# Contents

# Todo list

# 1 Introduction

In 1894, Albert Michelson remarked that "it seems probable that most of the grand underlying principles have been firmly established"[1] [1, p. 159].

What to put in introduction?

At the end of the 19th and the beginning of the 20th century, cooling technology made great progress. Liquifying gases, were able to reach temperatures as low as 4 K (the boiling point of Helium). Using that, SC was discovered in mercury in 1911 by Heike Onnes [2]. Superconductivity describes the phenomenon of the electrical resistance of a material suddenly dropping to zero below a critical temperature $T_C$. Discovery of Meissner effect, perfect expulsion of external magnetic fields in 1933 [3]. This started almost half a century of intensive theoretical research, which culminated in John Bardeen, Leon Cooper and J. Robert Schrieffer developing the microscopic theory now know as BCS theory [4]. 1986 and 1987: discovery of superconductivity with very high $T_C$ found in cuprates [5, 6]. Cuprate superconductors are made up of layers of cooper oxide and charge reservoirs in between. The specific charge reservoir layers determine the properties of the SC and varying them lead to a rich zoo of materials with high $T_C$ [7].

Largest commercial application to date is in magnetic resonance imaging, a medical technique using strong magnetic fields and field gradients [8]. Enabled due to the fact, that SCs can carry much stronger currents and thus generate much higher magnetic field strength. Technical applications in research are much wider, ranging from strong superconducting magnets in the LHC [9] and other particle accelerators over detectors of single photons in astrophysics [10] to extremely sensitive measurement devices for magnetic fields [11] and voltages [12] based on the Josesphon effect [13].

Since the first discovery of SC in cuprates, there has been a lot of work to develop superconductors with higher transition temperatures. One interesting development in is in twisted multilayer systems, first realized as twisted bilayer

[1] Variations of this quote have been attributed to Lord Kelvin, although the poetry having it said by someones, whose experiment would eventually lead to the development of special relativitiy is undeniable.

Graphene [14]. In comparison to the complex crystal structure of e.g. the Cuprates, twisted multilayer systems have a very simple structure and can be tuned very easily: the angle of twist between the layers can be easily accessed experimentally. The defining feature of these systems are flat electronic bands due to folding of the Brilluoin zone. Superconductivity in these systems is enhanced due to the fact that in the flat bands, interactions between the electrons are very strongly enhanced. Thus these systems are a very interesting playground to study strongly correlation effects in general and superconductivity in particular.

What I am doing: calculating length scales, why is that important?

# 2 Superconductivity

Superconductivity is an example of an emergent phenomenon: the Schrödinger equation describing all interactions between electrons gives no indication that there exists parameters for which the electrons condense into phase coherent pairs. In this chapter we review theoretical concepts needed for understanding superconductivity and introduce the tools used to study superconductivity in the later chapters. There are many textbooks covering these topics which can be referenced for a more detailed treatment, such as refs. [15–19].

Macroscopially, the superconducting state can be described by a spontaneous breaking of a $U(1)$ phase rotation symmetry that is associated with an order parameter. Theory of spontaneous symmetry breaking and associated phase transitions is Ginzburg-Landau theory discussed in section 2.1. Ginzburg-Landau theory introduces two length scales: the coherence length $\xi_0$ describing the length scale of amplitude variations of the order parameter and the London penetration depth $\lambda_L$, which is connected to energy cost of phase variations of the order parameter. The interplay of these length scales determine To this end, section 2.1 introduces a theoretical framework based on Cooper pairs with finite momentum [20] that will be used in later chapters to calculate these length scales from microscopic theories.

What is influenced by length scales? See Niklas 2024 npj

Ginzburg Landau theory is a macroscopic theory, but it can be connected to microscopic theories: if a theory finds an expression for the order parameter describing the symmetry breakdown, it can be connected to quantities expressed by Ginzburg-Landau theory, such as the superconducting current. One such theory to describe superconductivity from a microscopic perspective is BCS (Bardeen-Cooper-Schrieffer) theory in section 2.2. A method to treat local interactions non-perturbatively is DMFT (Dynamical Mean Field Theory). Section 2.3 briefly introduces the Greens function method to treat many-body problems and outlines the DMFT self-consistency cycle.

## 2.1 Ginzburg-Landau Theory of Superconductivity

Introduction with more history and what will be tackled in this section

This review partially follows the introduction given in refs. [15, 21].

