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Introduction | 1

Quantum Materials

What are quantum materials, connect to SC

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 low energy regime with quantum mechanics and the large and high energy regime 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 know 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 cooper oxide and charge reservoirs in between. The specific charge reservoir layers determine the properties of the SC and varying them lead to a rich zoo of materials with high T_C [7].

Largest commercial application to date is in magnetic resonance imaging, a medical technique using strong magnetic fields and field gradients [8]. Enabled due to the fact, that SCs can carry much stronger currents and thus generate much higher magnetic field strength. Technical applications in research are much wider, ranging from strong superconducting magnets in the LHC [9, 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 Josesphon 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 ξ_0 describing the length scale of amplitude variations of the order parameter and the London penetration depth λ_L, which is connected to energy cost of phase variations of the order parameter. They also connect to the energy gap Δ 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 Ψ which generally can be a complex-valued vector that becomes non-zero below the transition temperature T_C

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

In the example of a ferromagnet, a finite magnetization of a material is associated with a finite expectation value for the z-component of the spin operator, $m_z = \langle \hat{S_z} \rangle$. The order parameter describes the ‘degree of order‘ [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 the microscopic properties of the order parameter, but describes the changes in thermodynamic properties of matter with the development of an order parameter. In superconductivity, the order parameter is described by coherent pairs of electrons with opposite momentum and spin. This will be explained in more detail later, but might be helpful to think of Cooper pairs already when discussing Ginzburg-Landau theory.

Landau and Ginzburg-Landau Theory

The free energy is a thermodynamic quantity:

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

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

$$F_L[\Psi] = \int \mathrm{d}^d x f_L[\Psi] \;, \tag{2.3}$$

where

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

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

$$r = a(T - T_C) \;. \tag{2.5}$$

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

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

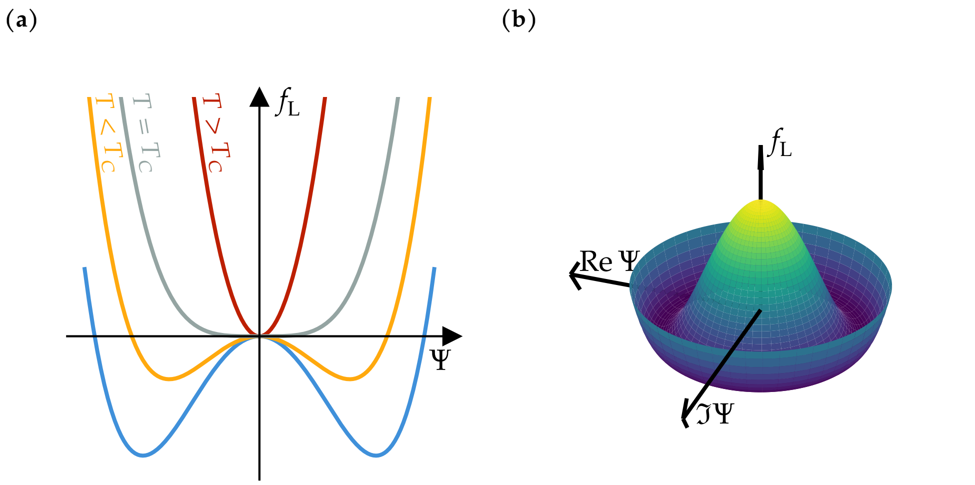

Figure 2.1 – Landau free energy and Mexican hat potential (**a**) Landau free energy f_L for a real-valued order parameter Ψ at different temperatures T. (b) Landau free energy for a complex order parameter Ψ.

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

$$|\Psi|^2 \propto T_C - T\,. \tag{2.7}$$

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

$$\Psi = \Psi_1 + \mathrm{i}\Psi_2 = |\Psi| e^{\mathrm{i}\phi}\,. \tag{2.8}$$

The Landau free energy then takes the form

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

with again

$$r = a(T_C - T)\,. \tag{2.10}$$

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

$$f_L[\Psi] = f_L[e^{\mathrm{i}\phi}\Psi] \ . \tag{2.11}$$

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 Landaus theory of phase transitions [27]. Where Landau theory as described above has an uniform order parameters, Ginzburg-Landau theory accounts for it being inhomogeneous, so an order parameter with spatially varying amplitude or direction. This in turn leads to the order parameter developing a fixed phase, which is the underlying mechanism of the superflow in superconductors.

