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I Introduction

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

What to put in introduction?

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

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

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

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

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

II Superconductivity

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

Macroscopially, the superconducting state can be described by a spontaneous breaking of a $U(1)$ phase rotation symmetry that is associated with an order parameter. Theory of spontaneous symmetry breaking and associated phase transitions is Ginzburg-Landau theory discussed in section II.1.

Talk about finite q specifically!

Ginzburg Landau theory is not a macroscopic theory, but it can be connected to microscopic theories: if a theory finds an expression for the order parameter describing the symmetry breakdown, it can be connected to quantities expressed by Ginzburg-Landau theory, such as the superconducting current. One such theory to describe superconductivity from a microscopic perspective is Bardeen-Cooper-Schrieffer (BCS) theory in section II.2.

A method to treat local interactions non-perturbatively is Dynamical Mean Field Theory (DMFT). Section II.3 briefly introduces the Greens function method to treat many-body problems and outlines the DMFT self-consistency cycle.

II.1 Ginzburg-Landau Theory of Superconductivity

This review partially follows the introduction given in refs. [15, 20].

Sponteneous Symmetry Breaking Symmetries are a powerful concept in physics. Noethers theorem [21] 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 Sponteneous Symmetry Breaking (SSB) 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.

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

$$|\Psi| = \begin{cases} 0 & T > T_C \\ |\Psi_0| > 0 & T < T_C \end{cases} . \tag{II.1}$$

In the example of a ferromagnet, a finite measurable magnetization of a material is associated with a finite expectation value for the z-component of the spin operator, $m_z = \langle \hat{S}_z \rangle$. This [22]

Work over paragraph

Similarly to a magnetically ordered state, the SC state is characterized by [23]

Order parameters from observables -> in contrast to microscopic OP

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

It does not need microscopic expression for order parameter, it provides corse-grained description of the properties of matter. The order parameter description is good at length scales above ξ_0, the coherence length (e.g. size of Cooper pairs for SC). On length scales above ξ_0, the order parameter behaves as a smoothly varying function.

Work over paragraph

Landau theory

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

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

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

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

Minimum of free energy occurs for:

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

Make graphic for Landau free energy

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

Make graphic for Landau OP and BCS OP

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

$$\psi = \psi_1 + \mathrm{i}\psi_2 = |\psi|e^{\mathrm{i}\phi} \tag{II.5}$$

The Landau free energy takes the form:

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

As before:

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

Figure II.1 shows the Landau free energy as function of ψ.

Make my own graphic for mexican hat potential

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

$$f[\psi] = f[e^{\mathrm{i}a}\psi] \tag{II.8}$$

In this 'Mexican hat' potential: order parameter can be rotated continuously from one broken-symmetry state to another. If we want the phase to be rigid, we need to introduce an There is a topological argument for the fact that the phase is rigid. This leads to Ginzburg-Landau theory. Will see later: well-defined phase is associated with persistent currents or superflow.

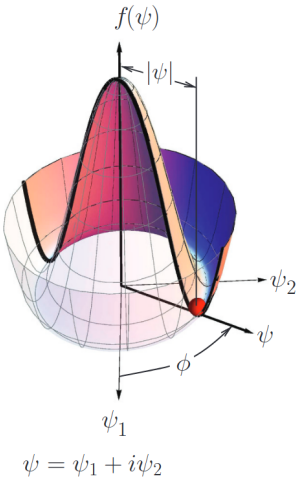

Figure II.1: *Mexican hat potential*

Work over paragraph

Ginzburg-Landau theory

Landau theory: energy cost of a uniform order parameter, more general theory needs to account for inhomogenous order parameters, in which the amplitude varies or direction of order parameter is twisted -> GL theory. First: one-component, 'Ising' order parameter. GL introduces additional energy $\delta f \propto |\Delta\psi|^2, f_{GL}[\psi, \Delta\psi] = \frac{s}{2}|\Delta\psi|^2 + f_L[\psi(s)]$, or in full:

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

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

Symbol for correlation and coherence length

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

sets characteristic length scale of order-parameter fluctuations, where the zero temperature value

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

is the microscopic coherence length ξ_0. Near transition $\xi(T)$ diverges, but far from transition it becomes comparable with the coherence length.

