Contents

Todo list

I EG-X Model

I.1 Lattice Structure of Graphene

Following [1].

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

Primitive lattice vectors of the hexagonal lattice:

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

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

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

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

with the nearest-neighbour distance a_0.

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

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

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

$$\boldsymbol{\delta}_{BA,1} = \tag{I.5}$$
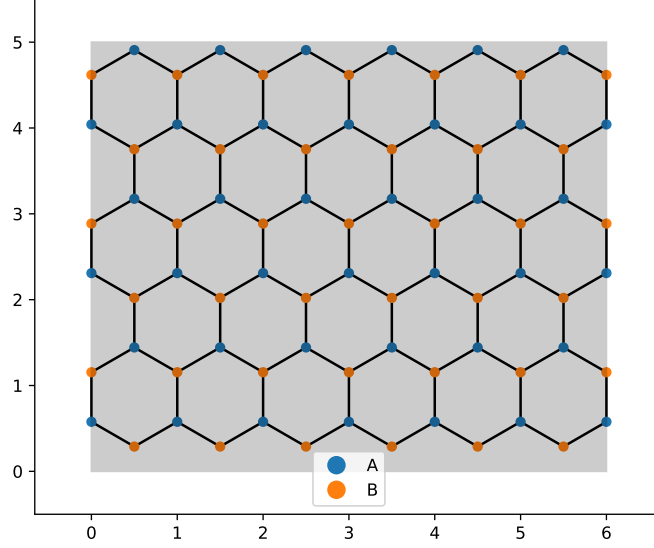
Figure I.1: *Graphene lattice structure*

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

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

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

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

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

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

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

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

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

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

so we have:

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

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

Points of high symmetry in the Brillouin zone are:

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

$$\mathrm{M} = \frac{\pi}{3a_0} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \tag{I.17}$$

$$\mathrm{K} = \frac{2\pi}{3a_0} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.18}$$

I.2 EG-X Model

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

Without interaction:

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

with:
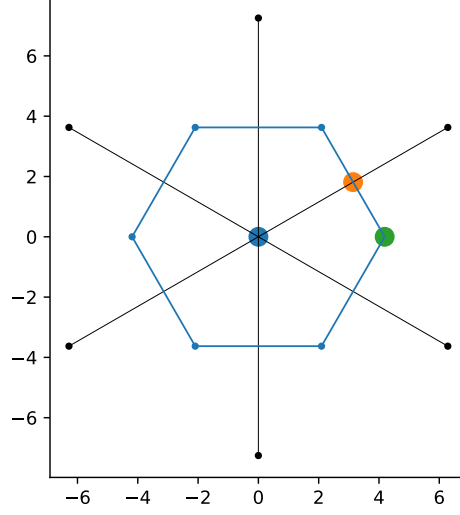
Figure I.2: *Graphene Brillouin Zone*

- 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:

$$H_{\mathrm{int}} = U_{\mathrm{X}} \sum_i d_{i,\uparrow}^\dagger d_{i,\downarrow}^\dagger d_{i,\downarrow} d_{i,\uparrow} + U_{\mathrm{Gr}} \sum_{i,\epsilon=A,B} c_{i,\uparrow}^{(\epsilon)\dagger} c_{i,\downarrow}^{(\epsilon)\dagger} c_{i,\downarrow}^\epsilon c_{i,\uparrow}^\epsilon \qquad (\mathrm{I.20})$$

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

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

example of the X atoms:

$$-t_{\mathrm{X}} \sum_{\langle ij \rangle, \sigma\sigma'} d^\dagger_{i,\sigma} d_{j,\sigma'} = -\frac{t_X}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma'} \tag{I.21}$$

$$\tag{I.22}$$

(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. I.21

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathbf{i k r}_i} c_{\mathbf{k}} \tag{I.23}$$

$$c^\dagger_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-\mathbf{i k r}_i} c^\dagger_{\mathbf{k}} \tag{I.24}$$

with the completeness relation:

$$\sum_i e^{\mathbf{i k r}_i} e^{-\mathbf{i k' r}_i} = N \delta_{\mathbf{k},\mathbf{k}'} . \tag{I.25}$$

