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In 1894, Albert Michelson remarked that “it seems probable that most of the grand underlying principles have been firmly established” [1, p. 159]. The 20th century then fundamentally changed our view of the world in the small and cold with quantum mechanics and the large and hot with general relativity. Among the events fuelling this revolution was the 1911 discovery of the phenomenon of superconductivity in Mercury by Heike Onnes [2]. Superconductivity is 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].

## High-Temperature Superconductivity

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, 10] and other particle accelerators over detectors of single photons in astrophysics [11] to extremely sensitive measurement devices for magnetic fields [12] and voltages [13] based on the Josephson effect [14].

Since the first discovery of SC in cuprates, there has been a lot of work to develop superconductors with higher transition temperatures.

## Flat Bands: Pairing and Supercurrent

### Twisted Bilayer Graphene

One interesting development in is in twisted multilayer systems, first realized as twisted bilayer Graphene [15]. 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.

I have system that is similar

### Organization of this thesis

# Superconductivity

# 2

In this chapter I 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. [16–20].

Macroscopically, the superconducting state can be described by a spontaneous breaking of a  $U(1)$  phase rotation symmetry that is associated with an order parameter. The theory of spontaneous symmetry breaking and associated phase transitions is Ginzburg-Landau theory discussed in section 2.1, following refs. [16, 21]. 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. They also connect to the energy gap  $\Delta$  and the condensate stiffness  $D_S$ , which are often competing energy scales in superconductors. The interplay of these length (energy) scales determine the macroscopic properties of a superconductors, so there is a great interest in accessing them in computational ways. To this end, section 2.1 also introduces a theoretical framework based on Cooper pairs with finite momentum [22] that will be used in later chapters to calculate these length scales from microscopic theories.

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 breakdown of symmetry, it can be connected to quantities expressed by Ginzburg-Landau theory. One such theory to describe superconductivity from a microscopic perspective is BCS (Bardeen-Cooper-Schrieffer) theory in section 2.2, which is 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.

Furthermore, section 2.4 introduces an emerging perspective in the study of novel superconductors: it turns out that the superfluid weight is connected to

a quantity of the electronic band structure called the quantum metric [23, 24], which is connected to

## 2.1 Ginzburg-Landau Theory of Superconductivity

### Spontaneous Symmetry Breaking and Order Parameter

Symmetries are a powerful concept in physics. Noethers theorem [25] 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 spontaneous 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 I 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  $T_C$

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

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’ [26]. 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 [27]. Landau theory and conversely

Ginzburg-Landau theory is not concerned with the microscopic properties of the order parameter, but describes the changes in thermodynamic properties of matter with the development of an order parameter.

### Landau and Ginzburg-Landau Theory

The free energy is a thermodynamic quantity:

$$F = E - TS \quad (2.2)$$

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:

$$F_L[\Psi] = \int d^d x f_L[\Psi], \quad (2.3)$$

where

$$f_L[\Psi] = \frac{r}{2}\Psi^2 + \frac{u}{4}\Psi^4 \quad (2.4)$$

is called the free energy density. Provided the parameters  $r$  and  $u$  are greater than 0, there is a minimum of  $f_L[\Psi]$  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

$$r = a(T - T_C). \quad (2.5)$$

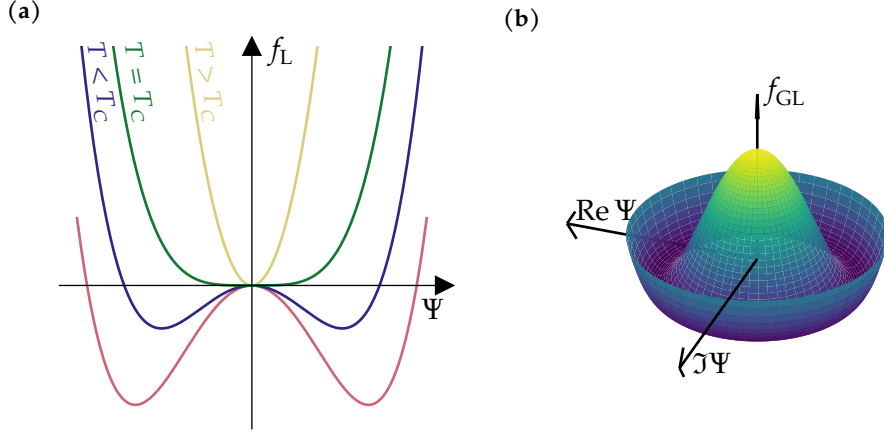
Figure 2.1a shows the free energy as a function of a single-component, real order parameter  $\Psi$  and it illustrates the essence of Landau theory: there are two cases for the minima of the free energy  $f$

$$\Psi = \begin{cases} 0 & T \geq T_C \\ \pm \sqrt{\frac{a(T_C - T)}{u}} & T < T_C \end{cases}, \quad (2.6)$$

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

$$|\Psi|^2 \propto T_C - T. \quad (2.7)$$





**Figure 2.1. Landau free energy and Mexican hat potential** (a) Landau free energy  $f_L$  at different temperatures  $T$ . (b)

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

$$\Psi = \Psi_1 + i\Psi_2 = |\Psi|e^{i\phi}. \quad (2.8)$$

The Landau free energy then takes the form

$$f_L[\Psi] = r\Psi^*\Psi + \frac{u}{2}(\Psi^*\Psi)^2 = r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \quad (2.9)$$

with again

$$r = a(T_C - T). \quad (2.10)$$

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

$$f_L[\Psi] = f_L[e^{i\phi}\Psi]. \quad (2.11)$$

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 symmetry-broken state to another.

In 1950, Ginzburg and Landau published their theory of superconductivity, based on Landau's theory of phase transitions [27]. Where Landau theory as described above has a uniform order parameter, 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

$$f_{GL}[\Psi, \Delta\Psi] = \frac{\hbar^2}{2m^*} |\Delta\Psi|^2 + r|\Psi|^2 + \frac{u}{2} |\Psi|^4, \quad (2.12)$$

where the gradient term  $\Delta\Psi$  is added in comparison to the Landau free energy. The prefactor  $\frac{\hbar^2}{2m^*}$  is chosen to illustrate the interpretation of the Ginzburg-Landau free energy as the energy of a condensate of bosons, where the gradient term  $|\Delta\Psi|^2$  is the kinetic energy. The free energy in eq. (2.12) is sensitive to a twist of the phase of the order parameter. Substituting the expression  $\Psi = |\Psi|e^{i\phi}$ , the gradient term reads

$$\Delta\Psi = (\Delta|\Psi| + i\Delta\phi|\Psi|)e^{i\phi}. \quad (2.13)$$

With that, eq. (2.12) becomes

$$f_{GL} = \frac{\hbar^2}{2m^*} |\Psi|^2 (\Delta\phi)^2 + \left[ \frac{\hbar^2}{2m^*} (\Delta|\Psi|)^2 + r|\Psi|^2 + \frac{u}{2} |\Psi|^4 \right]. \quad (2.14)$$