Complex order and superflow

Work over paragraph

Now: GL theory of complex or two-component order parameters, so superfluids and superconductors. Heart of discussion: emergence of a 'macroscopic wavefunction', where the microscopic field operators $\hat{\psi}(x)$ acquire an expectation value:

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

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

Magnitude determines density of particles in the superfluid:

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

Density operator is

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

so expectation value of that is the formula above.

Twist/gradient of phase determines superfluid velocity:

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

We will derive this later in the chapter. Counterintuitive from quantum mechanics: GL suggested that $\Phi(x)$ is a macroscopic manifestation of a macroscopic number of particles condensed into precisely the same quantum state. Emergent phenomenon, collective properties of mater not a-priori evident from microscopic physics.

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

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

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

$$H = \int \mathrm{d}^D x \frac{\hbar^2}{2m}|\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \tag{II.17}$$

Interpret GL free energy as energy density of a condensate of bosons in which the field operator behaves as a complex order parameter. Gives interpretation of gradient term as kinetic energy:

$$s|\Delta\psi|^2 = \frac{\hbar^2}{2m}\langle\Delta\hat{\psi}^\dagger\Delta\hat{\psi}\rangle \implies s = \frac{\hbar^2}{2m} \tag{II.18}$$

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

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

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

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

Freeze out fluctuations in amplitude (no x-dependence in amplitude) $\psi(x) = \sqrt{n_s}e^{i\phi(x)}$, then $\Delta\psi = i\Delta\phi\psi$ and $|\Delta\psi|^2 = n_s(\Delta\phi)^2$, dependency of kinetic energy on the phase twist is (bringing it into the form $\frac{m}{2}v^2$):

$$\frac{\hbar^2 n_s}{2m}(\Delta\phi)^2 = \frac{mn_s}{2}(\frac{\hbar}{m}\Delta\phi)^2 \tag{II.20}$$

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

$$\mathbf{v}_s = \frac{\hbar}{m}\Delta\phi \tag{II.21}$$

(this is explained in detail later).

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

$$\hat{\psi}(x)\,|\psi\rangle = \psi(x)\,|\psi\rangle \tag{II.22}$$

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

Phase rigidity and superflow In GL theory, energy is sensitive to a twist of the phase. Substitute $\psi = |\psi|e^{i\phi}$ into GL free energy, gradient term is:

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

So:

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

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

Phase rigidity and superflow

II.1.1 Superconducting length scales

From [24].

Better introduction

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

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

$$\psi_{\mathbf{q}}(\mathbf{r}) = |\psi_{\mathbf{q}}|e^{i\mathbf{qr}} \tag{II.25}$$

Then the free energy density is

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

Stationary point of the system:

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

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

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

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

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

Specifically: take

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

with $\mathbf{Q}$ such that

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

Depairing current from FMP

Full formula for supercurrent, with sum over orbitals

DS from FMP

Write more about the connection between all the things here

The Cooper pair [25, 26]

II.2 Bardeen-Coooper-Schrieffer Theory

First phenomenological description of SC: Fritz London in 1937 [27]. He was motivated by the discovery of the Meissner effect in 1933 [3], where magnetic flux inside of the superconductor is always pushed out in contrast to a perfectly conducting material, which would hold a 'memory' of the magnetic field at the time of the phase transition. This suggests that transition to the SC state is reversible and a SC is not just the limiting case of a conductor with infinite conductivity, in which according to the Maxwell equations, the magnetic flux would not change. Londons first descriptions is based on a one-particle wave function $\phi(x)$. He proposed that persistent supercurrent is a property of the ground state associated with its rigidity against the application of a field.