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

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

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 $\Psi = |\Psi|e^{\mathrm{i}\phi}$, the gradient term reads

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

With that, eq. (2.12) becomes

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

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.

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

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

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 ξ, the physics is entirely controlled by the phase degrees of freedom, i.e.

Work over paragraph

$$\begin{aligned} f_{\mathrm{GL}} &= \frac{\hbar^2}{2m^*}|\Psi|^2(\Delta\phi)^2 + \text{const.} && (2.16)\\ &= \frac{\hbar^2}{4m^*}n_{\mathrm{S}}(\Delta\phi)^2 + \text{const.} && (2.17)\\ &= D_{\mathrm{S}}(\Delta\phi)^2 + \text{const.} && (2.18) \end{aligned}$$

where $\frac{n_{\mathrm{S}}}{2} = |\Psi|^2$ is the density of single electrons that form the Cooper pairs (also called the superfluid/superconducting density). It is derived by looking at the superconducting state as a coherent state, the density n_S describes the average number of particles. A coherent state trades a small uncertainty in particle number for a very high certainty in phase. See for information chapter 14 in ref. [16]. So see that twisting the phase of the condensate is associated with an energy cost. This energy cost is characterized by the superfluid phase stiffness D_{S}.

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

$$|\Psi| = |\Psi_0|\sqrt{1 - \xi^2|\Delta\phi(\mathbf{r})|^2} \tag{2.19}$$

This shows that the superconducting order gets suppressed and eventually destroyed by short-ranged (below ξ) 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 ξ.

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

$$f_{\mathrm{GL}}[\Psi, \mathbf{A}] = \frac{\hbar^2}{2m^*}\left|\left(\Delta - \frac{\mathrm{i}e^*}{\hbar}\mathbf{A}\right)\Psi\right|^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \tag{2.20}$$

Describes really two intertwined Ginzburg-Landau theories for Ψ and $\mathbf{A}$ respectively. This mean there are two length scales, the coherence length ξ governing amplitude fluctuations of Ψ and the London penetration depth λ_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 $\mathbf{A}$:

$$\frac{\delta f_{\mathrm{GL}}}{\delta \mathbf{A}} = 0 = -\mathbf{j} + \frac{1}{\mu_0}\nabla \times \mathbf{B} \tag{2.21}$$

with the supercurrent density

$$\mathbf{j} = -\mathrm{i}\frac{e\hbar}{m^*}\left(\Psi^*\,\Delta\Psi - \Psi\,\Delta\Psi^*\right) - \frac{4e^2}{m^*}|\Psi|^2\mathbf{A}\,. \tag{2.22}$$

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

$$\mathbf{j} = 2e|\Psi|^2\frac{\hbar}{m^*}\left(\nabla\phi - \frac{2\pi}{\Phi_0}\mathbf{A}\right) \tag{2.23}$$

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. The equation can be gauge-transformed to

$$\mathbf{j} = -\frac{4e^2 n_S}{m^*}\mathbf{A} = \tilde{D_S}\mathbf{A} \tag{2.24}$$

which shows that the superfluid phase stiffness

$$D_S = \frac{\hbar^2}{(2e)^2}\tilde{D_S} \tag{2.25}$$

also encodes the linear response of a system to a small applied vector field $\mathbf{A}$.

Connection of SF weight and London penetration depth

Rewriting using $|\Psi|^2 = n_S/2$ and introducing the superfluid velocity $\mathbf{v}_S$:

$$\mathbf{j} = en_S\mathbf{v}_S \tag{2.26}$$

where even for $\mathbf{A} = 0$, there is finite current because of the phase twist of the condensate ground state (which is quite remarkable).

Section about BCS-BEC crossover? Can especially talk about what is optimised!