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. Twisting the phase of the condensate is associated with an energy cost. This energy cost is characterized by the stiffness  $D_S$

The dominating fluctuation is determined by the ratio of the factors  $\frac{\hbar^2}{2m^*}$  and  $r$ , which has the dimension  $\text{Length}^2$ , from which define the correlation length.

$$\xi = \sqrt{\frac{\hbar^2}{2m^*|r|}} = \xi_0 \left(1 - \frac{T}{T_C}\right)^{-\frac{1}{2}} \quad (2.15)$$

Introduce superfluid density properly

Energy cost of phase bending via GL energy

Explanation phase stiffness

Explanation superfluid weight as linear response

where I define the zero temperature value as the coherence length  $\xi_0 = \xi(T = 0) = \sqrt{\frac{\hbar^2}{2maT_C}}$ . On length scales above  $\xi$ , the physics is entirely controlled by the phase degrees of freedom, i.e.

$$f_{GL} = \frac{\hbar^2}{2m^*} |\Psi|^2 (\Delta\phi)^2 + \text{const.} \quad (2.16)$$

Take case of frozen amplitude fluctuations, i.e.  $\Delta|\Psi(\mathbf{r})| = 0$ . Stationary point condition for eq. (2.14) gives:

$$|\Psi| = |\Psi_0| \sqrt{1 - \xi^2 |\Delta\phi(\mathbf{r})|^2} \quad (2.17)$$

This shows that the superconducting order gets suppressed and eventually destroyed by short-ranged (below  $\xi$ ) phase fluctuations. By introducing a particular form of phase fluctuations  $\phi = \mathbf{q} \cdot \mathbf{r}$  into a microscopic model, it is possible to probe this breakdown of superconductivity and thus gain insight into the nature of superconductivity, in particular this gives access to  $\xi$ .

Work over paragraph

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

$$f_{GL}[\Psi, \mathbf{A}] = \frac{\hbar^2}{2m^*} \left| \left( \Delta - \frac{ie^*}{\hbar} \mathbf{A} \right) \Psi \right|^2 + r|\Psi|^2 + \frac{u}{2} |\Psi|^4 \quad (2.18)$$

Describes really two intertwined Ginzburg-Landau theories for  $\Psi$  and  $\mathbf{A}$  respectively. This mean there are two length scales, the coherence length  $\xi$  governing amplitude fluctuations of  $\Psi$  and the London penetration depth  $\lambda_L$ , which determines the distance magnetic fields penetrate into the superconductor. Can get the current density from the stationary point condition of the free energy for the vector potential  $\mathbf{A}$ :

$$\frac{\delta f_{GL}}{\delta \mathbf{A}} = 0 = -\mathbf{j} + \frac{1}{\mu_0} \nabla \times \mathbf{B} \quad (2.19)$$

with the supercurrent density

$$\mathbf{j} = -i \frac{e\hbar}{m^*} (\Psi^* \Delta \Psi - \Psi \Delta \Psi^*) - \frac{4e^2}{m^*} |\Psi|^2 \mathbf{A} . \quad (2.20)$$

Introducing the OP with phase  $\Psi = |\Psi|e^{i\phi}$ :

$$\mathbf{j} = 2e|\Psi|^2 \frac{\hbar}{m^*} \left( \nabla\phi - \frac{2\pi}{\Phi_0} \mathbf{A} \right) \quad (2.21)$$

with the magnetic flux quantum  $\Phi_0 = \frac{\pi\hbar}{e}$ . Shows that not only an applied field  $\mathbf{A}$  can induce a supercurrent, but also the twist of the phase of the condensate. Rewriting using  $|\Psi|^2 = n_s/2$  and introducing the superfluid velocity  $\mathbf{v}_s$ :

$$\mathbf{j} = en_s \mathbf{v}_s \quad (2.22)$$

## 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. Can be seen in the phenomenon of BCS-BEC crossover physics [28]. The picture of this crossover is the following: for a small attractive interaction, pairs of electrons are very loosely bound, which are pretty mobile, enabling superconductivity, while for a stronger interaction the pairs

The crossover region

These two energy scales are equivalently defined via the coherence length  $\xi_0$  and the London penetration depth introduced in section 2.1, 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 this [22]. As already discussed in the context of eq. (2.17), strong phase fluctuations destroy superconducting order.

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 [29–31]

Procedure: 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:

$$\Psi_{\mathbf{q}}(\mathbf{r}) = |\Psi_{\mathbf{q}}|e^{i\mathbf{q}\cdot\mathbf{r}} \quad (2.23)$$

Make clear: supercurrent just because of twisting of phase in ground state

Write introduction better

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

Write better: connection of the section above and this theory

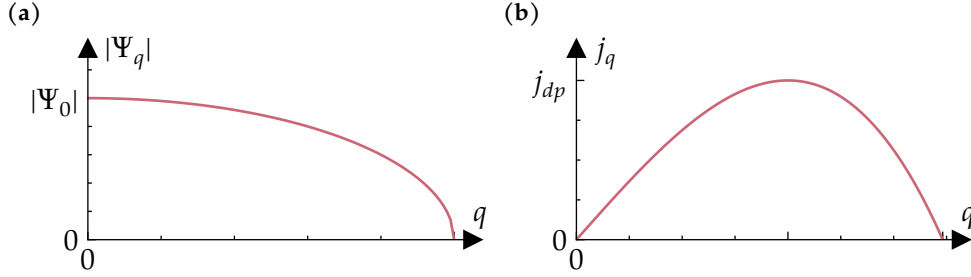


Figure 2.2. a and b

Then the free energy density eq. (2.12) is

$$f_{GL}[\Psi_{\mathbf{q}}] = r|\Psi_{\mathbf{q}}|^2 + \frac{u}{2}|\Psi_{\mathbf{q}}|^4 + \frac{\hbar^2 q^2}{2m^*}|\Psi_{\mathbf{q}}|^2 \quad (2.24)$$

Stationary point of the system:

$$\frac{\delta f_{GL}}{\delta \Psi_{\mathbf{q}}^*} = 2\Psi_{\mathbf{q}} [r(1 - \xi^2 q^2) + u|\Psi_{\mathbf{q}}|^2] = 0 \quad (2.25)$$

