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# I INTRODUCTION

In 1894, Albert Michelson remarked that “it seems probable that most of the grand underlying principles have been firmly established”<sup>1</sup> [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 known 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 copper 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 Josephson 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 is in twisted multilayer systems, first realized as twisted bilayer

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<sup>1</sup>Variations of this quote have been attributed to Lord Kelvin, although the poetry having it said by someone, whose experiment would eventually lead to the development of special relativity 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.

## II SUPERCONDUCTIVITY

In this chapter: review theoretical concepts needed for describing SC.

Macroscopically, SC state can be described by a spontaneous breaking of a  $U(1)$  phase rotation symmetry, that is associated with an order parameter. Theory of this: GL theory section II.1.

One tool to describe superconductivity from a microscopic perspective: BCS theory section II.2.

Taking fluctuations beyond mean field into account: DMFT section II.3.

There are many textbooks covering these topics which can be referenced for a more detailed treatment, such as refs. [15–18].

### II.1 GINZBURG-LANDAU THEORY OF SUPERCONDUCTIVITY

For this review, follow chapter 11 in ref. [15].

More extensive introduction

#### ORDER PARAMETER

Similarly to a magnetically ordered state, the SC state is characterized by [19, 20]

Work over paragraph

Such a symmetry breaking (e.g. iron becomes magnetic, water freezes, superfluidity/superconductivity) is associated with the development of an order parameter  $\Psi$  when the temperature drops below the transition temperature  $T_C$ .

Introduce spontaneous symmetry breaking

$$|\Psi| = \begin{cases} 0, & T > T_C \\ |\Psi_0| > 0, & T < T_C \end{cases} \quad (\text{II.1})$$

Ginzburg-Landau theory is concerned with the the properties of the

Intuitive understanding why that is?

It does not need microscopic expression for order parameter, it provides coarse-grained description of the properties of matter. The order parameter description is good at length scales above  $\xi_0$ , the coherence length (e.g. size of Cooper pairs for SC). On length scales above  $\xi_0$ , the order parameter behaves as a smoothly varying function.

Work over paragraph

## LANDAU THEORY

Basic idea of Landau theory: write free energy as function  $F[\psi]$  of the order parameter. Region of small  $\psi$ , expand free energy of many-body system as simple polynomial:

$$f_L = \frac{1}{V}F[\psi] = \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 \quad (\text{II.2})$$

Provided  $r$  and  $u$  are greater than 0: minimum of  $f_L[\psi]$  lies at  $\psi = 0$ . Landau theory assumes: at phase transition temperature  $r$  changes sign, so:

$$r = a(T - T_C) \quad (\text{II.3})$$

Minimum of free energy occurs for:

$$\psi = \begin{cases} 0 \\ \pm \sqrt{\frac{a(T_C - T)}{u}} \end{cases} \quad (\text{II.4})$$

Make graphic for Landau free energy

Make graphic for Landau OP and BCS OP

Two minima for free energy function for  $T < T_C$ . With this, we can extract  $T_C$  from the knowledge of the dependence of  $|\psi|^2$  on  $T$  via a linear fit. This is only valid for an area near  $T_C$  (where Landau theory holds), but can be used to get  $T_C$  from microscopic theories.

Going from a one to a  $n$ -component order parameters, OP acquires directions and magnitude. Particularly important example: complex or two component order parameter in superfluids and superconductors:

$$\psi = \psi_1 + i\psi_2 = |\psi|e^{i\phi} \quad (\text{II.5})$$

The Landau free energy takes the form:

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

As before:

$$r = a(T - T_C) \quad (\text{II.7})$$

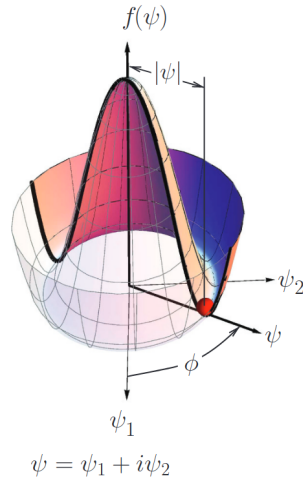
Make my own graphic for mexican hat potential

Figure II.1 shows the Landau free energy as function of  $\psi$ .