Superconducting Length Scales

Write introduction better

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 and mobile, while for a stronger interaction the pairs are bound together stronger and are not mobile, because hopping of a pair would involve a virtual hopping, thus breaking up the pair. This is highly suppressed. The crossover region between these two regimes is the BCS-BEC crossover. The energy scales characterizing the crossover are the superconducting gap/order parameter describing how strong the order is and the superfluid weight describing how mobile the Cooper pairs are. These two energy scales are equivalently defined via the coherence length ξ_0 and the London penetration depth introduced in section 2.1. To understand the physics of the BCS-BEC crossover and eventually use it to optimize current and future superconductors it is thus imperative to have access to the superconducting length scales in ab initio approaches Witt et al. introduced a framework for doing this [22]. As already discussed in the context of eq. (2.19), strong phase fluctuations destroy superconducting order. A particular choice of phase fluctuations would be

$$\phi(\mathbf{r}) = \mathbf{q} \cdot \mathbf{r} \tag{2.27}$$

which corresponds to Cooper pairs with a finite momentum $\mathbf{q}$. 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 in the paper: enforce FMP states via constraints on pair-center-of-mass momentum $\mathbf{q}$, access characteristic lenght scales ξ_0, λ_L through analysis of the momentum and temperature-dependent OP. FF-type pairing with Cooper pairs carrying finite momentum:

$$\Psi_{\mathbf{q}}(\mathbf{r}) = |\Psi_{\mathbf{q}}| e^{i\mathbf{q}\mathbf{r}} \tag{2.28}$$

Then the free energy density eq. (2.12) is

$$f_{GL}[\Psi_{\mathbf{q}}] = r|\Psi_{\mathbf{q}}|^2 + \frac{u}{2}|\Psi_{\mathbf{q}}|^4 + \frac{\hbar^2 q^2}{2m^*}|\Psi_{\mathbf{q}}|^2 \tag{2.29}$$

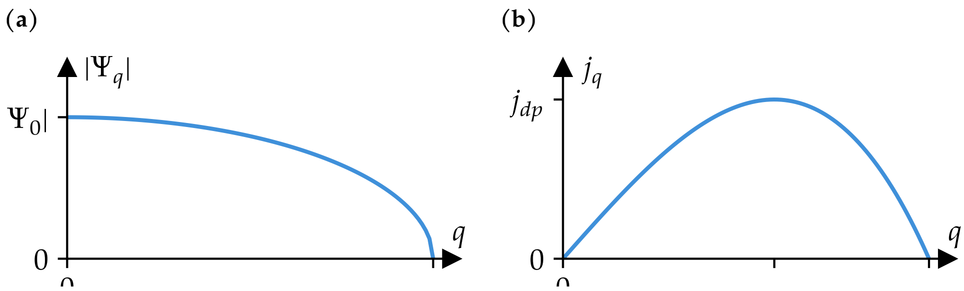

Figure 2.2 – a and b

Stationary point of the system:

$$\frac{\delta f_{GL}}{\delta \Psi^*_{\mathbf{q}}} = 2\Psi_{\mathbf{q}}\left[r(1-\xi^2 q^2) + u|\Psi_{\mathbf{q}}|^2\right] = 0 \tag{2.30}$$

which results in the **q**-dependence of the OP

$$|\Psi_{\mathbf{q}}|^2 = |\Psi_0|^2\left(1-\xi(T)^2 q^2\right) \tag{2.31}$$

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)

$$\xi(T) = \xi_0\left(1-\frac{T}{T_C}\right)^{-\frac{1}{2}} \tag{2.32}$$

The Cooper pair

Depairing current from FMP

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

$$\lambda_L(T) = \sqrt{\frac{\Phi_0}{3\sqrt{3}\pi\mu_0\xi(T)j_{\mathrm{dp}}(T)}} = \lambda_{L,0}\left(1-\left(\frac{T}{T_C}\right)^4\right)^{-\frac{1}{2}} \tag{2.33}$$

The superfluid phase stiffness can then be calculated via

Where does this formula come from? Second London equation

$$D_S \propto \lambda_L^{-2} \tag{2.34}$$

The finite-momentum method in the limit of $\mathbf{q} \to 0$ is related to linear response techniques to calculate the superfluid weight [23, 34].