In 1950 [23]: GL interpreted this wave function as a complex order parameter as explained in section II.1.

Following [15, ch. 14].

II.2.1 BCS Hamiltonian

Microscopic description of SC: 1957 by John Bardeen, his postdoc Leon Cooper and the graduate in the group, J. Robert Schrieffer [4]. Description is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [28]. The final element in this description was the origin of the attractive interaction $V_{\mathbf{k},\mathbf{k}'}$ between electrons, which Bardeen, Cooper and Schrieffer identified as a retarded electron-phonon interaction [4]. BCS-Hamiltonian:

$$H_{\text{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{II.32}$$

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

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

More about mean field theory in section II.2.2

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.

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 [29, 30] and the band gap measured by Giaever in 1960 [31]. On the other hand, it established electronic pairing as the microscopic mechanism behind SC, which holds still today even for high T_C/unconventional superconductors, so SCs that cannot be described by BCS theory [32].

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

II.2.2 Attractive Hubbard Model

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [33], Kanamori [34] and Gutzweiler [35].

$$H_{\text{int}} = U \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{II.34}$$

where $U > 0$.

Besides

[36]

This simple Hubbard model can be extended in a multitude of ways to model a variety of physical system. In this work: extension to multiple orbitals (i.e. atoms in the unit cell for lattice systems) and an attractive interaction, i.e. a negative U. Physical motivation for taking a negative-U Hubbard model: electrons can experience a local attraction interaction, for example through electrons

Some relevance of the repulsive Hubbard model

coupling with phononic degrees of freedom or with electronic excitations that can be described as bosons [37]. The form of the interaction term is then:

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{II.35}$$

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).

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Order of op
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equations!

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

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

there are other combinations, talk about that

$$d_{i,\alpha} = c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} - \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{II.36}$$

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{II.37}$$

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

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{II.38}$$

$$= -\sum_{i,\alpha} U_\alpha \left(d^\dagger_{i,\alpha} + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \right) \left(e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) \tag{II.39}$$

$$= -\sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{II.40}$$

$$+ \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{II.41}$$

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

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

$$= -\sum_{i,\alpha} U_\alpha (c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \tag{II.43}$$

$$- \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) \tag{II.44}$$

$$= \tag{II.45}$$

with the expectation values

$$\Delta \tag{II.46}$$

General multi-band mean field theory theory

$$H_{\text{int}} \approx \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{II.47}$$

Mean field with finite momentum

Fourier transformation:

$$H_{int} = -\frac{1}{N^2} \sum_{\alpha,\mathbf{k}_{1,2,3,4}} U_\alpha e^{\mathrm{i}(\mathbf{k}_1+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_3) r_{i\alpha}} c^\dagger_{\mathbf{k}_1\alpha\uparrow} c^\dagger_{\mathbf{k}_3\alpha\downarrow} c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \tag{II.48}$$

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

$$H_{int} = -\sum_{\alpha,\mathbf{k},\mathbf{k}'} U_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \tag{II.49}$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{II.50}$$

with

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

$$\Delta^*_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\alpha\uparrow} c^\dagger_{-\mathbf{k}'\alpha\downarrow} \rangle \tag{II.52}$$

This gives the BCS mean field Hamiltonian:

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

Nambu spinor

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c^\dagger_{1,-\mathbf{k}\downarrow} \\ c^\dagger_{2,-\mathbf{k}\downarrow} \\ c^\dagger_{3,-\mathbf{k}\downarrow} \end{pmatrix} \tag{II.54}$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \tag{II.55}$$

with

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

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

Self-consistency Formula for OP using the Bogoliubov operators

$$\Delta_\alpha = -U \tag{II.57}$$

How to solve mean field theory self-consistently

Finite momentum To include finite momentum, take the ansatz of a Fulde-Ferrel (FF) type pairing [38]:

How to include finite momentum

$$\Delta \tag{II.58}$$

II.3 Dynamical Mean-Field Theory (DMFT)