### 2.1.1 Sponteneous Symmetry Breaking and Order Parameter

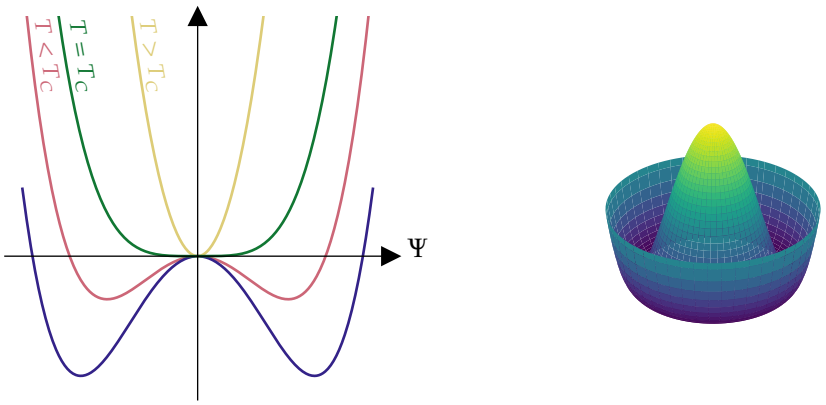
Symmetries are a powerful concept in physics. Noethers theorem [22] connects the symmetries of physical theories to associated conservation laws. An interesting facet of symmetries in physical theories is the fact, that a ground state of a system must not necessarily obey the same symmetries of its Hamiltonian, i.e. for a symmetry operation that is described by a unitary operator $U$, the Hamiltonian commutes with $U$ (which results in expectation values of the Hamiltonian being invariant under the symmetry operation) but the states $|\phi\rangle$ and $U|\phi\rangle$ are different. This phenomenon is called SSB (Sponteneous Symmetry Breaking) and the state $|\phi\rangle$ is said to be symmetry-broken.

One consequence of this fact is that for a given symmetry-broken state $|\phi\rangle$, there exists multiple states that can be reached by repeatedly applying $U$ to $|\phi\rangle$ and all have the same energy. To differentiate the symmetry-broken states an operator can be defined that has all these equivalent states as eigenvectors with different eigenvalues and zero expectation value for symmetric states. This is the microscopic notion of an order parameter.

The original notion of an order parameter was motivated from macroscopic observables that can then be related to the microscopic order parameter operator introduced above. Macroscopically we characterize the symmetry breaking by an order parameter $\Psi$ which generally can be a complex-valued vector that becomes non-zero below the transition temperature $T_C$

$$|\Psi| = \begin{cases} 0 & T > T_C \\ |\Psi_0| > 0 & T < T_C \end{cases} . \tag{2.1}$$

In the example of a ferromagnet, a finite magnetization of a material is associated with a finite expectation value for the $z$-component of the spin operator, $m_z = \langle \hat{S}_z \rangle$. The order parameter describes the 'degree of order' [23]. Similarly to a magnetically ordered state, the SC state is characterized by an order parameter. The theory of phase transitions in superconductors was developed by Ginzburg and Landau [24]. Landau theory and conversely Ginzburg-Landau theory is not concerned with the the microscopic properties




(a) (b)

of the order parameter, but describes the changes in thermodynamic properties of matter with the development of an order parameter.

### 2.1.2 Landau and Ginzburg-Landau Theory

The free energy is a thermodynamic quantity:

$$F = E - TS \tag{2.2}$$

with the energy of the system $E$, temperature $T$ and entropy $S$. A system in thermodynamic equilibrium has minimal free energy. The fundamental idea underlying Landau theory is to write the free energy $F[\Psi]$ as function of the order parameter $\Psi$ and expand it as a polynomial:

$$F[\Psi] = \frac{r}{2}\Psi^2 + \frac{u}{4}\Psi^4 \,. \tag{2.3}$$

Provided the parameters $r$ and $u$ are greater than 0, there is a minimum of $F[\Psi]$ that lies at $\Psi = 0$. Landau theory assumes that at the phase transition temperature $T_C$ the parameter $r$ changes sign, so it can be written in first order as

$$r = a(T - T_C) \,. \tag{2.4}$$

Work over graphic for mexican hat potential

Figure 2.1a shows the free energy as a function of a single-component, real order parameter $\Psi$ and it illustrates the essence of Landau theory: there are two cases for the minima of the free energy $F$

$$\Psi = \begin{cases} 0 & T \geq T_C \\ \pm\sqrt{\frac{a(T_C - T)}{u}} & T < T_C \end{cases}, \tag{2.5}$$

so there is a for $T < T_C$ there are two minima corresponding to ground states with broken symmetry. When the order parameter can be calculated from some microscopic theory, the critical temperature $T_C$ can be extracted from the behavior of the order parameter near $T_C$ via a linear fit of