2.2 Bardeen-Coooper-Schrieffer Theory

The BCS (Bardeen-Cooper-Schrieffer) description of superconductivity describes superconductivity as the condensation of electrons into pairs that form a macroscopic quantum state. 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 (BCS) mean-field theory for the multiband Hubbard model.

Better introduction

BCS Hamiltonian

Work over paragraph

BCS-Hamiltonian:

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{2.35}$$

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

$$\Delta = -\frac{U}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -U \langle c_{-\mathbf{r}=0\downarrow} c_{\mathbf{r}=\mathbf{0}\uparrow} \rangle \simeq U\Psi \,. \tag{2.36}$$

A finite Δ 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 Δ 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. In particular, the model Hamiltonian can be expanded with other types of pairing interactions to give a picture of superconductivity in the cuprates, compare ch. 15 in [16].

BCS theory 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 Gutzweiler [42]. The Hamiltonian of the singleband Hubbard model is

Kinetic term as well

$$H = H_0 + H_{\text{int}} = -t \sum_{\langle ij \rangle} + U \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{2.37}$$

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

Besides

[43]

Some relevance of the repulsive Hubbard model

The Hubbard model in the form of eq. (2.37) 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:

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

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{2.38}$$

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

where α 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. (2.38). Mean-field approximation (here specifically for superconductivity i.e. pairing): operators do not deviate much from their average value, i.e. the deviation operators

there are other combinations, talk about that

$$d_{i,\alpha} = c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} - \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.39}$$

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{2.40}$$

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

deviations with small deltas

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{2.41}$$

$$= -\sum_{i,\alpha} U_\alpha \left(d^\dagger_{i,\alpha} + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \right) \left(e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \tag{2.42}$$

$$= -\sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.43}$$

$$+ \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{2.44}$$

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

$$H_{\text{int}} \approx -\sum_{i,\alpha} U_\alpha \left(d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \tag{2.45}$$

$$= -\sum_{i,\alpha} U_\alpha (c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{2.46}$$

$$- \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{2.47}$$

$$= \sum_{i,\alpha} \left(\Delta_{i,\alpha} c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} + \Delta^*_{i,\alpha} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha} \right) \tag{2.48}$$

with the expectation value

$$\Delta_{i,\alpha} = -U_\alpha \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{2.49}$$

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]:

How to include finite momentum, rewrite equations

$$\Delta_{i,\alpha} = \Delta_\alpha e^{i\mathbf{q}\mathbf{r}_{i\alpha}} \tag{2.50}$$

Using the Fourier transform

$$c_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{i\alpha}} c_{\mathbf{k}\alpha\sigma} \tag{2.51}$$

can write mean-field interaction term as

$$\sum_{i,\alpha} \left(\Delta_{i,\alpha} c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} + \Delta^*_{i,\alpha} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha} \right) \tag{2.52}$$

there are phase factors introduced by the orbital positions

can write

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{2.53}$$

The Hamiltonian in eq. (2.53) can be written as

Get the remaining terms here

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}} \mathbf{C}^\dagger_{\mathbf{k}} H_{\mathrm{BdG}}(\mathbf{k}) \mathbf{C}_{\mathbf{k}} \tag{2.54}$$

$$C_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}1\uparrow} & c_{\mathbf{k}2\uparrow} & \cdots & c_{\mathbf{k}n_{\mathrm{orb}}\uparrow} & c^\dagger_{-\mathbf{k}1\downarrow} & c^\dagger_{-\mathbf{k}2\downarrow} & \cdots & c^\dagger_{-\mathbf{k}n_{\mathrm{orb}}\downarrow} \end{pmatrix}^T \tag{2.55}$$

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

$$H_{\mathrm{BdG}}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H^*_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{2.56}$$

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

$$H_{\mathrm{BdG}} = U_{\mathbf{k}} \epsilon_{\mathbf{k}} U^\dagger_{\mathbf{k}} \tag{2.57}$$

and

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \epsilon_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}} \tag{2.58}$$

with quasi-particle operators

$$\gamma_{\mathbf{k}} = U_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \tag{2.59}$$

Write indeces everywhere without comma

Using the gap equation

gap equation

$$\Delta_{\alpha} = -U \tag{2.60}$$

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 Δ_{α} again, until a converged value is found.