We get:

$$-\frac{t_X}{2} \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma'} = -\frac{t_X}{2} \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} \sum_{\mathbf{k},\mathbf{k}'} e^{-\mathbf{i k r}_i} d^\dagger_{\mathbf{k},\sigma} e^{\mathbf{i k' r}_i} e^{\mathbf{i k' \delta_{\mathrm{X}}}} d_{\mathbf{k}',\sigma'} \tag{I.26}$$

$$= -\frac{t_X}{2} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{\mathbf{k},\sigma} e^{\mathbf{i k' \delta_{\mathrm{X}}}} d_{\mathbf{k}',\sigma'} \sum_i e^{-\mathbf{i k r}_i} e^{\mathbf{i k' r}_i} \tag{I.27}$$

$$= -\frac{t_X}{2} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_{\mathrm{X}}} d^\dagger_{\mathbf{k},\sigma} e^{\mathbf{i k' \delta_{\mathrm{X}}}} d_{\mathbf{k}',\sigma'} N \delta_{\mathbf{k},\mathbf{k}'} \tag{I.28}$$

$$= -\frac{t_X}{2} \sum_{\mathbf{k},\sigma,\sigma'} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma'} \sum_{\delta_{\mathrm{X}}} e^{\mathbf{i k \delta_{\mathrm{X}}}} \tag{I.29}$$

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

Do the calculation right!

$$f_{\mathrm{X}}(\mathbf{k}) = -\frac{t_X}{2} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{\mathrm{X}}} = -\frac{t_X}{2} \left(e^{\mathrm{i}\sqrt{3}a_0(\frac{\sqrt{3}}{2}k_x + \frac{1}{2}k_y)} + e^{\mathrm{i}\sqrt{3}a_0(\frac{\sqrt{3}}{2}k_x - \frac{1}{2}k_y)} + e^{\mathrm{i}\sqrt{3}a_0(-k_y)} \right.$$

$$\tag{I.30}$$

$$\left. + e^{\mathrm{i}\sqrt{3}a_0(-\frac{\sqrt{3}}{2}k_x - \frac{1}{2}k_y)} + e^{\mathrm{i}\sqrt{3}a_0(-\frac{\sqrt{3}}{2}k_x + \frac{1}{2}k_y)} + e^{\mathrm{i}\sqrt{3}a_0 k_y} \right) \tag{I.31}$$

$$= -\frac{t_X}{2} \left(2\cos{(\sqrt{3}a_0 k_y)} + 2e^{\mathrm{i}\sqrt{3}a_0(\frac{\sqrt{3}}{2}k_x)} \cos{(\frac{\sqrt{3}}{2}a_0 k_y)} \right. \tag{I.32}$$

$$\left. + 2e^{-\mathrm{i}\sqrt{3}a_0(\frac{\sqrt{3}}{2}k_x)} \cos{(\frac{\sqrt{3}}{2}a_0 k_y)} \right) \tag{I.33}$$

$$= -t_X \left(\cos{(\sqrt{3}a_0 k_y)} + 2\cos{(\frac{\sqrt{3}}{2}a_0 k_y)} \cos{(\frac{3}{2}a_0 k_x)} \right) \tag{I.34}$$

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

$$-t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma\sigma'} c_{i,\sigma}^{(B),\dagger} c_{j,\sigma'}^{(A)} = -\frac{t_{\mathrm{Gr}}}{2} \sum_{i,\sigma\sigma'} \sum_{\boldsymbol{\delta}_{AB}} c_{i,\sigma}^{(B),\dagger} c_{i+\boldsymbol{\delta}_{AB},\sigma'}^{(B)} \tag{I.35}$$

$$= -\frac{t_{GR}}{2} \sum_{\mathbf{k},\sigma,\sigma'} c_{\mathbf{k},\sigma}^{(A)\dagger} c_{\mathbf{k},\sigma'}^{(B)} \sum_{\boldsymbol{\delta}_{BA}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}} \tag{I.36}$$