$$|\Psi|^2 \propto T_C - T \,. \tag{2.6}$$

Generalizing this from a one to an $n$-component order parameters is straightforward. One example is the complex or two component order parameter that will become important for

$$\Psi = \Psi_1 + \mathrm{i}\Psi_2 = |\Psi| e^{\mathrm{i}\phi} \,. \tag{2.7}$$

The Landau free energy then takes the form

$$F[\Psi] = r\Psi^*\Psi + \frac{u}{2}(\Psi^*\Psi)^2 = r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \tag{2.8}$$

with again

$$r = a(T_C - T) \,. \tag{2.9}$$

Instead of the two minima, the free energy here is rotational symmetry, because it is independent of the phase of the order parameter:

$$F[\Psi] = f[e^{\mathrm{i}a}\Psi] \,. \tag{2.10}$$

This gives the so called 'Mexican hat' potential shown in fig. 2.1b. In this potential, the order parameter can be rotated continuously from one broken-symmetry state to another.

In 1950, Ginzburg and Landau published their theory of superconductivity based on Landaus theory of phase transitions [24]. Where Landau theory as described above has an uniform order parameters, Ginzburg-Landau theory accounts for it being inhomogeneous, so an order parameter with spatially

varying amplitude or direction. This in turn leads to the order parameter developing a fixed phase, which is the underlying mechanism of the superflow in superconductors.

Ginzburg-Landau theory can be developed for a general $n$-component order parameter, but in superfluids and superconductors the order parameter is complex, i.e. two-component. The Ginzburg-Landau free energy for a complex order parameter is

$$F_{\mathrm{GL}}[\Psi, \Delta\Psi] = s|\Delta\Psi|^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \,, \tag{2.11}$$

where the gradient term $\Delta\Psi$ is added in comparison to the Landau free energy. The free energy in eq. (2.11) is sensitive to a twist of the phase of the order parameter. Substituting the expression $\Psi = |\Psi|e^{\mathrm{i}\phi}$, the gradient term reads

Introduce gradient term as kinetic energy (with mass)

$$\Delta\Psi = (\Delta|\Psi| + \mathrm{i}\,\Delta\phi|\Psi|)e^{\mathrm{i}\phi} \,. \tag{2.12}$$

With that, eq. (2.11) becomes

$$F_{GL} = s|\Psi|^2(\Delta\phi)^2 + \left[s(\Delta|\Psi|)^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4\right] \,. \tag{2.13}$$

Now the contributions of phase and amplitude variations are split up: the first term describes energy cost of variations in the phase of the order parameter and the second term describes energy cost of variations in the magnitude of the order parameter. The dominating fluctuation is determined by the ratio of the factors $s$ and $r$, which has the dimension Length$^2$, from which define the correlation length

$$\xi = \sqrt{\frac{s}{|r|}} = \xi_0 \left(1 - \frac{T}{T_C}\right)^{-\frac{1}{2}} \tag{2.14}$$

where $\xi_0 = \xi(T=0) = \sqrt{\frac{s}{aT_C}}$ is the coherence length.

significance of coherence length: only phase fluctuations

Superconductors: charged superfluids, coupling to electromagnetic fields. Free energy with minimal coupling to an electromagnetic field:

Work over paragraph

$$F_{\mathrm{GL}}[\Psi, \mathbf{A}] = s|\Delta\Psi|^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \tag{2.15}$$

Explanation London penetration depth

$$|\Psi| = |\Psi_0|\sqrt{1 - \xi^2|\Delta\phi(\mathbf{r})|^2} \tag{2.16}$$

Explanation supercurrent

Explanation superfluid weight

Explanation: phase fluctuations destroy SC order -> introducing q gives access to SC properties

Be proper about what is a free energy density and what is

### 2.1.3 Superconducting Length Scales

One of the challenges in achieving high-temperature superconductivity is the fact, that the two intrinsic energy scales of superconductors i.e. the pairing amplitude and the phase coherence often compete.

Competing energy scales via interaction strength: higher U gives more tightly bound pairs

[25]

These two energy scales are equivalently defined via the coherence length $\xi_0$ and the London penetration depth introduced in section 2.1.2, so having access to these scales from microscopic models and ab initio approaches is very important in the search for high $T_C$-superconductors. Witt et al. introduced a framework for doing exactly that [20]. As already eq. (2.16)

In most materials: Cooper pairs do not carry finite center-of-mass momentum. In presence of e.g. external fields or magnetism: SC states with FMP might arise [26–28]