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

$$|\Psi_{\mathbf{q}}|^2 = |\Psi_0|^2 (1 - \xi(T)^2 q^2) \quad (2.26)$$

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 eq. (2.15)

$$\xi(T) = \xi_0 \left(1 - \frac{T}{T_C}\right)^{-\frac{1}{2}} \quad (2.27)$$

### The Cooper pair

The momentum of the Cooper pairs entails a charge supercurrent  $\mathbf{j}_{\mathbf{q}}$ . For small  $q$

The depairing current is an upper boundary for the maximal current that can flow through a material, also called the critical current  $\mathbf{j}_c$ . The value of

Depairing  
current from  
FMP

$j_c$  is strongly dependent on the geometry of the sample [32, 33], so  $j_{dp}$  is not necessarily experimentally available, but it can be used to calculate the London penetration depth [17]

$$\lambda_L(T) = \sqrt{\frac{\Phi_0}{3\sqrt{3}\pi\mu_0\zeta(T)j_{dp}(T)}} = \lambda_{L,0} \left(1 - \left(\frac{T}{T_C}\right)^4\right)^{-\frac{1}{2}} \quad (2.28)$$

## 2.2 Bardeen-Cooper-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].

The BCS (Bardeen-Cooper-Schrieffer) description of superconductivity is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [34]. 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 refs. [16, 17]. This section gives an introduction to the relevant physics of BCS theory as originally proposed, then derives the

### BCS Hamiltonian

BCS-Hamiltonian:

$$H_{\text{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \quad (2.29)$$

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

$$\Delta = -\frac{U}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -U \langle c_{-\mathbf{r}=0\downarrow} c_{\mathbf{r}=0\uparrow} \rangle \simeq U\Psi. \quad (2.30)$$

Where does this formula come from? Second London equation

$D_S$

What else can be done with the FMP method?

Connection of the FMP method to linear response techniques

Better introduction

Work over paragraph

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 [35, 36] and the band gap measured by Giaever in 1960 [37]. On the other hand, it established electronic pairing, i.e. the picture of a quantum-mechanical wave function with a defined phase as already described by Fritz London in 1937 [38] as the microscopic mechanism behind SC. This picture still holds today even for high  $T_C$ /unconventional superconductors, so SCs that cannot be described by BCS theory [39].

### Multiband BCS Theory

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [40], Kanamori [41] and Gutzwiller [42].

$$H_{\text{int}} = U \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow} c_{i,\uparrow} \quad (2.31)$$

where  $U > 0$ . It describes a repulsive interaction between electrons of different spin at the same lattice site.

Besides  
[43]

The Hubbard model in the form of eq. (2.31) can be extended in a multitude of ways to model a variety of physical system. Here: 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 [44]. The form of the interaction term is then:

$$H_{\text{int}} = - \sum_{i,\alpha} U_\alpha c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \quad (2.32)$$

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

Kinetic term as well

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 equa-

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. [16]. The review follows ref. [45]. A more intuitive way based on ref. [18] discussed here looks at the operators and which one are small.

Look at interaction term eq. (2.32). Mean-field approximation (here specifically for superconductivity i.e. pairing): operators do not deviate much from their average value, i.e. the deviation operators

$$d_{i,\alpha} = c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger - \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \quad (2.33)$$

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \quad (2.34)$$

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

$$H_{\text{int}} = - \sum_{i,\alpha} U_\alpha c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \quad (2.35)$$

$$= - \sum_{i,\alpha} U_\alpha (d_{i,\alpha}^\dagger + \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle) (e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (2.36)$$

$$= - \sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \quad (2.37)$$

$$+ \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (2.38)$$

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

$$H_{\text{int}} \approx - \sum_{i,\alpha} U_\alpha (d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle + \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (2.39)$$

$$= - \sum_{i,\alpha} U_\alpha (c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \quad (2.40)$$

$$- \langle c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \quad (2.41)$$

$$= \sum_{i,\alpha} \left( \Delta_{i,\alpha} c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger + \Delta_{i,\alpha}^* c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha} \right) \quad (2.42)$$

there are other combinations, talk about that

deviations with small deltas



with the expectation value

$$\Delta_{i,\alpha} = -U_\alpha \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \quad (2.43)$$

which is called the superconducting gap and is the order parameter introduced in Ginzburg-Landau theory in section 2.1. To include finite momentum in BCS theory, take the ansatz of a Fulde-Ferrel (FF) type pairing [46]:

$$\Delta_{i,\alpha} = \Delta_\alpha e^{i\mathbf{q}\cdot\mathbf{r}_{i\alpha}} \quad (2.44)$$

Using the Fourier transform

$$c_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_{i\alpha}} c_{\mathbf{k}\alpha\sigma} \quad (2.45)$$

can write mean-field interaction term as

$$\sum_{i,\alpha} \left( \Delta_{i,\alpha} c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger + \Delta_{i,\alpha}^* c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha} \right) \quad (2.46)$$

can write

$$H_{\text{MF}} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\beta\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c_{\mathbf{k}\alpha\uparrow}^\dagger c_{-\mathbf{k}\alpha\downarrow}^\dagger + \Delta_\alpha^* c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (2.47)$$

The Hamiltonian in eq. (2.47) can be written as

$$H_{\text{MF}} = \sum_{\mathbf{k}} \mathbf{C}_{\mathbf{k}}^\dagger H_{\text{BdG}}(\mathbf{k}) \mathbf{C}_{\mathbf{k}} \quad (2.48)$$

$$\mathbf{C}_{\mathbf{k}} = (c_{\mathbf{k}1\uparrow} \quad c_{\mathbf{k}2\uparrow} \quad \dots \quad c_{\mathbf{k}n_{\text{orb}}\uparrow} \quad c_{-\mathbf{k}1\downarrow}^\dagger \quad c_{-\mathbf{k}2\downarrow}^\dagger \quad \dots \quad c_{-\mathbf{k}n_{\text{orb}}\downarrow}^\dagger)^T \quad (2.49)$$

with the so-called Bogoliubov-de Gennes (BdG) matrix

$$H_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H_{0,\downarrow}^*(-\mathbf{k}) + \mu \end{pmatrix} \quad (2.50)$$

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

$$H_{\text{BdG}} = U_{\mathbf{k}} \epsilon_{\mathbf{k}} U_{\mathbf{k}}^\dagger \quad (2.51)$$

How to include finite momentum, rewrite equations

there are phase factors introduced by the orbital positions

Get the remaining terms here

and

$$H_{\text{MF}} = \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \epsilon_{\mathbf{k}} \gamma_{\mathbf{k}}^{\dagger} \quad (2.52)$$

with quasi-particle operators

$$\gamma_{\mathbf{k}} = U_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \quad (2.53)$$

Using the gap equation

$$\Delta_{\alpha} = -U \quad (2.54)$$

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.