We note

$$\sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} = \left(\sum_{\boldsymbol{\delta}_{BA}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}} \right)^* \tag{I.37}$$

and calculate

$$f_{Gr} = -\frac{t_{Gr}}{2} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} = \tag{I.38}$$

Doing the same for the hoppings between the A and B Graphene sites as well as the hybridisaton between X and Graphene A lattice sites,

we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \tag{I.39}$$

$$= \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c_{k,\sigma}^{A,\dagger} & c_{k,\sigma}^{B,\dagger} & d_{k,\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{k,\sigma}^{A} \\ c_{k,\sigma}^{B} \\ d_{k,\sigma} \end{pmatrix} \tag{I.40}$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. I.40. This was done in fig. I.3.

Values used for calculation:

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

V is the control parameter. (According to Niklas), a range from $V = 0.1$ to $V = 2$ can be crudely onto real experimental materials.
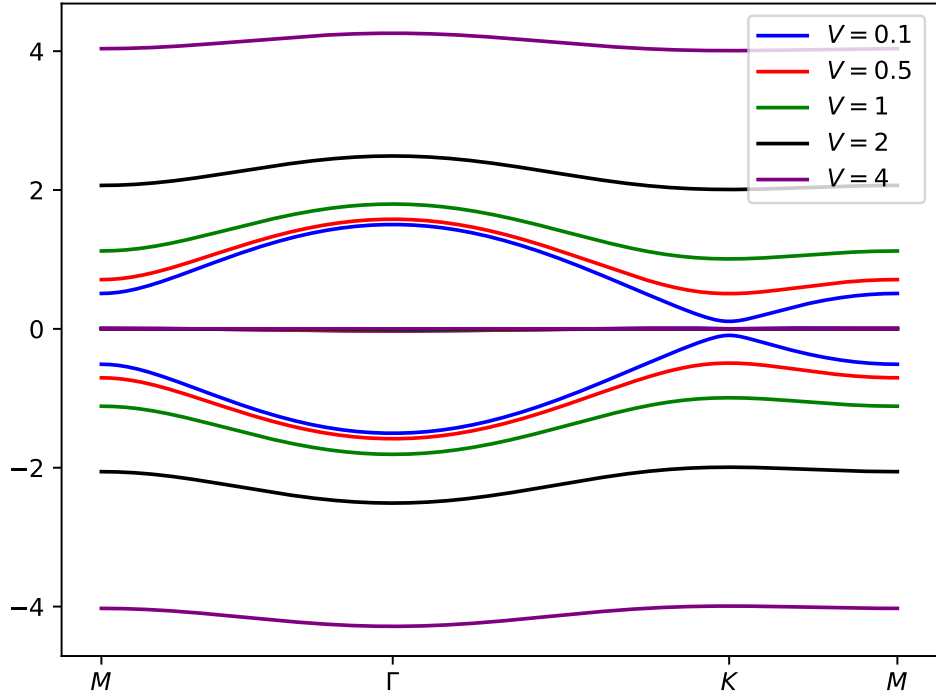
Figure I.3: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

II Green's Function Formalism

Source: [2]

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.

Most general non-interacting electronic Hamiltonian in second quantization:

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

with lattice coordinates i, j and spin σ.

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

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

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

The Dyson equation

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

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!).

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

II.1 Nambu-Gorkov GF

Order parameter can be chosen as the anomalous GF:

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

or the superconducting gap

$$\Delta = Z\Sigma^{\text{AN}} \tag{II.5}$$

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

Sources for these?

How to get quasiparticle weight?

III 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.

IV Superconductivity

IV.0.1 Extracting T_{C}

From Niklas

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

> 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 $P_{\mathrm{SC}}(T) \propto \sqrt{T_c - T}$ 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 ($P_{\mathrm{SC}} \gtrsim 0.01$). Then, T_c is determined by

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

Figure IV.1: *Formula for extracting T_{C}*

V d-wave Superconductivity

Source: Coleman - *Introduction to Many-Body Physics* [6, ch. 15]

V.1 BCS theory with momentum dependent coupling

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

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

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

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

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!

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

or at $T = 0$:

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

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?