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 encompassing all non-local correlation effects, as seen in fig. 2.3.

This

What is the basic idea of DMFT?

DMFT has

What has been achieved with DMFT

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].

Green's Function Formalism

Work over the paragraph

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 exampple, 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

$$t \to -\mathrm{i}\tau \tag{2.61}$$

where τ is real and has the dimension time. This enables the simultaneous expansion of exponential $e^{-\beta H}$ coming from the thermodynamic average and $e^{-\mathrm{i}Ht}$ coming from the time evolution of operators.

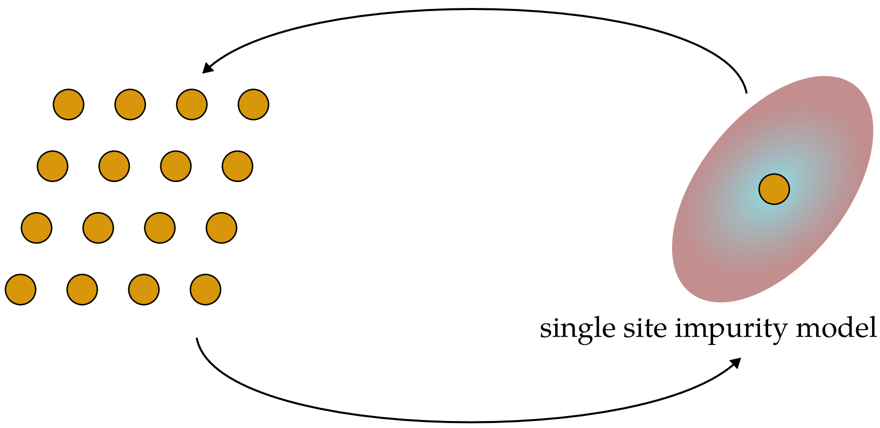

Figure 2.3 – Mapping of the full lattice problem . This also

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

$$G(\mathbf{k}, \tau) = -\langle T_\tau(A(\tau)B(0))\rangle \tag{2.62}$$

with time-ordering operator in imaginary time :

also time-ordering without Delta

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau-\tau')A(\tau)B(\tau') \pm \Theta(\tau'-\tau)B(\tau')A(\tau) \tag{2.63}$$

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

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

$$-\beta < \tau < \beta \tag{2.64}$$

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

Definition of Matsubara frequencies

$$G_{AB}(\mathbf{k}, \mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{2.65}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{2.66}$$

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

Connection to experimental observables

$$G^R_{AB}(\omega) = G_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{2.67}$$

What is the eta there?

Spectral representation of Matsubara and retarded GF

How to get real frequency information from Matsubara GF?

Dyson Equation

Dyson equation:

Dyson equation

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}-\Sigma_\sigma(\mathbf{k},\mathrm{i}\omega_n)}} \tag{2.68}$$

Self energy

Anderson Impurity Model

Nambu-Gorkov Green's Functions

To describe superconductivity,

Order parameter can be chosen as the anomalous GF:

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

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{2.69}$$

DMFT with NG GFs

2.4 Quantum Metric

Topic in quantum materials: quantum geometry and its influence on a many (quantum) material properties [24]. First (?) example: the Integer quantum Hall effect [49] that was explained by Thouless et al. to be a consequence of the unique topology of the ground state of the electron [50].

Concept of quantum geometry first formulated in 1980 by Provost and Vallee [51].

Parameter dependent Hamiltonian $\{H(\lambda)\}$, smooth dependence on parameter $\lambda = (\lambda_1, \lambda_2, \ldots) \in \mathcal{M}$ (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 $\mathrm{d}\lambda$:

Dont get it here

$$\mathrm{d}s^2 = ||\psi(\lambda+\mathrm{d}\lambda) - (\lambda)||^2 = \langle\delta\psi|\,\delta\psi\rangle = \langle\partial_\mu\psi|\,\partial_\nu\psi\rangle\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu = (\gamma_{\mu\nu} + \mathrm{i}\sigma_{\mu\nu})\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu \tag{2.70}$$

Last part is splitting up into real and imaginary part

Recently, the Quantum Geometric Tensor (and in turn the quantum metric) was measured [52].