Write inde-  
gap equation  
where with-  
out comma

SC current in  
BCS

## 2.3 Dynamical Mean-Field Theory

The foundational idea of Dynamical Mean Field Theory (DMFT) is to map the full interacting problem to the problem of a single lattice site (or a small cluster of lattice sites) embedded in a mean field

as seen in fig. 2.3.

This

DMFT has

This section describes the method of Green's function, which is the language DMFT is formulated in, the mapping of the lattice problem onto the impurity problem and the resulting self-consistency loop of DMFT. Additionally, I will also briefly describe how to describe the superconducting state in terms of Green's function and the consequences for a DMFT implementation. I will not fully derive the equations of DMFT here, for a more (pedagogical) introduction see refs. [16, 18, 47, 48].

What is the  
basic idea of  
DMFT?

What  
has been  
achieved  
with DMFT

### Green's Function Formalism

Green's functions: method to encode influence of many-body effects on propagation of particles in a system. Depending on the context, different kinds of Green's functions are employed. For example, Matsubara Green's functions naturally includes finite temperatures. This is done via a so-called Wick rotation of the time variable  $t$  into imaginary time

$$t \rightarrow -i\tau \quad (2.55)$$

Work over  
the para-  
graph

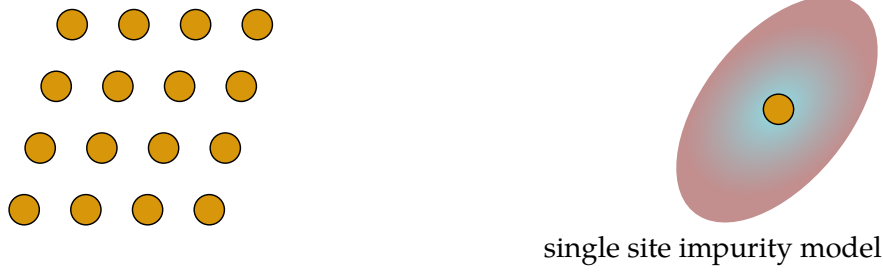


Figure 2.3. AIM mapping

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.

For our context (translationally invariant and systems), Matsubara GF are defined as

$$G(\mathbf{k}, \tau) = -\langle T_\tau(A(\tau)B(0)) \rangle \quad (2.56)$$

with time-ordering operator in imaginary time :

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau - \tau')A(\tau)B(\tau') \pm \Theta(\tau' - \tau)B(\tau')A(\tau) \quad (2.57)$$

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

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

$$-\beta < \tau < \beta \quad (2.58)$$

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

$$G_{AB}(\mathbf{k}, i\omega_n) = \int_0^\beta d\tau \quad (2.59)$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} & \text{for bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{for fermions} \end{cases} \quad (2.60)$$

also time-ordering without Delta

Definition of Matsubara frequencies

Can get the retarded GF  $G_{AB}^R(\omega)$  by analytic continuation:

$$G_{AB}^R(\omega) = G_{AB}(i\omega_n \rightarrow \omega + i\eta) \quad (2.61)$$

Connection to experimental observables

What is the eta there?

## Dyson Equation

Dyson equation:

$$G_{\sigma}(\mathbf{k}, i\omega_n) = \frac{G_{\sigma}^0(\mathbf{k}, i\omega_n)}{1 - G_{\sigma}^0(\mathbf{k}, i\omega_n) \Sigma_{\sigma}(\mathbf{k}, i\omega_n)} = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma_{\sigma}(\mathbf{k}, i\omega_n)} \quad (2.62)$$

Spectral representation of Matsubara and retarded GF

## Anderson Impurity Model

### Nambu-Gorkov Green's Functions

To describe superconductivity,

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\text{loc}}(\tau = 0^-) \quad (2.63)$$

How to get real frequency information from Matsubara GF?

Dyson equation

Self energy

## 2.4 Quantum Metric

First formulated in [49]

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  $|\phi_n(\lambda)\rangle$  at every point in  $\mathcal{M}$

Infinitesimal variation of the parameter  $d\lambda$ :

$$ds^2 = \|\psi(\lambda + d\lambda) - \psi(\lambda)\|^2 = \langle \delta\psi | \delta\psi \rangle = \langle \partial_{\mu}\psi | \partial_{\nu}\psi \rangle d\lambda^{\mu} d\lambda^{\nu} = (\gamma_{\mu\nu} + i\sigma_{\mu\nu}) d\lambda^{\mu} d\lambda^{\nu} \quad (2.64)$$

Last part is splitting up into real and imaginary part

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

DMFT with NG GFs

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

Dont get it here

## Quantum Metric and Superfluid Weight

---

[23]

Write up  
notes about  
quantum  
metric and  
superfluid  
weight

# Dressed Graphene Model

3

This thesis concerned with a specific model. Idea: Graphene with an added orbital on one of the lattice site with a low hopping, as to provide a flat band. I will call this model dressed Graphene from here on. This chapter reviews the lattice structure in section 3.1.

## 3.1 Lattice Structure

There exist a few different ways to define the lattice structure of Graphene which are all equivalent, but intermediate steps in calculating tight-binding models look different depending on the definition. This review on follows ref. [50].

Monolayer graphene forms a honeycomb lattice, which is a hexagonal Bravais lattice with a two atom basis, as can be seen in fig. 3.1a. The primitive lattice vectors of the hexagonal lattice are:

$$\mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \mathbf{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \quad (3.1)$$

with lattice constant  $a = \sqrt{3}a_0 \approx 2.46 \text{ \AA}$ , using the nearest-neighbour distance  $a_0$ . The vectors to the nearest-neighbor atoms  $B_i$  ( $i = 1, 2, 3$ ) from atom  $A$  are and the vectors to the nearest-neighbor atoms  $A_i$  ( $i = 1, 2, 3$ ) from atom  $B$  are The vectors between the Graphene  $A$  atom and the six neighbours on the same sub lattice are:

$$\delta_{AA,1} = \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \delta_{AA,2} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \delta_{AA,3} = a \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad (3.2)$$

$$\delta_{AA,4} = a \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \quad \delta_{AA,5} = a \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad \delta_{AA,6} = a \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \quad (3.3)$$

