{\alpha n} \tag{IX.41}$$

$$= \sum_{\alpha \mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} \left\langle c_{-k'\alpha\downarrow} c_{k'\alpha\uparrow} \right\rangle [G_{-k\downarrow}]^*_{\alpha n} \tag{IX.42}$$

$$= \sum_{\alpha \mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} [G_{-k\downarrow}]^*_{\alpha n} \sum_m [G_{-k'\downarrow}]_{\alpha m} [G_{k'\uparrow}]_{\alpha m} \left\langle d_{-k'm\downarrow} d_{k'm\uparrow} \right\rangle \tag{IX.43}$$

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

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow} \rangle = \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \tau = 0^+) \tag{IX.44}$$

$$= \frac{1}{\beta} \sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+} \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \mathrm{i}\omega_n) \tag{IX.45}$$

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

$$\frac{1}{\beta}\sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+}\mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}',\mathrm{i}\omega_n) \tag{IX.46}$$

$$= \sum_{z_0 \mathrm{poles of} \mathcal{F}} e^{-z_0 0^+} n_F(z_0) Res_{z_0}\mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}',z_0) \tag{IX.47}$$

$$= e^{-E_{m\mathbf{k}}0^+} n_F(E_{m\mathbf{k}}) Res_{E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} + e^{E_{m\mathbf{k}}0^+} n_F(-E_{m\mathbf{k}}) Res_{-E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} \tag{IX.48}$$

with residue:

$$Res_{E_{m\mathbf{k}}} \frac{1}{(\mathrm{i}\omega_n)^2 - z_0^2} = \frac{1}{\partial_z|_{z_0=E_{m\mathbf{k}}}((\mathrm{i}\omega)^2 - z_0^2)} = \frac{1}{2E_{m\mathbf{k}}} \tag{IX.49}$$

So we have

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow}\rangle = -\Delta_m \left(\frac{n_F(E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} - \frac{n_F(-E_{m\mathbf{k}})}{2E_{m\mathbf{k}}}\right) \tag{IX.50}$$

The n_F term can be written as:

$$n_F(E_{m\mathbf{k}'}) - n_F(-E_{m\mathbf{k}'}) = \frac{1}{e^{\beta E_{m\mathbf{k}'}}+1} - \frac{1}{e^{-\beta E_{m\mathbf{k}'}}+1} \tag{IX.51}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{\beta E_{m\mathbf{k}'}}+1} - \frac{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{-\beta E_{m\mathbf{k}'}}+1} \tag{IX.52}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}} - e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}} + e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \tag{IX.53}$$

$$= -\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right) \tag{IX.54}$$

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

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m\mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n}[G_{-k\downarrow}]^*_{\alpha n}[G_{-k'\downarrow}]_{\alpha m}[G_{k'\uparrow}]_{\alpha m}\Delta_m(\mathbf{k}')\frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{2E_{m\mathbf{k}'}} \tag{IX.55}$$

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

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m \mathbf{k}'} U_\alpha |[G_{k\uparrow}]_{\alpha n}|^2 |[G_{k'\uparrow}]_{\alpha m}|^2 \Delta_m(\mathbf{k}') \frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{2E_{m\mathbf{k}'}} \tag{IX.56}$$

IX.1.2 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):

$$x = \begin{pmatrix} \Re(\Delta_1(\mathbf{k}_1)) \\ \Re(\Delta_1(\mathbf{k}_2)) \\ \vdots \\ \Re(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Re(\Delta_3(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_1(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_3(\mathbf{k}_1)) \\ \vdots \end{pmatrix} \tag{IX.57}$$

so that accessing a certain element takes the form:

$$\Re\Delta_n(\mathbf{k}) = x\left[\text{index}(\mathbf{k}) + \frac{\text{len}(x)\cdot n}{6}\right] \tag{IX.58}$$

$$\Im\Delta_n(\mathbf{k}) = x\left[\text{index}(\mathbf{k}) + \frac{\text{len}(x)\cdot n}{6} + \frac{1}{2}\text{len}(x)\right] \tag{IX.59}$$

X Conclusion

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List of Symbols

Symbol	Meaning	Definition
τ	general imaginary time variable	2
$\mathcal{C}_{AB}(\tau, 0)$	Correlation function in imaginary time	2

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