Quantum Metric and Superfluid Weight

In the context of superconductivity:
[23, 34, 53]

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.

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

Connection with Niklas/Siheeon paper on dressed Graphene

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. [54].

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:

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

with lattice constant $a = \sqrt{3}a_0 \approx 2.46$ Å, 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:

Labels on vectors

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

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

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

labels on vectors

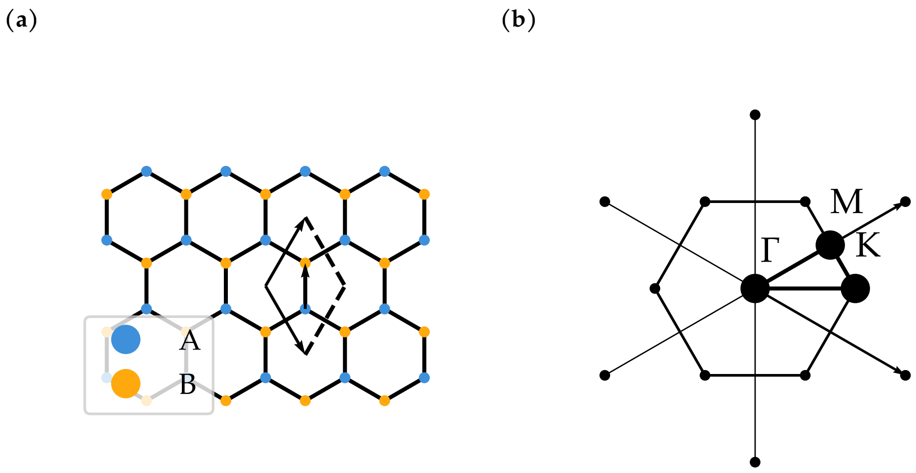

Figure 3.1 – (a) Graphene lattice structure and (b) Brillouin zone

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{3.4}$$
$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{3.5}$$

so we have:

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

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

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \; \mathrm{M} = \frac{\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \; \mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\,. \tag{3.7}$$

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

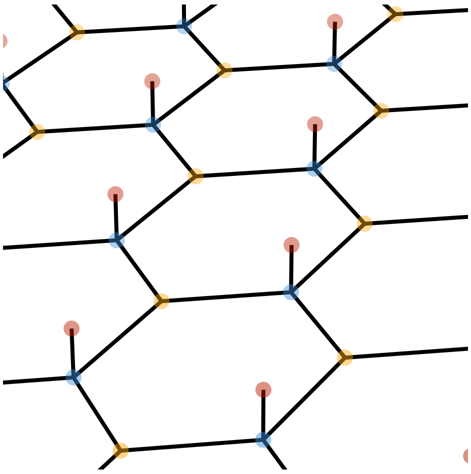

Figure 3.2 – Dressed Graphene model

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

$$H_0 = -t_\mathrm{X} \sum_{\langle ij \rangle, \sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_\mathrm{Gr} \sum_{\langle ij \rangle, \sigma} c^{(\mathrm{A}),\dagger}_{i,\sigma} c^{(\mathrm{B})}_{j,\sigma} + V \sum_{i,\sigma\sigma'} d^\dagger_{i,\sigma} c^{(\mathrm{A})}_{i,\sigma'} + \mathrm{h.c.} \tag{3.8}$$

with

- d - operators on the X atom
- $c^{(\epsilon)}$ - operators on the graphene sites ($\epsilon = \mathrm{A}, \mathrm{B}$)
- 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:

$$H_\mathrm{int} = -U_\mathrm{X} \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} - U_\mathrm{Gr} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{3.9}$$

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

$$\alpha = 1, 2, 3 \tag{3.10}$$

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

$$H_0 = \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{3.11}$$

with the matrix in the sublattice indices

$$\mathbf{t} = \begin{pmatrix} 0 & -t_{\mathrm{Gr}} & V\delta_{ij} \\ -t_{\mathrm{Gr}} & 0 & 0 \\ V\delta_{ij} & 0 & -t_{\mathrm{X}} \end{pmatrix} \tag{3.12}$$

Also write the interaction part as

$$H_{\mathrm{int}} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \,. \tag{3.13}$$

Using the Fourier transformation appendix A

Clean up the section from here

$$H_0 = \sum_{\mathbf{k}, \sigma, \sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^\dagger_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^A_{k,\sigma} \\ c^B_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{3.14}$$

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.