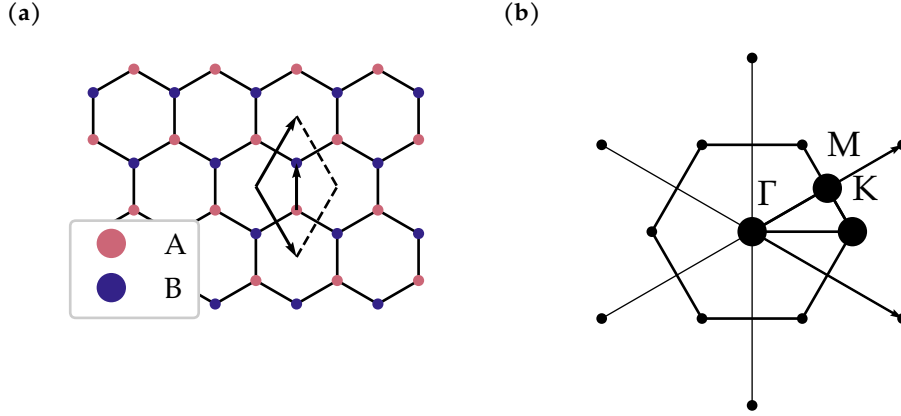
The primitive reciprocal lattice vectors  $\mathbf{b}_1, \mathbf{b}_2$  fulfill

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

Connection with Niklas/Si-heeon paper on dressed Graphene

Labels on vectors

labels on vectors



**Figure 3.1.** (a) Graphene lattice structure and (b) Brilluoin zone

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \quad (3.4)$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0, \quad (3.5)$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \quad (3.6)$$

The first Brilluoin zone of the hexagonal lattice is shown in fig. 3.1b, with the points of high symmetry

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \mathbf{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \mathbf{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (3.7)$$

### 3.2 Dressed Graphene Model

The model I am concerned with in this thesis consists of a Hubbard Hamiltonian (as introduced in section 2.2) on a Graphene lattice, with one additional atom at one of the two sites in a unit cell, which I will call X. This is shown in fig. 3.2. The kinetic term is

Work over  
image for  
dressed  
graphene  
lattice

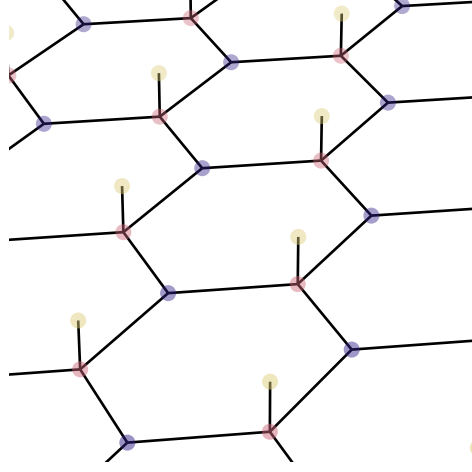


Figure 3.2. Dressed Graphene model

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma} d_{i, \sigma}^\dagger d_{j, \sigma} - t_{Gr} \sum_{\langle ij \rangle, \sigma} c_{i, \sigma}^{(A), \dagger} c_{j, \sigma}^{(B)} + V \sum_{i, \sigma \sigma'} d_{i, \sigma}^\dagger c_{i, \sigma'}^{(A)} + \text{h.c.} \quad (3.8)$$

with

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

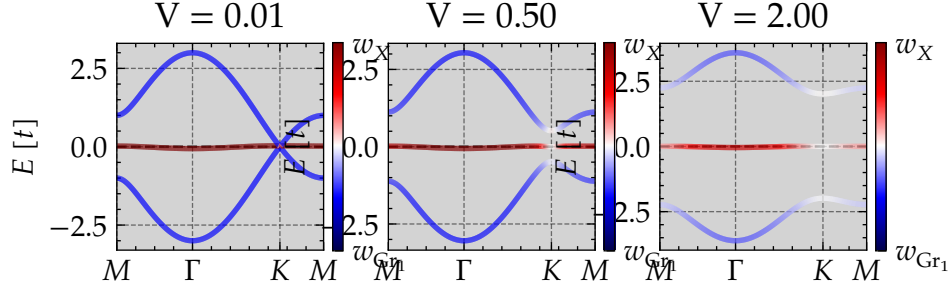
The (attractive) Hubbard interaction has the following form:

$$H_{\text{int}} = -U_X \sum_i d_{i, \uparrow}^\dagger d_{i, \downarrow}^\dagger d_{i, \downarrow} d_{i, \uparrow} - U_{Gr} \sum_{i, \epsilon=A, B} c_{i, \uparrow}^{(\epsilon), \dagger} c_{i, \downarrow}^{(\epsilon), \dagger} c_{i, \downarrow}^\epsilon c_{i, \uparrow}^\epsilon \quad (3.9)$$

The notation using different letters for the sites connects intuitively to the physical picture, but it is more economical and in line with the notation for mean field-theory established in section 2.2 to write the Hamiltonian using a sublattice index

$$\alpha = 1, 2, 3 \quad (3.10)$$





**Figure 3.3.** Bands of the non-interacting dressed Graphene model, with parameters  $t_X = 0 \cdot t_{Gr}$

with  $1 \cong Gr_A$ ,  $2 \cong Gr_B$ ,  $3 \cong X$ . Then we can write the non-interacting term as

$$H_0 = \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta} c_{i\alpha}^\dagger c_{j\beta} \quad (3.11)$$

with the matrix in the sublattice indices

$$\mathbf{t} = \begin{pmatrix} 0 & -t_{Gr} & V\delta_{ij} \\ -t_{Gr} & 0 & 0 \\ V\delta_{ij} & 0 & -t_X \end{pmatrix} \quad (3.12)$$

Also write the interaction part as

$$H_{int} = - \sum_{i\alpha} U_\alpha c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\alpha\downarrow} c_{i\alpha\uparrow} . \quad (3.13)$$

Using the Fourier transformation appendix A

$$H_0 = \sum_{\mathbf{k}, \sigma, \sigma'} \begin{pmatrix} c_{\mathbf{k}, \sigma}^{A, \dagger} & c_{\mathbf{k}, \sigma}^{B, \dagger} & d_{\mathbf{k}, \sigma}^\dagger \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}, \sigma}^A \\ c_{\mathbf{k}, \sigma}^B \\ d_{\mathbf{k}, \sigma} \end{pmatrix} \quad (3.14)$$

Clean up the section from here

The band structure for the non-interacting dressed graphene model is easily obtained by diagonalising the matrix in eq. (3.14). This was done in fig. 3.3.