Theory/procedure in the paper: enforce FMP states via constraints on pair-center-of-mass momentum $\mathbf{q}$, access characteristic lenght scales $\xi_0, \lambda_L$ through analysis of the momentum and temperature-dependent OP. FF-type pairing with Cooper pairs carrying finite momentum:

$$\psi_{\mathbf{q}}(\mathbf{r}) = |\psi_{\mathbf{q}}| e^{i\mathbf{q}\mathbf{r}} \tag{2.17}$$

Then the free energy density is

$$f_{GL}[\psi_{\mathbf{q}}] = \alpha|\psi_{\mathbf{q}}|^2 + \frac{b}{2}|\psi_{\mathbf{q}}|^4 + \frac{\hbar^2 q^2}{2m^*}|\psi_{\mathbf{q}}|^2 \tag{2.18}$$

Stationary point of the system:

$$\frac{\delta f_{GL}}{\delta \psi^*_{\mathbf{q}}} = 2\psi_{\mathbf{q}}\left[\alpha(1 - \xi^2 q^2) + b|\psi_{\mathbf{q}}|^2\right] = 0 \tag{2.19}$$

which results in the $\mathbf{q}$-dependence of the OP

$$|\psi_{\mathbf{q}}|^2 = |\psi_0|^2(1 - \xi(T)^2 q^2) \tag{2.20}$$

For some value, SC order breaks down, $\psi_{\mathbf{q}_c} = 0$, because the kinetic energy from phase modulation exceeds the gain in energy from pairing. In GL theory: $q_c = \xi(T)^{-1}$. The temperature dependence of the OP and extracted $\xi(T)$ gives access to the coherence length via

$$\xi(T) = \xi_0(1 - \frac{T}{T_C})^{-\frac{1}{2}} \tag{2.21}$$

Depairing current from FMP

Full formula for supercurrent, with sum over orbitals

DS from FMP

What else can be done with the FMP method?

Make graphic for Landau OP and BCS OP with q

The Cooper pair

## 2.2 Bardeen-Coooper-Schrieffer Theory

It took nearly 50 years after the first discovery of superconductivity in mercury by Heike Kamerlingh Onnes in 1911 [2] for the first microscopic description of this phenomenon to be published in 1957 by John Bardeen, Leon Cooper and J. Robert Schrieffer [4]. This BCS (Bardeen-Cooper-Schrieffer) theory is one of the great successes in physics history.

The BCS description of superconductivity is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [29]. The origin of the attractive interaction $V_{\mathbf{k},\mathbf{k}'}$, which Bardeen, Cooper and Schrieffer identified as a retarded electron-phonon interaction [4].

There exist many textbooks tackling BCS theory from different angles, such as chapter 14 in refs. [15, 16]. This section gives an introduction to the relevant physics of BCS theory as originally proposed, then derives the

Better introduction

### 2.2.1 BCS Hamiltonian

Work over paragraph

BCS-Hamiltonian:

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{2.22}$$

This Hamiltonian can be solved exactly using a mean field approach, because it involves an interaction at zero momentum and thus infinite range. Order parameter in mean field BCS theory is the pairing amplitude

$$\Delta = -\frac{U}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -U \langle c_{-\mathbf{r}=0\downarrow} c_{\mathbf{r}=0\uparrow} \rangle \simeq U\Psi \, . \tag{2.23}$$

More about mean field theory in section 2.2.2

A finite $\Delta$ corresponds to the pairing introduced above: there is a finite expectation value for a coherent creation/annihilation of a pair of electrons with opposite momentum and spin. A finite $\Delta$ also introduces a band gap into the spectrum. BCS theory brings multiple aspects together: concept of paired electrons with the pairing amplitude being the order parameter in SC, an explanation for the attractive interaction overcoming Coulomb repulsion and a model Hamiltonian that very elegantly captures the essential physics.

It is very successful in two ways: on the one hand it could quantitatively predict effects in the SCs known at the time, for example the Hebel-Slichter peak

that was measured in 1957 [30, 31] and the band gap measured by Giaever in 1960 [32]. On the other hand, it established electronic pairing as the microscopic mechanism behind SC, which holds still today even for high $T_C$/unconventional superconductors, so SCs that cannot be described by BCS theory [33].

Other pairing interactions can be taken, gives explanations for a lot of different SCs

### 2.2.2 Multiband BCS Mean Field Theory

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [34], Kanamori [35] and Gutzweiler [36].

$$H_{\text{int}} = U \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{2.24}$$

where $U > 0$.