II.3.1 Green's Function Formalism

Work over the paragraph

Following [17]

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

Have different kinds of Green's functions, for example the retarded Green's function:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(t')\}\rangle \tag{II.59}$$

They give the amplitude of a particle inserted at point $\mathbf{r}'$ at time t' to propagate to position $\mathbf{r}$ at time t. For time-independent Hamiltonians and systems in equilibrium, the GFs only depend on time differences:

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

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

$$G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) = -\mathrm{i}\Theta(t)\,\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(0)\}\rangle \tag{II.61}$$

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

$$G^R(\mathbf{k}, \sigma, \sigma' t) = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma'}(0)\}\rangle \tag{II.62}$$

Define Fourier-transform:

$$G^R(\mathbf{k}, \sigma, \sigma', \omega) = \int_{-\infty}^{\infty} \mathrm{d}t G^R(\mathbf{k}, \sigma, \sigma' t) \tag{II.63}$$

Can define the spectral function from this:

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

Looking at the diagonal elements of G^R here. The spectral function can be thought of as the energy resolution of a particle with energy ω. This mean, for non-interacting systems, the spectral function is a delta-function around the single-particle energies:

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

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

Show GFs can be related to observables

Mathematical technique to calculate retarded GFs involves defining GFs on imaginary times τ:

$$t \to -\mathrm{i}\tau \tag{II.66}$$

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.

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

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

with time-ordering operator in imaginary time:

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

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

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

$$-\beta < \tau < \beta \tag{II.69}$$

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

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

with fermionic/bosonic Matsubara frequencies

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

How to resolve ambiguity at borders of integral

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

$$C^R_{AB}(\omega) = C_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{II.72}$$

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

So in particular the extrapolation of the Matsubara GF to zero is proportional to the density of states at the chemical potential. Gapped: density is zero (Matsubara GF goes to 0), metal: density is finite (Matsubara GF goes to finite value) [17, p. 8.3.4].

single-particle Matsubara GF

II.3.2 Perturbation theory, Dyson equation

Short introduction to diagrams

Dyson equation:

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}-\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}} \tag{II.73}$$

Self energy

Dyson equation

II.3.3 Nambu-Gorkov GF

Introduction following [15, ch. 14.7]

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

Order parameter can be chosen as the anomalous GF:

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

or the superconducting gap

$$\Delta = Z\Sigma^{\text{AN}} \tag{II.75}$$

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

Sources for these?

How to get quasiparticle weight?

II.3.4 DMFT

Following [39].

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \tag{II.76}$$

with lattice coordinates i, j and spin σ.

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

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

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

The Dyson equation

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \left(G_0(\mathbf{k}, \mathrm{i}\omega_n) - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)\right)^{-1} \tag{II.78}$$

relates the non-interacting Greens function $G_0(\mathbf{k}, \mathrm{i}\omega_n)$ and the fully-interacting Greens function $G(\mathbf{k}, \mathrm{i}\omega_n)$ (inversion of a matrix!).

III Quantum Metric

First formulated in [40]

Following Cheng - a pedagogical Introduction

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

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

Dont get it here

$$\mathrm{d}s^2 = \||\psi(\lambda+\mathrm{d}\lambda)-(\lambda)\||^2 = \langle\delta\psi|\,\delta\psi\rangle = \langle\partial_\mu\psi|\,\partial_\nu\psi\rangle\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu = (\gamma_{\mu\nu}+\mathrm{i}\sigma_{\mu\nu})\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu \tag{III.1}$$

Last part is splitting up into real and imaginary part

III.1 Quantum Metric and superfluid weight

[41]

Write up notes about quantum metric and superfluid weight

IV Dressed Graphene Model

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

IV.1 Lattice Structure

Structure of honeycomb lattice following [42].