# Superconducting Length Scales

4

Specifically: take

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

with  $\mathbf{Q}$  such that

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

Explain how to get the length scales in the different ways

# Dressed Graphene Hamiltonian in Reciprocal Space

A

In this chapter, the Hamiltonian

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

from section 3.2 will be treated to obtain the electronic band structure shown in the chapter. 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. For example, for the X atoms this gives:

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

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

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. Now, using 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:

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

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

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

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

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

$$\mathbf{k} \cdot \delta_{AA,1} = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = k_x + \sqrt{3}k_y \quad (\text{A.10})$$

Clear up  
definition  
NN vectors  
and results

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad (\text{A.11})$$

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

$$+ e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \quad (\text{A.13})$$

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

$$= -2t_X \left( \cos(ak_x) + 2 \cos(\frac{a}{2}k_x) \cos(\sqrt{3}\frac{a}{2}k_y) \right). \quad (\text{A.15})$$

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

$$-t_{\text{Gr}} \sum_{\langle ij \rangle, \sigma, \sigma'} c_{i,\sigma}^{(A)\dagger} c_{j,\sigma'}^{(B)} = -t_{\text{Gr}} \sum_{i,\sigma,\sigma'} \sum_{\delta_{AB}} c_{i,\sigma}^{(A)\dagger} c_{i+\delta_{AB},\sigma'}^{(B)} \quad (\text{A.16})$$

$$= -t_{\text{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c_{\mathbf{k},\sigma}^{(A)\dagger} c_{\mathbf{k},\sigma'}^{(B)} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{A.17})$$

with again the sum over  $\delta_{AB}$

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

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

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

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

We note

Show that!

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left( \sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \quad (\text{A.22})$$

All in all:

$$H_0 = \sum_{\mathbf{k}, \sigma, \sigma'} \begin{pmatrix} c_{\mathbf{k}, \sigma}^{A, \dagger} & c_{\mathbf{k}, \sigma}^{B, \dagger} & d_{\mathbf{k}, \sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}, \sigma}^A \\ c_{\mathbf{k}, \sigma}^B \\ d_{\mathbf{k}, \sigma} \end{pmatrix} \quad (\text{A.23})$$

# Notes on the Computational Implementation

B

## BCS code

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

All the data,

For reproducibility, Datalad [51] is used.

The implementation relies on the work of many contributors of packages in Python's ecosystem, most important among them NumPy [52], SciPy [53], Matplotlib [54], Pandas [55, 56] and Parasweep [57].

Data availability

What software for what?

## DMFT

DMFT loop using TRIQS [58]

# Bibliography

- [1] U. of Chicago. *Annual Register*. 1893-1930., 1896. 462 pp. (cit. on p. 1).
- [2] H. K. Onnes. "Further Experiments with Liquid Helium. G. On the Electrical Resistance of Pure Metals, Etc. VI. On the Sudden Change in the Rate at Which the Resistance of Mercury Disappears." In: *Through Measurement to Knowledge: The Selected Papers of Heike Kamerlingh Onnes 1853-1926*. Ed. by K. Gavroglu and Y. Goudaroulis. Dordrecht: Springer Netherlands, 1991, pp. 267-272. ISBN: 978-94-009-2079-8. DOI: 10.1007/978-94-009-2079-8\_17 (cit. on pp. 1, 11).
- [3] W. Meissner and R. Ochsenfeld. "Ein neuer Effekt bei Eintritt der Supraleitfähigkeit". In: *Naturwissenschaften* 21.44 (Nov. 1, 1933), pp. 787-788. ISSN: 1432-1904. DOI: 10.1007/BF01504252 (cit. on p. 1).
- [4] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. "Theory of Superconductivity". In: *Physical Review* 108.5 (Dec. 1, 1957), pp. 1175-1204. DOI: 10.1103/PhysRev.108.1175 (cit. on pp. 1, 11).
- [5] J. G. Bednorz and K. A. Müller. "Possible High Tc Superconductivity in the Ba-La-Cu-O System". In: *Zeitschrift für Physik B Condensed Matter* 64.2 (June 1, 1986), pp. 189-193. ISSN: 1431-584X. DOI: 10.1007/BF01303701 (cit. on p. 1).
- [6] S.-i. Uchida et al. "High Tc Superconductivity of La-Ba-Cu Oxides". In: *Japanese Journal of Applied Physics* 26 (1A Jan. 1, 1987), p. L1. ISSN: 1347-4065. DOI: 10.1143/JJAP.26.L1 (cit. on p. 1).
- [7] D. Rybicki et al. "Perspective on the Phase Diagram of Cuprate High-Temperature Superconductors". In: *Nature Communications* 7.1 (May 6, 2016), p. 11413. ISSN: 2041-1723. DOI: 10.1038/ncomms11413 (cit. on p. 1).
- [8] P. A. Rinck. *Magnetic Resonance in Medicine - A Critical Introduction*. ISBN: 978-628-01-2260-1. URL: <http://www.magnetic-resonance.org/> (cit. on p. 1).

- [9] A. Tollestrup and E. Todesco. “The Development of Superconducting Magnets for Use in Particle Accelerators: From the Tevatron to the LHC”. In: *Reviews of Accelerator Science and Technology* 1.01 (2008), pp. 185–210 (cit. on p. 1).
- [10] L. Rossi. “Particle Accelerators and Cuprate Superconductors”. In: *Physica C: Superconductivity and its Applications* 614 (Nov. 15, 2023), p. 1354360. ISSN: 0921-4534. DOI: 10.1016/j.physc.2023.1354360 (cit. on p. 1).
- [11] K. Irwin and G. Hilton. “Transition-Edge Sensors”. In: *Cryogenic Particle Detection*. Ed. by C. Enss. Berlin, Heidelberg: Springer, 2005, pp. 63–150. ISBN: 978-3-540-31478-3. DOI: 10.1007/10933596\_3 (cit. on p. 1).
- [12] M. I. Faley et al. “High-Tc SQUID Biomagnetometers”. In: *Superconductor Science and Technology* 30.8 (July 2017), p. 083001. ISSN: 0953-2048. DOI: 10.1088/1361-6668/aa73ad (cit. on p. 1).
- [13] A. M. Klushin et al. “Present and Future of High-Temperature Superconductor Quantum-Based Voltage Standards”. In: *IEEE Instrumentation & Measurement Magazine* 23.2 (Apr. 2020), pp. 4–12. ISSN: 1941-0123. DOI: 10.1109/MIM.2020.9062678 (cit. on p. 1).
- [14] B. D. Josephson. “Possible New Effects in Superconductive Tunnelling”. In: *Physics Letters* 1.7 (July 1, 1962), pp. 251–253. ISSN: 0031-9163. DOI: 10.1016/0031-9163(62)91369-0 (cit. on p. 1).
- [15] Y. Cao et al. “Unconventional Superconductivity in Magic-Angle Graphene Superlattices”. In: *Nature* 556.7699 (Apr. 2018), pp. 43–50. ISSN: 1476-4687. DOI: 10.1038/nature26160 (cit. on p. 2).
- [16] P. Coleman. *Introduction to Many-Body Physics*. Cambridge University Press, Nov. 2015. ISBN: 978-0-521-86488-6. DOI: 10.1017/CBO9781139020916 (cit. on pp. 3, 11, 13, 15).
- [17] M. Tinkham. *Introduction to Superconductivity*. 2. ed. International Series in Pure and Applied Physics. New York: McGraw-Hill, 1996. 454 pp. ISBN: 978-0-07-064878-4 (cit. on pp. 3, 11).
- [18] H. Bruus and K. Flensberg. *Many-Body Quantum Theory in Condensed Matter Physics: An Introduction*. Oxford Graduate Texts. Oxford, New York: Oxford University Press, Nov. 11, 2004. 466 pp. ISBN: 978-0-19-856633-5 (cit. on pp. 3, 13, 15).