15

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

$$\text{sign}\left(\Delta_{\mathbf{k}}\right) = -\text{sign}\left(V_{\mathbf{k},\mathbf{k}'}\right)\text{sign}\left(\Delta_{\mathbf{k}'}\right) \tag{V.5}$$

So for an attractive interaction we have:

$$\text{sign}\left(\Delta_{\mathbf{k}}\right) = -(-1)\text{sign}\left(\Delta_{\mathbf{k}'}\right) \tag{V.6}$$

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

Two cases :

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

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

V.2 Anisotropic pairing

V.2.1 Hubbard interaction

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

$$V_{\mathbf{k},\mathbf{k}'}\Psi_{\mathbf{k}}^{\dagger}\Psi_{\mathbf{k}'} \tag{V.7}$$

We start from a Hubbard-like interaction term

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

Margin notes:
- Why large gap?
- Connection from gap to transition temperature?
- Are there more?
- 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

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

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

and we can split up the interaction term

> Show why the third line works!

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

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

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

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

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

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

First we treat $V^{\uparrow\downarrow}_{\text{BCS}}$. 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?

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

We define spatial parity of this wavefunction:

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

as well as the spin parity:

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

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

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

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

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

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

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

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

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

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

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

With everything we write the unequal spin pairing as:

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

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

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

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

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

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

Margin notes:

How exactly?

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

explain last step here

vector arrows over the psi (or bold)

How can we access that information in experiment?

Source for that?

V.2.2 Magnetic interaction

Starting point here is a magnetic interaction:

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

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

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

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

These eigenvalues enter as prefactors into the pairing potentials:

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

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

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.

V.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

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

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

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

In momentum space:

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

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

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

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

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

Looking at the gap equation

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

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

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

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

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

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

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

Margin notes:

$V_q^{singlet}$ 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?

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

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

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

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

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

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

couples to cooper pairs via d-wave interaction , because

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

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

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

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

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

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

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

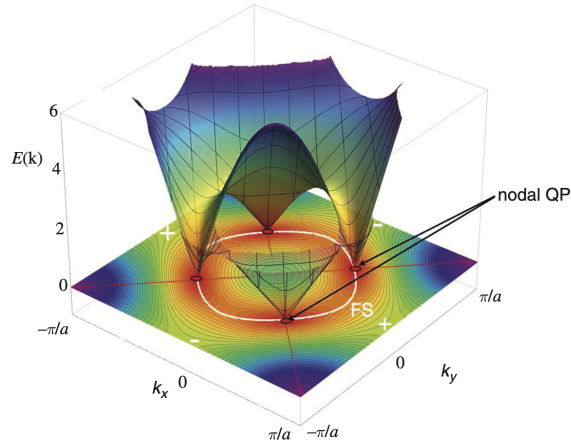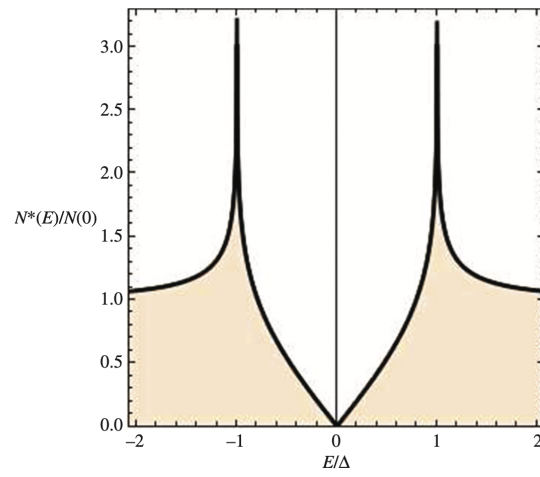The dependence $\Delta \propto \cos(2\theta)$ is typical for an $l = 2$ Cooper pair. The

Figure V.1

quasiparticle energy is then

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

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 V.2

VI Coherence length and penetration depth in strongly correlated superconductors

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

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

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.

VI.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

$$1 \qquad (VI.2)$$

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

$$\xi(T) = \qquad (VI.3)$$

with the zero temperature value ξ_0 being the coherence length.

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