Rotational symmetry, because free energy is independent of the global phase of the OP:

$$f[\psi] = f[e^{ia}\psi] \quad (\text{II.8})$$





**Figure II.1:** Mexican hat potential

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.

#### GINZBURG-LANDAU THEORY

Work over paragraph

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:

$$f_{GL}[\psi, \Delta\psi, h] = \frac{s}{2}(\Delta\psi)^2 + \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 \quad (\text{II.9})$$

GL theory is only valid near critical point, where OP is small enough to permit leading-order expansion. Dimensional analysis shows:  $\frac{s}{r} = L^2$  has dimension of length squared. Length scale introduced by the gradient term: correlation

length

$$\xi(T) = \sqrt{\frac{s}{|r(T)|}} = \xi_0 \left| 1 - \frac{T}{T_C} \right|^{-\frac{1}{2}} \quad (\text{II.10})$$

sets characteristic length scale of order-parameter fluctuations, where

$$\xi_0 = \xi(T = 0) = \sqrt{\frac{s}{\alpha T_C}} \quad (\text{II.11})$$

is a measure of the microscopic coherence length. Near transition  $\xi(T)$  diverges, but far from transition it becomes comparable with the coherence length.

Work over paragraph

#### COMPLEX ORDER AND SUPERFLOW

Now: GL 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:

$$\langle \hat{\psi}(x) \rangle = \psi(x) = |\psi(x)| e^{i\theta(x)} \quad (\text{II.12})$$

Reminder: Field operators are the real space representations of creation/annihilation operators. They can be thought of the super position of all ways of creating a particle at position  $x$  via the basis coefficients.

Magnitude determines density of particles in the superfluid:

$$|\psi(x)|^2 = n_s(x) \quad (\text{II.13})$$

Density operator is

$$\hat{\rho} = \hat{\psi}(x) \hat{\psi}^\dagger(x) \quad (\text{II.14})$$

so expectation value of that is the formula above.

Twist/gradient of phase determines superfluid velocity:

$$\mathbf{v}_s(x) = \frac{\hbar}{m} \Delta \phi(x) \quad (\text{II.15})$$

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 matter not a-priori evident from microscopic physics.

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

$$f_{GL}[\psi, \Delta\psi] = s|\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \quad (\text{II.16})$$

Compare with the energy density of a bosonic field (with a quartic interaction):

$$H = \int d^Dx \frac{\hbar^2}{2m} |\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \quad (\text{II.17})$$

Interpret GL free energy 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:

$$s|\Delta\psi|^2 = \frac{\hbar^2}{2m} \langle \Delta\hat{\psi}^\dagger \Delta\hat{\psi} \rangle \Rightarrow s = \frac{\hbar^2}{2m} \quad (\text{II.18})$$

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

$$\xi = \sqrt{\frac{s}{|r|}} = \sqrt{\frac{\hbar^2}{2m|r|}} = \xi_0 \left(1 - \frac{T}{T_C}\right)^{-\frac{1}{2}} \quad (\text{II.19})$$

where  $\xi_0 = \xi(T=0) = \sqrt{\frac{\hbar^2}{2maT_C}}$  is the coherence length. Beyond this length scale: 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  $\frac{m}{2}v^2$ ):

$$\frac{\hbar^2 n_s}{2m} (\Delta\phi)^2 = \frac{mn_s}{2} \left(\frac{\hbar}{m} \Delta\phi\right)^2 \quad (\text{II.20})$$

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

$$\mathbf{v}_s = \frac{\hbar}{m} \Delta\phi \quad (\text{II.21})$$

(this is explained in detail later).

I dont know why that is. Can I support that somehow better? -> See Niklas thesis

For interpretation of superfluid states: coherent states. These are eigenstates of the field operator

$$\hat{\psi}(x) |\psi\rangle = \psi(x) |\psi\rangle \quad (\text{II.22})$$

and don't have a definite particle number. Importantly, this small uncertainty in particle number enables a high degree of precision in phase (which is the property of a condensate).