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

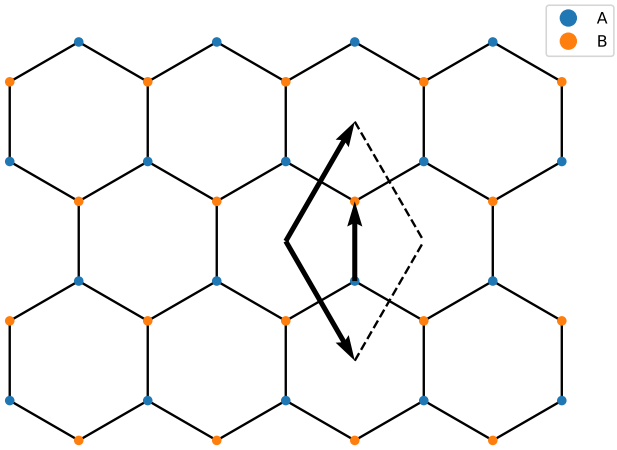

Figure IV.1: *Graphene lattice structure*

Primitive lattice vectors of the hexagonal lattice:

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

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

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

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

with the nearest-neighbour distance a_0.

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

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

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

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

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

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

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

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

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

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

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

First BZ vs this Gamma centered one

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

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

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

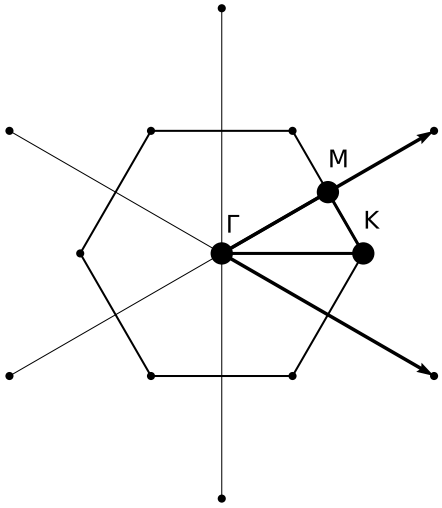

Figure IV.2: *Graphene Brillouin Zone*

so we have:

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

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

Points of high symmetry in the Brillouin zone are:

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

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

$$\mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{IV.18}$$

IV.2 Dressed Graphene Model

Graphene lattice and a site X.

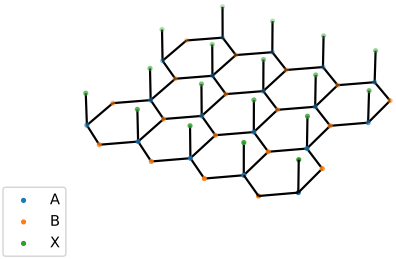

Figure IV.3: *EG-X model*

Without interaction:

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

with:

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

We can also introduce an onsite Hubbard interaction:

$$H_{\mathrm{int}} = U_X \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{\mathrm{Gr}} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{IV.20}$$

Hamilto-
n orbital

Define sublattice index

$$\alpha = 1, 2, 3 \tag{IV.21}$$

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

$$H_0 = -\sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{IV.22}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{IV.23}$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{IV.24}$$

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

$$H_{int} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{IV.25}$$

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^\dagger_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_{\mathrm{X}} \end{pmatrix} \begin{pmatrix} c^A_{k,\sigma} \\ c^B_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{IV.26}$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. (IV.26). This was done in fig. IV.4.

Values used for calculation:

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

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

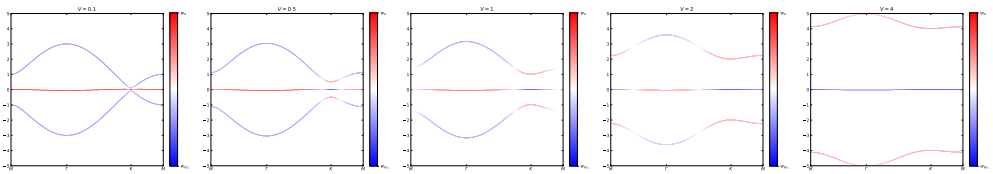

Figure IV.4: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

V Results

Parameter sweeps using [43].