Some relevance of the repulsive Hubbard model

Besides
[37]
This simple Hubbard model can be extended in a multitude of ways to model a variety of physical system. In this work: extension to multiple orbitals (i.e. atoms in the unit cell for lattice systems) and an attractive interaction, i.e. a negative $U$. Physical motivation for taking a negative-U Hubbard model: electrons can experience a local attraction interaction, for example through electrons coupling with phononic degrees of freedom or with electronic excitations that can be described as bosons [38]. The form of the interaction term is then:

There are some more specific papers to the specific mechanisms (and also some more mechanism), could cite these here and say some more things

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{2.25}$$

where $\alpha$ counts orbitals and the minus sign in front is taken so that $U > 0$ now corresponds to an attractive interaction (this is purely convention).

There are a multitude of ways to derive a mean field description of a given interacting Hamiltonian. Very rigorous in path integral formulations as saddle points, given for example in ref. [15]. The review follows [39]. A more intuitive way based on ref. [17] discussed here looks at the operators and which one are small.

Order of operators? -> also in all other equations!

Look at interaction term eq. (2.25). Mean-field approximation (here specifically for superconductivity i.e. pairing): operators do not deviate much from their average value, i.e. the deviation operators

there are other combinations, talk about that

$$d_{i,\alpha} = c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} - \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.26}$$

deviations with small deltas

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{2.27}$$

are small (dont contribute much to expectation values and correlation functions), so that in the interaction part of the Hamiltonian

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{2.28}$$

$$= -\sum_{i,\alpha} U_\alpha \left( d^\dagger_{i,\alpha} + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \right) \left( e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \tag{2.29}$$

$$= -\sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.30}$$

$$+ \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{2.31}$$

the first term is quadratic in the deviation and can be neglected. Thus arrive at the approximation

$$H_{\text{int}} \approx -\sum_{i,\alpha} U_\alpha \left( d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \tag{2.32}$$

$$= -\sum_{i,\alpha} U_\alpha (c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.33}$$

$$- \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{2.34}$$

$$= \sum_{i,\alpha} (\Delta_{i,\alpha} c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} + \Delta^*_{i,\alpha} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha}) \tag{2.35}$$

with the expectation value

$$\Delta_{i,\alpha} = -U_\alpha \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{2.36}$$

which is called the superconducting gap. Using the Fourier transform

$$c_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{i\alpha}} c_{\mathbf{k}\alpha\sigma} \tag{2.37}$$

can write

$$H_{\text{MF}} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{2.38}$$

Look at that Hamiltonian again, is that correct and can I write it better?

To include finite momentum, take the ansatz of a Fulde-Ferrel (FF) type pairing [40]:

How to include finite momentum, rewrite equations

$$\Delta \tag{2.39}$$

The Hamiltonian in eq. (2.38) can be writen as

Get the rem terms here

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}} \mathbf{C}_{\mathbf{k}}^{\dagger} H_{\mathrm{BdG}}(\mathbf{k}) \mathbf{C}_{\mathbf{k}} \tag{2.40}$$

$$C_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}1\uparrow} & c_{\mathbf{k}2\uparrow} & \dots & c_{\mathbf{k}n_{\mathrm{orb}}\uparrow} & c^{\dagger}_{-\mathbf{k}1\downarrow} & c^{\dagger}_{-\mathbf{k}2\downarrow} & \dots & c^{\dagger}_{-\mathbf{k}n_{\mathrm{orb}}\downarrow} \end{pmatrix}^{T} \tag{2.41}$$

with the so-called Bogoliubov-de-Gennes matrix

$$H_{\mathrm{BdG}}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^{\dagger} & -H^{*}_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{2.42}$$

with $H_{0,\sigma}$ being the F.T. of the kinetic term and $\Delta = \mathrm{diag}(\Delta_1, \Delta_2, \dots, \Delta_{n_{\mathrm{orb}}})$. Problem is now reduced to diagonalization of the BdG matrix. Write

$$H_{\mathrm{BdG}} = U_{\mathbf{k}} \epsilon_{\mathbf{k}} U_{\mathbf{k}}^{\dagger} \tag{2.43}$$

and

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \epsilon_{\mathbf{k}} \gamma_{\mathbf{k}}^{\dagger} \tag{2.44}$$

with quasi-particle operators

$$\gamma_{\mathbf{k}} = U_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \tag{2.45}$$

Write indeces everywhere without comma

Using the gap equation

$$\Delta_{\alpha} = -U \tag{2.46}$$

gap equation

the order parameter can be determined self-consistently, i.e. starting from an initial value, the BdG matrix needs to be set up, diagonalized and then used to determine $\Delta_{\alpha}$ again, until a converged value is found.

SC current in BCS

## 2.3 Dynamical Mean-Field Theory (DMFT)

Introduction DMFT, citing what has been achieved with it so far, what is the basic idea etc.