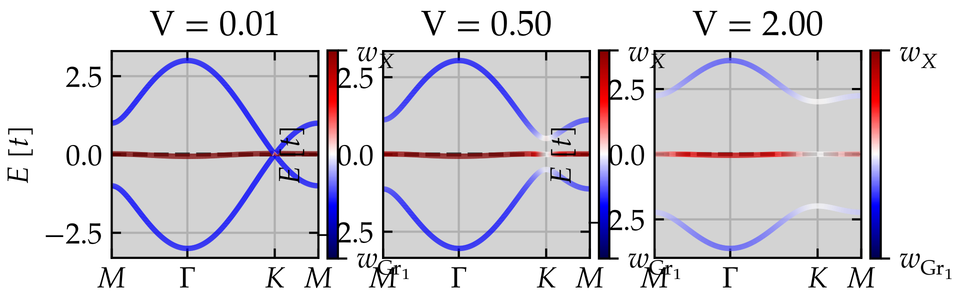

Figure 3.3 – Bands of the non-interacting dressed Graphene model, with parameters $t_X = 0 \cdot t_{\mathrm{Gr}}$

4 Superconducting Length Scales

Explain how to get the length scales in the different ways

Specifically: take

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

with $\mathbf{Q}$ such that

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

A Dressed Graphene Hamiltonian in Reciprocal Space

In this chapter, the Hamiltonian

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

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 $\delta_{\mathrm{X}}, \delta_{\epsilon}$ $(\epsilon = A, B)$ for the vectors to the nearest neighbors of the X atoms and Graphene A, B sites. For example, for the X atoms this gives:

$$-t_{\mathrm{X}} \sum_{\langle ij \rangle,\sigma} (d^{\dagger}_{i,\sigma} d_{j,\sigma} + d^{\dagger}_{j,\sigma} d_{i,\sigma}) = -\frac{t_{\mathrm{X}}}{2} \sum_{i,\delta_{\mathrm{X}},\sigma} d^{\dagger}_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma} - \frac{t_{\mathrm{X}}}{2} \sum_{j,\delta_{\mathrm{X}},\sigma} d^{\dagger}_{j,\sigma} d_{j+\delta_{\mathrm{X}},\sigma} \tag{A.2}$$

$$= -t_{\mathrm{X}} \sum_{i,\sigma} \sum_{\delta_{\mathrm{X}}} d^{\dagger}_{i,\sigma} d_{i+\delta_{\mathrm{X}},\sigma} \quad . \tag{A.3}$$

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

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

with the completeness relation

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

eq. (A.3) reads:

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

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

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

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

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

Clear up definition NN vectors and results

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

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

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

$$\left. + e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \tag{A.13}$$

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

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

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

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

$$= -t_{\mathrm{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{A.17}$$

with again the sum over δ_{AB}

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

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

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

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

We note Show that!

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

All in all:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{\mathbf{k},\sigma} & c^{B,\dagger}_{\mathbf{k},\sigma} & d^{\dagger}_{\mathbf{k},\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{\mathbf{k},\sigma} \\ c^{B}_{\mathbf{k},\sigma} \\ d_{\mathbf{k},\sigma} \end{pmatrix} \tag{A.23}$$

B Notes on the Computational Implementation

BCS code

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

All the data,

For reproducibility, Datalad [55] is used.

The implementation relies on the work of many contributors of packages in Pythons ecosystem, most important among them NumPy [56], SciPy [57], Matplotlib [58], Pandas [59, 60] and Parasweep [61].

Data availability

What software for what?

DMFT

DMFT loop using TRIQS [62]

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