**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:

$$\Delta\psi = (\Delta|\psi| + i\Delta\phi|\psi|)e^{i\phi} \quad (\text{II.23})$$

So:

$$f_{GL} = \frac{\hbar}{2m}|\psi|^2(\Delta\phi)^2 + \left[ \frac{\hbar}{2m}(\Delta|\psi|)^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \right] \quad (\text{II.24})$$

The second term resembles GL functional for an Ising order parameter, describes energy cost of variations in the magnitude of the order parameter.

Phase rigidity and superflow

### II.1.1 SUPERCONDUCTING LENGTH SCALES

Better introduction

From [21].

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.

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

$$\psi_{\mathbf{q}}(\mathbf{r}) = |\psi_{\mathbf{q}}|e^{i\mathbf{q}\cdot\mathbf{r}} \quad (\text{II.25})$$

Then the free energy density is

$$f_{GL}[\psi_{\mathbf{q}}] = \alpha|\psi_{\mathbf{q}}|^2 + \frac{b}{2}|\psi_{\mathbf{q}}|^4 + \frac{\hbar^2 q^2}{2m^*}|\psi_{\mathbf{q}}|^2 \quad (\text{II.26})$$

Stationary point of the system:

$$\frac{\delta f_{GL}}{\delta \psi_{\mathbf{q}}^*} = 2\psi_{\mathbf{q}} \left[ \alpha(1 - \xi^2 q^2) + b|\psi_{\mathbf{q}}|^2 \right] = 0 \quad (\text{II.27})$$

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

$$|\psi_{\mathbf{q}}|^2 = |\psi_0|^2(1 - \xi(T)^2 q^2) \quad (\text{II.28})$$

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

$$\xi(T) = \xi_0(1 - \frac{T}{T_C})^{-\frac{1}{2}} \quad (\text{II.29})$$

Specifically: take

$$\xi(T) = \frac{1}{\sqrt{2}|\mathbf{Q}|} \quad (\text{II.30})$$

with  $\mathbf{Q}$  such that

$$|\frac{\psi_{\mathbf{Q}}(T)}{\psi_0(T)}| = \frac{1}{\sqrt{2}} \quad (\text{II.31})$$

The Cooper pair [22, 23]

## II.2 BARDEEN-COOOPER-SCHRIEFFER THEORY

First phenomenological description of SC: Fritz London in 1937 [24]. He was motivated by the discovery of the Meissner effect in 1933 [3], where magnetic flux inside of the superconductor is always pushed out in contrast to a perfectly conducting material, which would hold a 'memory' of the magnetic field at the time of the phase transition. This suggests that transition to the SC state is reversible and a SC is not just the limiting case of a conductor with infinite conductivity, in which according to the Maxwell equations, the magnetic flux would not change. Londons first descriptions is based on a one-particle wave function  $\phi(x)$ . He proposed that persistent supercurrent is a property of the ground state associated with its rigidity against the application of a field.

In 1950 [20]: GL interpreted this wave function as a complex order parameter as explained in section II.1.

Following [15, ch. 14].

Depairing current from FMP

Full formula for supercurrent, with sum over orbitals

DS from FMP

Write more about the connection between all the things here

### II.2.1 BCS HAMILTONIAN

Microscopic description of SC: 1957 by John Bardeen, his postdoc Leon Cooper and the graduate in the group, J. Robert Schrieffer [4]. Description is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [25]. The final element in this description was the origin of the attractive interaction  $V_{\mathbf{k},\mathbf{k}'}$  between electrons, which Bardeen, Cooper and Schrieffer identified as a retarded electron-phonon interaction [4]. BCS-Hamiltonian:

$$H_{\text{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \quad (\text{II.32})$$

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

$$\Delta = -\frac{U}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -U \langle c_{-\mathbf{r}=0\downarrow} c_{\mathbf{r}=0\uparrow} \rangle \simeq U\Psi. \quad (\text{II.33})$$

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. 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.

What is explained by phononic pairing?