### 2.3.1 Green's Function Formalism

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

Following [17]

Give an introduction

Work over the paragraph

Slim down to relevant information

Have different kinds of Green's functions, for example the retarded Green's function (here with the $k$ for lattice systems):

$$G^R(\mathbf{k},\sigma,\sigma' t) = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma'}(0)\}\rangle \tag{2.47}$$

They give the amplitude of a particle inserted at momentum $\mathbf{k}'$ at time $t'$ to propagate to position $\mathbf{k}$ at time $t$. Define Fourier-transform:

$$G^R(\mathbf{k},\sigma,\sigma',\omega) = \int_{-\infty}^{\infty} \mathrm{d}t G^R(\mathbf{k},\sigma,\sigma' t) \tag{2.48}$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma,\omega) = -2\Im G^R(\mathbf{k}\sigma,\omega) \tag{2.49}$$

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 $\omega$. This mean, for non-interacting systems, the spectral function is a delta-function around the single-particle energies:

$$A_0(\mathbf{k}\sigma,\omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}\sigma}) \tag{2.50}$$

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

Show GFs can be related to observables

A mathematical trick to calculate GFs in praxis is to introduce the imaginary time variable $\tau$

$$t \to -\mathrm{i}\tau \tag{2.51}$$

where $\tau$ 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 Matsubara GF $C_{AB}(\tau,0)$:

Introduce Greens functions instead of correlation functions

$$C_{AB}(\tau,0) = -\left\langle T_\tau(A(\tau)B(0))\right\rangle \tag{2.52}$$

with time-ordering operator in imaginary time:

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau-\tau')A(\tau)B(\tau') \pm \Theta(\tau'-\tau)B(\tau')A(\tau) \tag{2.53}$$

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

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

$$-\beta < \tau < \beta \tag{2.54}$$

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

$$C_{AB}(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{2.55}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{2.56}$$

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

$$C^R_{AB}(\omega) = C_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{2.57}$$

What is the eta there -> need to define it in retarded GF

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).

single-particle Matsubara GF

### 2.3.2 Self Energy

Short introduction to diagrams

Self energy

Dyson equation

Dyson equation:

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}-\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}} \tag{2.58}$$

### 2.3.3 Nambu-Gorkov GF

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

Introduction following [15, ch. 14.7]

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{2.59}$$

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{2.60}$$

Sources for these?

How to get quasiparticle weight?

that can be calculated from the anomalous self-energy $\Sigma^{\mathrm{AN}}$ and quasiparticle weight $Z$

### 2.3.4 DMFT

Following [41].

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \tag{2.61}$$

with lattice coordinates $i, j$ and spin $\sigma$.

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

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)} \tag{2.62}$$

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

The Dyson equation

$$G(\mathbf{k}, \mathrm{i}\omega_n) = (G_0(\mathbf{k}, \mathrm{i}\omega_n) - \Sigma(\mathbf{k}, \mathrm{i}\omega_n))^{-1} \tag{2.63}$$

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!).

# 3 Dressed Graphene Model

Write introduction to the model and what is done in this chapter

## 3.1 Lattice Structure

Structure of honeycomb lattice following [42].

Monolayer graphene forms a honeycomb lattice, which is a hexagonal Bravais lattice with a two atom basis.

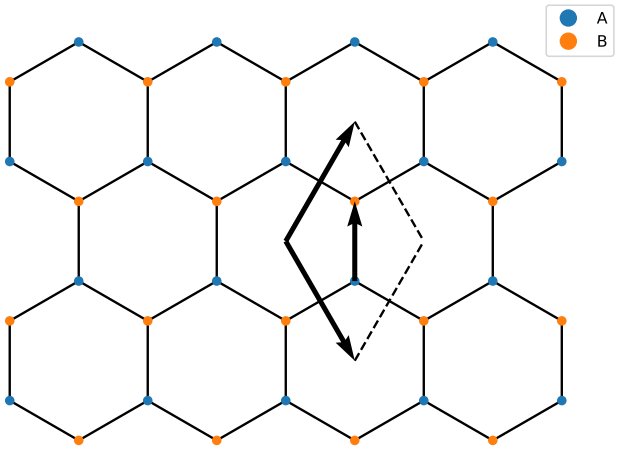



**Figure 3.1:** *Graphene lattice structure*

Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \tag{3.1}$$

$$\mathbf{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \tag{3.2}$$

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

$$a = \sqrt{3}a_0 \tag{3.3}$$

with the nearest-neighbour distance $a_0$.