V.1 Gaps

V.2 Superfluid Weight

V.3 Breakdown of SC with finite momentum

V.4 Coherence length etc.

A Dressed Graphene Hamiltonian in Reciprocal Space

Clean up this section

In this chapter, the model Hamiltonian from section IV.2

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

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

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

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

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

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

with the completeness relation

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

eq. (A.3) reads:

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

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

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

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

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

Correct exp expressions

Example for a vector product

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

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

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

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

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

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

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

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

Show that!

We note

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

and calculate

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

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

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

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

All together, we get:

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

B Notes on the Computational Implementation

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

All the data,

For reproducibility, Datalad [44] is used.

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

Data availability

What software for what?

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 p. 1).

[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 pp. 1, 10).

[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, 10).

[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] 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).

[11] 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).

[12] 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).

[13] 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).

[14] 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).

[15] 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, 10, 12, 17).

[16] M. Tinkham. *Introduction to Superconductivity*. 2. ed. International Series in Pure and Applied Physics. New York: McGraw-Hill, 1996. 454 pp. ISBN: 978-0-07-064878-4 978-0-07-114782-8 (cit. on p. 3).

[17] 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, 12, 14, 16).

[18] 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).

[19] K. H. Bennemann and J. B. Ketterson, eds. *Superconductivity*. Berlin, Heidelberg: Springer Berlin Heidelberg, 2008. ISBN: 978-3-540-73252-5 978-3-540-73253-2. DOI: 10.1007/978-3-540-73253-2 (cit. on p. 3).

[20] 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).

[21] 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. 3).

[22] L. D. Landau. "On the Theory of Phase Transitions". In: *Collected Papers of L.D. Landau*. Pergamon, Jan. 1, 1965, pp. 193–216. ISBN: 978-0-08-010586-4. DOI: 10.1016/B978-0-08-010586-4.50034-1 (cit. on p. 4).

[23] L. D. Landau. "On The Theory of Superconductivity". In: *Collected Papers of L.D. Landau*. Ed. by D. Ter haar. Pergamon, Jan. 1, 1965, pp. 546–568. ISBN: 978-0-08-010586-4. DOI: 10.1016/B978-0-08-010586-4.50078-X (cit. on pp. 4, 10).

[24] N. Witt et al. *Bypassing the Lattice BCS-BEC Crossover in Strongly Correlated Superconductors: Resilient Coherence from Multiorbital Physics*. July 11, 2024. DOI: 10.48550/arXiv.2310.09063. Pre-published (cit. on p. 9).

[25] 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. 10).

[26] R. Shimano and N. Tsuji. "Higgs Mode in Superconductors". In: *Annual Review of Condensed Matter Physics* 11 (Volume 11, 2020 Mar. 10, 2020), pp. 103–124. ISSN: 1947-5454, 1947-5462. DOI: 10.1146/annurev-conmatphys-031119-050813 (cit. on p. 10).

[27] 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. 10).

[28] 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. 10).

[29] 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. 11).

[30] 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. 11).

[31] 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. 11).

[32] 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. 11).

[33] 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. 11).

[34] 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. 11).

[35] 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. 11).

[36] 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. 11).

[37] 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).

[38] 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).

[39] 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. 17).

[40] 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. 19).

[41] 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 p. 19).

[42] 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. 21).

[43] 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 pp. 27, 33).

[44] 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. 33).

[45] 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. 33).

[46] 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. 33).

[47] 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. 33).

[48] 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. 33).

[49] T. pandas development team. *Pandas-Dev/Pandas: Pandas*. Version v2.2.3. Zenodo, Sept. 20, 2024. DOI: 10.5281/ZENODO.3509134 (cit. on p. 33).

Not cited

[50] 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.

List of Symbols

Symbol	Meaning	Definition
ξ	Temperature dependent correlation length	6
ξ_0	Coherence length	7
τ	general imaginary time variable	15
$C_{AB}(\tau,0)$	Correlation function in imaginary time	16