It is very successful in two ways: on the one hand very in establishing electronic pairing as the microscopic mechanism behind SC, which holds still today even for high  $T_C$ /unconventional superconductors and secondly

Sources for that

This so-called BCS-theory of superconductivity is very successful in explaining experimental results in many compounds.

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

### II.2.2 ATTRACTIVE HUBBARD MODEL

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [26], Kanamori [27] and Gutzwiller [28].

$$H_{\text{int}} = U \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow} c_{i,\uparrow} \quad (\text{II.34})$$

where  $U > 0$ .

Besides

[29]

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 [30]. The form of the interaction term is then:

$$H_{\text{int}} = - \sum_{i,\alpha} U_{\alpha} c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \quad (\text{II.35})$$

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).

**MULTIBAND BCS MEAN FIELD THEORY** 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]. A more intuitive way based on ref. [17] discussed here looks at the operators and which one are small.

Look at interaction term eq. (II.35). Mean-field approximation (here specifically for superconductivity i.e. pairing): operators do not deviate much from their average value, i.e. the deviation operators

$$d_{i,\alpha} = c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} - \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \quad (\text{II.36})$$

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \quad (\text{II.37})$$

are small (don't contribute much to expectation values and correlation functions), so that in the interaction part of the Hamiltonian

$$H_{\text{int}} = - \sum_{i,\alpha} U_{\alpha} c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \quad (\text{II.38})$$

$$= - \sum_{i,\alpha} U_{\alpha} (d_{i,\alpha}^{\dagger} + \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle) (e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (\text{II.39})$$

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

$$+ \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (\text{II.41})$$

Some relevance of the repulsive Hubbard model

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

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

there are other combinations, talk about that

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

$$H_{\text{int}} \approx - \sum_{i,\alpha} U_{\alpha} \left( d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle + \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \quad (\text{II.42})$$

$$= - \sum_{i,\alpha} U_{\alpha} \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \quad (\text{II.43})$$

$$- \langle c_{i,\alpha,\uparrow}^{\dagger} c_{i,\alpha,\downarrow}^{\dagger} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \quad (\text{II.44})$$

$$= \quad (\text{II.45})$$

with the expectation values

$$\Delta \quad (\text{II.46})$$

$$H_{\text{int}} \approx \sum_{\alpha,\mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^* c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{II.47})$$

Fourier transformation:

$$H_{\text{int}} = - \frac{1}{N^2} \sum_{\alpha, \mathbf{k}_1, 2, 3, 4} U_{\alpha} e^{i(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_3) \cdot \mathbf{r}_{i\alpha}} c_{\mathbf{k}_1\alpha\uparrow}^{\dagger} c_{\mathbf{k}_3\alpha\downarrow}^{\dagger} c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \quad (\text{II.48})$$

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

$$H_{\text{int}} = - \sum_{\alpha, \mathbf{k}, \mathbf{k}'} U_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \quad (\text{II.49})$$

Mean-field approximation:

$$H_{\text{int}} \approx \sum_{\alpha, \mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^* c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{II.50})$$

with

$$\Delta_{\alpha} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \quad (\text{II.51})$$

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

General multi-band  
mean field theory  
theory

Mean field with fi-  
nite momentum



This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c_{\mathbf{k}\alpha\uparrow}^\dagger c_{-\mathbf{k}\alpha\downarrow}^\dagger + \Delta_\alpha^* c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{II.53})$$

with Nambu spinor

Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c_{1,-\mathbf{k}\downarrow}^\dagger \\ c_{2,-\mathbf{k}\downarrow}^\dagger \\ c_{3,-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \quad (\text{II.54})$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \quad (\text{II.55})$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H_{0,\downarrow}^*(-\mathbf{k}) + \mu \end{pmatrix} \quad (\text{II.56})$$

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

SELF-CONSISTENCY Formula for OP using the Bogoliubov operators

$$\Delta_\alpha = -U \quad (\text{II.57})$$

How to solve mean field theory self-consistently

FINITE MOMENTUM To include finite momentum, take the ansatz of a Fulde-Ferrel (FF) type pairing [31]:

$$\Delta \quad (\text{II.58})$$

How to include finite momentum

## II.3 DYNAMICAL MEAN-FIELD THEORY

### II.3.1 GREEN'S FUNCTION FORMALISM

Following [17]