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

$$\delta_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \tag{3.4}$$

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

$$\delta_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix} \tag{3.5}$$

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

$$\delta_{AA,1} = \mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = a\begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = a\begin{pmatrix} \sin(\frac{\pi}{6}) \\ \cos(\frac{\pi}{6}) \end{pmatrix} \tag{3.6}$$

$$\delta_{AA,2} = a\begin{pmatrix} \sin(\frac{3\pi}{6}) \\ \cos(\frac{3\pi}{6}) \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.7}$$

$$\delta_{AA,3} = a\begin{pmatrix} \sin(\frac{5\pi}{6}) \\ \cos(\frac{5\pi}{6}) \end{pmatrix} = a\begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \tag{3.8}$$

$$\delta_{AA,4} = a\begin{pmatrix} \sin(\frac{7\pi}{6}) \\ \cos(\frac{7\pi}{6}) \end{pmatrix} = a\begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \tag{3.9}$$

$$\delta_{AA,5} = a\begin{pmatrix} \sin(\frac{9\pi}{6}) \\ \cos(\frac{9\pi}{6}) \end{pmatrix} = a\begin{pmatrix} -1 \\ 0 \end{pmatrix} \tag{3.10}$$

$$\delta_{AA,6} = a\begin{pmatrix} \sin(\frac{11\pi}{6}) \\ \cos(\frac{11\pi}{6}) \end{pmatrix} = a\begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \tag{3.11}$$

First BZ vs this Gamma centered one

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

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{3.12}$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{3.13}$$

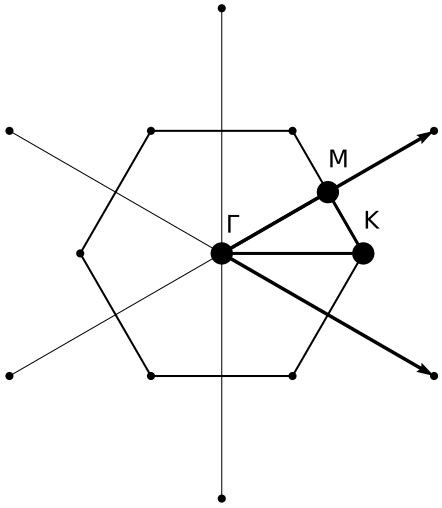



**Figure 3.2:** *Graphene Brillouin Zone*

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{3.14}$$

$$\mathbf{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{3.15}$$

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.16}$$

$$\mathrm{M} = \frac{\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{3.17}$$

$$\mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.18}$$

## 3.2 Dressed Graphene Model

Graphene lattice and a site X.

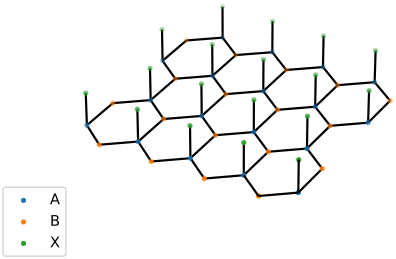



**Figure 3.3:** *EG-X model*

Without interaction:

$$H_0 = -t_X \sum_{\langle ij\rangle,\sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_{Gr} \sum_{\langle ij\rangle,\sigma} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + V \sum_{i,\sigma\sigma'} d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma'} + \text{h.c.} \tag{3.19}$$

with:

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

We can also introduce an onsite Hubbard interaction:

$$H_{\text{int}} = U_X \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{Gr} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{3.20}$$

Hamilto-
n orbital

Define sublattice index

$$\alpha = 1, 2, 3 \tag{3.21}$$

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

$$H_0 = -\sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{3.22}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{3.23}$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{3.24}$$

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

$$H_{int} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{3.25}$$

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^\dagger_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_{\mathrm{X}} \end{pmatrix} \begin{pmatrix} c^A_{k,\sigma} \\ c^B_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{3.26}$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. (3.26). This was done in fig. 3.4.

Values used for calculation:

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

$V$ is the control parameter. A range from $V = 0.1$ to $V = 2$ can be mapped onto materials in experiment.

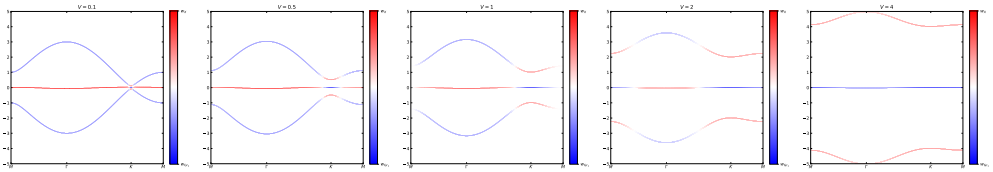


**Figure 3.4:** *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

# 4 Results

Parameter sweeps using [43].