- 
- [19] A. I. Larkin and A. A. Varlamov. *Theory of Fluctuations in Superconductors*. Oxford Science Publications 127. Oxford Oxford: Clarendon Press Oxford University Press, 2005. ISBN: 978-0-19-852815-9 (cit. on p. 3).
- [20] K. H. Bennemann and J. B. Ketterson, eds. *Superconductivity*. Berlin, Heidelberg: Springer Berlin Heidelberg, 2008. ISBN: 978-3-540-73252-5. DOI: 10.1007/978-3-540-73253-2 (cit. on p. 3).
- [21] A. Beekman, L. Rademaker, and J. van Wezel. “An Introduction to Spontaneous Symmetry Breaking”. In: *SciPost Physics Lecture Notes* (Dec. 4, 2019), p. 011. ISSN: 2590-1990. DOI: 10.21468/SciPostPhysLectNotes.11 (cit. on p. 3).
- [22] N. Witt et al. “Bypassing the Lattice BCS–BEC Crossover in Strongly Correlated Superconductors through Multiorbital Physics”. In: *npj Quantum Materials* 9.1 (Dec. 10, 2024), pp. 1–10. ISSN: 2397-4648. DOI: 10.1038/s41535-024-00706-7 (cit. on pp. 3, 9).
- [23] S. Peotta and P. Törmä. “Superfluidity in Topologically Nontrivial Flat Bands”. In: *Nature Communications* 6.1 (Nov. 20, 2015), p. 8944. ISSN: 2041-1723. DOI: 10.1038/ncomms9944 (cit. on pp. 4, 18).
- [24] J. Yu et al. *Quantum Geometry in Quantum Materials*. Dec. 30, 2024. DOI: 10.48550/arXiv.2501.00098. Pre-published (cit. on p. 4).
- [25] E. Noether. “Invariante Variationsprobleme”. In: *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse* 1918 (1918), pp. 235–257. URL: <https://eudml.org/doc/59024> (visited on 12/10/2024) (cit. on p. 4).
- [26] L. D. Landau. “On the Theory of Phase Transitions”. In: *Zhurnal Eksperimental’noi i Teoreticheskoi Fiziki* 7 (1937). Ed. by D. ter Haar, pp. 19–32. DOI: 10.1016/B978-0-08-010586-4.50034-1 (cit. on p. 4).
- [27] V. L. Ginzburg and L. D. Landau. “On the Theory of Superconductivity”. In: *Zhurnal Eksperimental’noi i Teoreticheskoi Fiziki* 20 (1950). Ed. by D. ter Haar, pp. 1064–1082. DOI: 10.1016/B978-0-08-010586-4.50078-x (cit. on pp. 4, 7).
- [28] Q. Chen et al. “When Superconductivity Crosses over: From BCS to BEC”. In: *Reviews of Modern Physics* 96.2 (May 23, 2024), p. 025002. DOI: 10.1103/RevModPhys.96.025002 (cit. on p. 9).

- 
- [29] A. Q. Chen et al. “Finite Momentum Cooper Pairing in Three-Dimensional Topological Insulator Josephson Junctions”. In: *Nature Communications* 9.1 (Aug. 28, 2018), p. 3478. ISSN: 2041-1723. DOI: 10.1038/s41467-018-05993-w (cit. on p. 9).
- [30] P. Wan et al. “Orbital Fulde–Ferrell–Larkin–Ovchinnikov State in an Ising Superconductor”. In: *Nature* 619.7968 (July 2023), pp. 46–51. ISSN: 1476-4687. DOI: 10.1038/s41586-023-05967-z (cit. on p. 9).
- [31] N. F. Q. Yuan and L. Fu. “Supercurrent Diode Effect and Finite-Momentum Superconductors”. In: *Proceedings of the National Academy of Sciences* 119.15 (Apr. 12, 2022), e2119548119. DOI: 10.1073/pnas.2119548119 (cit. on p. 9).
- [32] J. Bardeen. “Critical Fields and Currents in Superconductors”. In: *Reviews of Modern Physics* 34.4 (Oct. 1, 1962), pp. 667–681. DOI: 10.1103/RevModPhys.34.667 (cit. on p. 11).
- [33] K. Xu, P. Cao, and J. R. Heath. “Achieving the Theoretical Depairing Current Limit in Superconducting Nanomesh Films”. In: *Nano Letters* 10.10 (Oct. 13, 2010), pp. 4206–4210. ISSN: 1530-6984. DOI: 10.1021/nl102584j (cit. on p. 11).
- [34] L. N. Cooper. “Bound Electron Pairs in a Degenerate Fermi Gas”. In: *Physical Review* 104.4 (Nov. 15, 1956), pp. 1189–1190. DOI: 10.1103/PhysRev.104.1189 (cit. on p. 11).
- [35] L. C. Hebel and C. P. Slichter. “Nuclear Relaxation in Superconducting Aluminum”. In: *Physical Review* 107.3 (Aug. 1, 1957), pp. 901–902. DOI: 10.1103/PhysRev.107.901 (cit. on p. 12).
- [36] L. C. Hebel and C. P. Slichter. “Nuclear Spin Relaxation in Normal and Superconducting Aluminum”. In: *Physical Review* 113.6 (Mar. 15, 1959), pp. 1504–1519. DOI: 10.1103/PhysRev.113.1504 (cit. on p. 12).
- [37] I. Giaever and K. Megerle. “Study of Superconductors by Electron Tunneling”. In: *Physical Review* 122.4 (May 15, 1961), pp. 1101–1111. DOI: 10.1103/PhysRev.122.1101 (cit. on p. 12).
- [38] F. London. “A New Conception of Supraconductivity”. In: *Nature* 140.3549 (Nov. 1, 1937), pp. 793–796. ISSN: 1476-4687. DOI: 10.1038/140793a0 (cit. on p. 12).