Work over the paragraph

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:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -i\Theta(t - t') \langle \{c_{\mathbf{r}\sigma}(t), c_{\mathbf{r}'\sigma'}^\dagger(t')\} \rangle \quad (\text{II.59})$$

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:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t - t') \quad (\text{II.60})$$

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

$$G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) = -i\Theta(t) \langle \{c_{\mathbf{r}\sigma}(t), c_{\mathbf{r}'\sigma'}^\dagger(0)\} \rangle \quad (\text{II.61})$$

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

$$G^R(\mathbf{k}, \sigma, \sigma', t) = -i\Theta(t - t') \langle \{c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma'}^\dagger(0)\} \rangle \quad (\text{II.62})$$

Define Fourier-transform:

$$G^R(\mathbf{k}, \sigma, \sigma', \omega) = \int_{-\infty}^{\infty} dt G^R(\mathbf{k}, \sigma, \sigma', t) \quad (\text{II.63})$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma, \omega) = -2\Im G^R(\mathbf{k}\sigma, \omega) \quad (\text{II.64})$$

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:

$$A_0(\mathbf{k}\sigma, \omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}\sigma}) \quad (\text{II.65})$$

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  $\tau$ :

$$t \rightarrow -i\tau \quad (\text{II.66})$$

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  $e^{-iHt}$  coming from the time evolution of operators.

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

$$C_{AB}(\tau, 0) = -\langle T_\tau(A(\tau)B(0)) \rangle \quad (\text{II.67})$$

with time-ordering operator in imaginary time:

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau - \tau')A(\tau)B(\tau') \pm \Theta(\tau' - \tau)B(\tau')A(\tau) \quad (\text{II.68})$$

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

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

$$-\beta < \tau < \beta \quad (\text{II.69})$$

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

$$C_{AB}(i\omega_n) = \int_0^\beta d\tau \quad (\text{II.70})$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} & \text{for bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{for fermions} \end{cases} \quad (\text{II.71})$$

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  $C_{AB}^R(\omega)$  by analytic continuation:

$$C_{AB}^R(\omega) = C_{AB}(i\omega_n \rightarrow \omega + i\eta) \quad (\text{II.72})$$

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) [17, p. 8.3.4].

### II.3.2 PERTURBATION THEORY, DYSON EQUATION

Dyson equation:

$$G_\sigma(\mathbf{k}, i\omega_n) = \frac{G_\sigma^0(\mathbf{k}, i\omega_n)}{1 - G_\sigma^0(\mathbf{k}, i\omega_n)\Sigma_\sigma(\mathbf{k}, i\omega_n)} = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma_\sigma(\mathbf{k}, i\omega_n)} \quad (\text{II.73})$$

How to resolve ambiguity at borders of integral

single-particle Matsubara GF

equations of motion for Matsubara GF

Short introduction to diagrams

Self energy

Dyson equation

## II.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:

$$\Psi = F^{\text{loc}}(\tau = 0^-) \quad (\text{II.74})$$

or the superconducting gap

$$\Delta = Z\Sigma^{\text{AN}} \quad (\text{II.75})$$

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

Sources for these?

How to get quasiparticle weight?

## II.3.4 DMFT

Following [32].

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \quad (\text{II.76})$$

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

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

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)} \quad (\text{II.77})$$

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

The Dyson equation

$$G(\mathbf{k}, i\omega_n) = (G_0(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n))^{-1} \quad (\text{II.78})$$

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!).