## 4.1 Gaps

## 4.2 Superfluid Weight

## 4.3 Breakdown of SC with finite momentum

## 4.4 Coherence length etc.

Explain how to get the length scales in the different ways

Specifically: take

$$\xi(T) = \frac{1}{\sqrt{2}|\mathbf{Q}|} \tag{4.1}$$

with $\mathbf{Q}$ such that

$$|\frac{\psi_{\mathbf{Q}}(T)}{\psi_0(T)}| = \frac{1}{\sqrt{2}} \tag{4.2}$$

# A Dressed Graphene Hamiltonian in Reciprocal Space

Clean up this section

In this chapter, the model Hamiltonian from section 3.2

$$H_0 = -t_X \sum_{\langle ij\rangle,\sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_{Gr} \sum_{\langle ij\rangle,\sigma} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + V \sum_{i,\sigma} d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma} + \text{h.c.} \tag{A.1}$$

will be treated to obtain the electronic band structure. The first step is to write out the sums over nearest neighbors $\langle i,j\rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) for the vectors to the nearest neighbors of the X atoms and Graphene $A, B$ sites. Doing the calculation for example of the X atoms:

$$-t_X \sum_{\langle ij\rangle,\sigma} (d^\dagger_{i,\sigma} d_{j,\sigma} + d^\dagger_{j,\sigma} d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} - \frac{t_X}{2} \sum_{j,\sigma} \sum_{\delta_X} d^\dagger_{j,\sigma} d_{j+\delta_X,\sigma} \tag{A.2}$$

$$= -t_X \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} \tag{A.3}$$

The factor $1/2$ in eq. (A.2) is to account for double counting when going to the sum over all lattice sites $i$. By relabeling $j \to i$ in the second sum, the two sum are the same and eq. (A.3) is obtained. Using now the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}, \; c^\dagger_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c^\dagger_{\mathbf{k}} \tag{A.4}$$

with the completeness relation

$$\sum_i e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_i} = N \delta_{\mathbf{k},\mathbf{k}'} \,, \tag{A.5}$$

eq. (A.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_X} \left( e^{-i\mathbf{k}\mathbf{r}_i} d^\dagger_{\mathbf{k},\sigma} \right) \left( e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma} \right) \tag{A.6}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\delta_X,\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} e^{i\mathbf{k}'\delta_X} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \tag{A.7}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} \sum_{\delta_X} e^{i\mathbf{k}'\delta_X} \left( N \delta_{\mathbf{k},\mathbf{k}'} \right) \tag{A.8}$$

$$= -t_X \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \, . \tag{A.9}$$

This part is now diagonal in $\mathbf{k}$ space. The nearest neighbours vectors $\delta_X$ for the X atoms are the vectors $\delta_{AA,i}$ from section 3.1. With that, the sum over $\delta_X$ can be explicitly calculated:

Correct exp expressions

Example for a vector product

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \tag{A.10}$$

$$= -t_X \left[ \exp\left( ia \left( \frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) \right) + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right. \tag{A.11}$$

$$\left. + \, e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \tag{A.12}$$

$$= -t_X \left( 2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos\left(\frac{a}{2}k_x\right) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos\left(\frac{a}{2}k_x\right) \right) \tag{A.13}$$

$$= -2t_X \left( \cos(ak_x) + 2\cos\left(\frac{a}{2}k_x\right) \cos\left(\sqrt{3}\frac{a}{2}k_y\right) \right) \, . \tag{A.14}$$

The same can be done for the hopping between Graphene sites, for example :

$$-t_{\mathrm{Gr}} \sum_{\langle ij \rangle,\sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_{\mathrm{Gr}} \sum_{i,\sigma\sigma'} \sum_{\delta_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\delta_{AB},\sigma'} \tag{A.15}$$

$$= -t_{\mathrm{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{A.16}$$

Show that!

We note

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left( \sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \tag{A.17}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} \tag{A.18}$$

$$= -t_{Gr} \left( e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{A.19}$$

$$= -t_{Gr} \left( e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \left( e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x} \right) \right) \tag{A.20}$$

$$= -t_{Gr} \left( e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) \tag{A.21}$$

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{A.22}$$

# B Notes on the Computational Implementation

All the code is available at github.com/Ruberhauptmann/quant-met.

All the data,

For reproducibility, Datalad [44] is used.

The implementation relies on the work of many contributors of packages in Pythons ecosystem, most important among them NumPy [45], SciPy [46], Matplotlib [47], Pandas [48, 49] and Parasweep [43].

Data availability

What software for what?

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# List of Symbols

| Symbol | Meaning | Definition |
|---|---|---|
| $C_{AB}(\tau, 0)$ | Correlation function in imaginary time | 13 |