- [39] X. Zhou et al. “High-Temperature Superconductivity”. In: *Nature Reviews Physics* 3.7 (July 2021), pp. 462–465. ISSN: 2522-5820. DOI: 10.1038/s42254-021-00324-3 (cit. on p. 12).
- [40] J. Hubbard and B. H. Flowers. “Electron Correlations in Narrow Energy Bands”. In: *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* 276.1365 (Nov. 26, 1963), pp. 238–257. DOI: 10.1098/rspa.1963.0204 (cit. on p. 12).
- [41] J. Kanamori. “Electron Correlation and Ferromagnetism of Transition Metals”. In: *Progress of Theoretical Physics* 30.3 (Sept. 1, 1963), pp. 275–289. ISSN: 0033-068X. DOI: 10.1143/PTP.30.275 (cit. on p. 12).
- [42] M. C. Gutzwiller. “Effect of Correlation on the Ferromagnetism of Transition Metals”. In: *Physical Review Letters* 10.5 (Mar. 1, 1963), pp. 159–162. DOI: 10.1103/PhysRevLett.10.159 (cit. on p. 12).
- [43] M. Qin et al. “The Hubbard Model: A Computational Perspective”. In: *Annual Review of Condensed Matter Physics* 13 (Volume 13, 2022 Mar. 10, 2022), pp. 275–302. ISSN: 1947-5454, 1947-5462. DOI: 10.1146/annurev-conmatphys-090921-033948 (cit. on p. 12).
- [44] R. Micnas, J. Ranninger, and S. Robaszkiewicz. “Superconductivity in Narrow-Band Systems with Local Nonretarded Attractive Interactions”. In: *Reviews of Modern Physics* 62.1 (Jan. 1, 1990), pp. 113–171. DOI: 10.1103/RevModPhys.62.113 (cit. on p. 12).
- [45] K.-E. Huhtinen. “Superconductivity and Normal State Properties in Flat Bands”. Aalto University, 2023. URL: <https://aaltodoc.aalto.fi/handle/123456789/119970> (visited on 11/27/2024) (cit. on p. 13).
- [46] J. J. Kinnunen et al. “The Fulde–Ferrell–Larkin–Ovchinnikov State for Ultracold Fermions in Lattice and Harmonic Potentials: A Review”. In: *Reports on Progress in Physics* 81.4 (Feb. 2018), p. 046401. ISSN: 0034-4885. DOI: 10.1088/1361-6633/aaa4ad (cit. on p. 14).
- [47] E. Pavarini et al., eds. *Dynamical Mean-Field Theory of Correlated Electrons*. Schriften Des Forschungszentrums Jülich Reihe Modeling and Simulation Band/volume 12. Jülich: Forschungszentrum Jülich, Zentralbibliothek, Verlag, 2022. 1 p. ISBN: 978-3-95806-619-9 (cit. on p. 15).

- 
- [48] A. Georges et al. “Dynamical Mean-Field Theory of Strongly Correlated Fermion Systems and the Limit of Infinite Dimensions”. In: *Reviews of Modern Physics* 68.1 (Jan. 1, 1996), pp. 13–125. doi: 10.1103/RevModPhys.68.13 (cit. on p. 15).
- [49] J. P. Provost and G. Vallee. “Riemannian Structure on Manifolds of Quantum States”. In: *Communications in Mathematical Physics* 76.3 (Sept. 1, 1980), pp. 289–301. issn: 1432-0916. doi: 10.1007/BF02193559 (cit. on p. 17).
- [50] G. Yang et al. “Structure of Graphene and Its Disorders: A Review”. In: *Science and Technology of Advanced Materials* 19.1 (Aug. 29, 2018), pp. 613–648. issn: 1468-6996. doi: 10.1080/14686996.2018.1494493 (cit. on p. 19).
- [51] Y. O. Halchenko et al. “DataLad: Distributed System for Joint Management of Code, Data, and Their Relationship”. In: *Journal of Open Source Software* 6.63 (July 1, 2021), p. 3262. issn: 2475-9066. doi: 10.21105/joss.03262 (cit. on p. 27).
- [52] C. R. Harris et al. “Array Programming with NumPy”. In: *Nature* 585.7825 (Sept. 2020), pp. 357–362. issn: 1476-4687. doi: 10.1038/s41586-020-2649-2 (cit. on p. 27).
- [53] P. Virtanen et al. “SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python”. In: *Nature Methods* 17.3 (Mar. 2020), pp. 261–272. issn: 1548-7105. doi: 10.1038/s41592-019-0686-2 (cit. on p. 27).
- [54] J. D. Hunter. “Matplotlib: A 2D Graphics Environment”. In: *Computing in Science & Engineering* 9.3 (May 2007), pp. 90–95. issn: 1558-366X. doi: 10.1109/MCSE.2007.55 (cit. on p. 27).
- [55] W. McKinney. “Data Structures for Statistical Computing in Python”. In: *Python in Science Conference*. Austin, Texas, 2010, pp. 56–61. doi: 10.25080/Majora-92bf1922-00a (cit. on p. 27).
- [56] T. pandas development team. *Pandas-Dev/Pandas: Pandas*. Version v2.2.3. Zenodo, Sept. 20, 2024. doi: 10.5281/ZENODO.3509134 (cit. on p. 27).
- [57] E. Bach. “Parasweep: A Template-Based Utility for Generating, Dispatching, and Post-Processing of Parameter Sweeps”. In: *SoftwareX* 13 (Jan. 1, 2021), p. 100631. issn: 2352-7110. doi: 10.1016/j.softx.2020.100631 (cit. on p. 27).

- [58] O. Parcollet et al. “TRIQS: A Toolbox for Research on Interacting Quantum Systems”. In: *Computer Physics Communications* 196 (Nov. 1, 2015), pp. 398–415. issn: 0010-4655. doi: 10.1016/j.cpc.2015.04.023 (cit. on p. 27).

Not cited

- [59] T. Hazra, N. Verma, and M. Randeria. “Bounds on the Superconducting Transition Temperature: Applications to Twisted Bilayer Graphene and Cold Atoms”. In: *Physical Review X* 9.3 (Sept. 17, 2019), p. 031049. doi: 10.1103/PhysRevX.9.031049.

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## List of Abbreviations

<b>BCS</b>	Bardeen-Cooper-Schrieffer 3, 11
<b>DMFT</b>	Dynamical Mean Field Theory 3, 15
<b>BdG</b>	Bogoliubov-de Gennes 14