### III QUANTUM METRIC

First formulated in [33]

Following Cheng - a pedagogical Introduction

Parameter dependent Hamiltonian  $\{H(\lambda)\}$ , smooth dependence on parameter

$\lambda = (\lambda_1, \lambda_2, \dots) \in \mathcal{M}$  (base manifold)

Hamiltonian acts on parametrized Hilbert space  $\mathcal{H}(\lambda)$

Eigenenergies  $E_n(\lambda)$ , eigenstates  $|\phi_n(\lambda)\rangle$

System state  $|\psi(\lambda)\rangle$  is linear combination of  $|\psi_n(\lambda)\rangle$  at every point in  $\mathcal{M}$

Infinitesimal variation of the parameter  $d\lambda$  :

See what is specific to this paper, see that I can derive that myself

Dont get it here

$$ds^2 = \|\psi(\lambda+d\lambda) - \psi(\lambda)\|^2 = \langle \delta\psi | \delta\psi \rangle = \langle \partial_\mu \psi | \partial_\nu \psi \rangle d\lambda^\mu d\lambda^\nu = (\gamma_{\mu\nu} + i\sigma_{\mu\nu}) d\lambda^\mu d\lambda^\nu \quad (\text{III.1})$$

Last part is splitting up into real and imaginary part

#### III.1 QUANTUM METRIC AND SUPERFLUID WEIGHT

Write up notes about quantum metric and superfluid weight



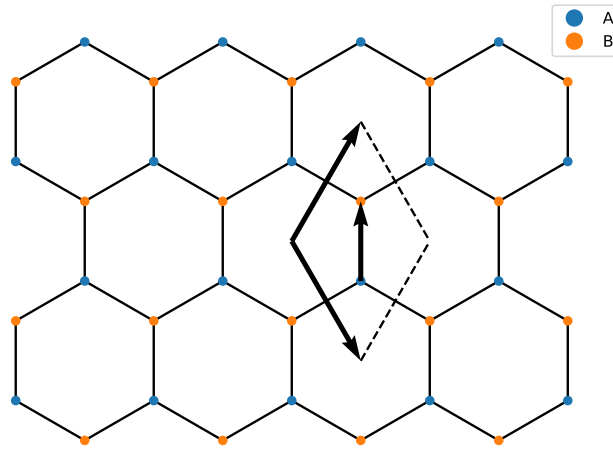
## IV DRESSED GRAPHENE MODEL

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

### IV.1 LATTICE STRUCTURE

Structure of honeycomb lattice following [34].

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



**Figure IV.1:** *Graphene lattice structure*

Primitive lattice vectors of the hexagonal lattice:

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

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

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

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

with the nearest-neighbour distance  $a_0$ .

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

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

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

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

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

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

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

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

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

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

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

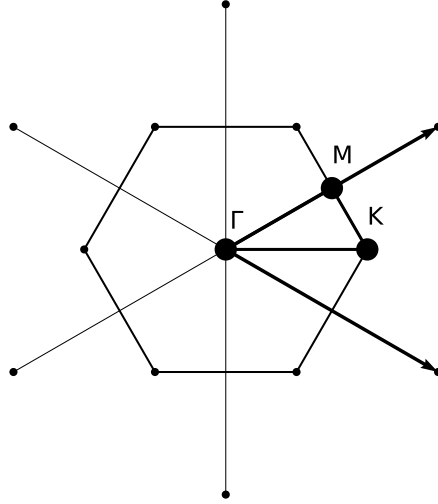
First BZ vs this  
Gamma centered  
one

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

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

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





**Figure IV.2:** *Graphene Brillouin Zone*

so we have:

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

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

Points of high symmetry in the Brillouin zone are:

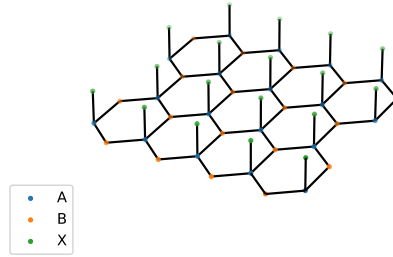
$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (\text{IV.16})$$

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

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

## IV.2 EG-X MODEL

Graphene lattice and a site X.



**Figure IV.3:** *EG-X model*

Without interaction:

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

with:

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

We can also introduce an onsite Hubbard interaction:

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

Hamilto-  
n orbital

Define sublattice index

$$\alpha = 1, 2, 3 \quad (\text{IV.21})$$

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

$$H_0 = - \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta} c_{i\alpha}^\dagger c_{j\beta} \quad (\text{IV.22})$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\text{Gr}} & 0 \\ t_{\text{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\text{X}} \end{pmatrix} \quad (\text{IV.23})$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \quad (\text{IV.24})$$

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

$$H_{int} = - \sum_{i\alpha} U_\alpha c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\alpha\downarrow} c_{i\alpha\uparrow} \quad (\text{IV.25})$$



## V RESULTS

Parameter sweeps using [35].

### V.1 GAPS

### V.2 SUPERFLUID WEIGHT

### V.3 BREAKDOWN OF SC WITH FINITE MOMENTUM

### V.4 COHERENCE LENGTH ETC.



## A DRESSED GRAPHENE HAMILTONIAN IN RECIPROCAL SPACE

Clean up this section

In the following chapter, the model Hamiltonian

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

will be treated to obtain the 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:

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

$$= -t_X \sum_{i,\sigma} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma} \quad (\text{A.3})$$

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  $j \rightarrow i$  in the second sum, the two sum are the same and eq. (A.3) is obtained. Using now the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}, \quad c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \quad (\text{A.4})$$

with the completeness relation

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

eq. (A.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_X} (e^{-i\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger) (e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma}) \quad (\text{A.6})$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\delta_X,\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k}',\sigma} e^{i\mathbf{k}'\delta_X} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \quad (\text{A.7})$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k}',\sigma} \sum_{\delta_X} e^{i\mathbf{k}'\delta_X} (N \delta_{\mathbf{k},\mathbf{k}'}) \quad (\text{A.8})$$

$$= -t_X \sum_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X}. \quad (\text{A.9})$$

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 ?? . With that, the sum over  $\delta_X$  can be explicitly calculated:

Correct exp expressions

Example for a vector product

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

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

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

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

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

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

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

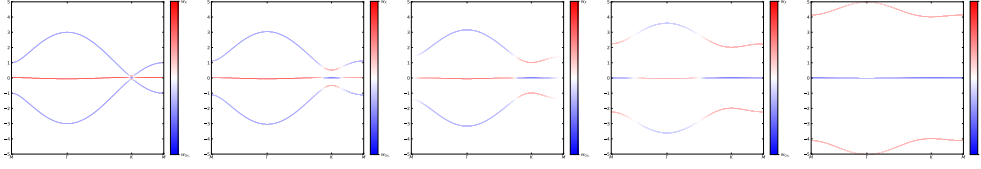
$$= -t_{\text{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c_{\mathbf{k},\sigma}^{(A)\dagger} c_{\mathbf{k},\sigma'}^{(B)} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{A.16})$$

Show that!

We note

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





**Figure A.1:** Bands of the non-interacting EG-X model. All the bands are spin-degenerate.

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{A.18})$$

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

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

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

All together, we get:

$$H_0 = \sum_{\mathbf{k}, \sigma, \sigma'} \begin{pmatrix} c_{\mathbf{k}, \sigma}^{A, \dagger} & c_{\mathbf{k}, \sigma}^{B, \dagger} & d_{\mathbf{k}, \sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}, \sigma}^A \\ c_{\mathbf{k}, \sigma}^B \\ d_{\mathbf{k}, \sigma} \end{pmatrix} \quad (\text{A.22})$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. ???. This was done in fig. A.1.

Values used for calculation:

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

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



## B NOTES ON THE COMPUTATIONAL IMPLEMENTATION

All the code is available at [github.com/Ruberhauptmann/quant-met](https://github.com/Ruberhauptmann/quant-met).

All the data, \_\_\_\_\_

Data availability

For reproducibility, Datalad [36] is used.

The implementation relies on the work of many contributors of packages in Python's ecosystem, most important among them NumPy [37], SciPy [38], Matplotlib [39], Pandas [40, 41] and Parasweep [35]. \_\_\_\_\_

What software for what?



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## LIST OF SYMBOLS

Symbol	Meaning	Definition
$\tau$	general imaginary time variable	14
$C_{AB}(\tau, 0)$	Correlation function in imaginary time	15