I 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. [1–5].

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 I.1. Ginzburg-Landau theory introduces two length scales: the coherence length ξ describing

Section I.1 also introduces the theoretical framework based on introducing a finite momentum for the Cooper pairs [6] that will be used in later chapters to calculate these length scales from microscopic theories.

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 BCS (Bardeen-Cooper-Schrieffer) theory in section I.2.

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

I.1 Ginzburg-Landau Theory of Superconductivity

This review partially follows the introduction given in refs. [1, 7].

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

I.1.1 Sponteneous Symmetry Breaking and Order Parameter

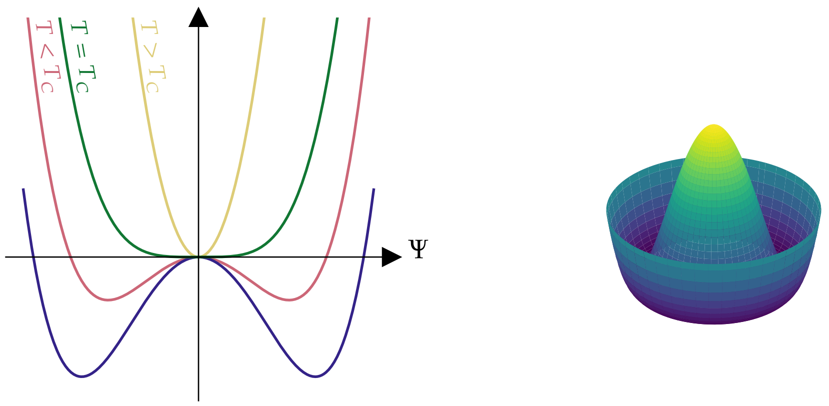
Symmetries are a powerful concept in physics. Noethers theorem [8] connects the symmetries of physical theories to associated conservation laws. An interesting facet of symmetries in physical theories is the fact, that a ground state of a system must not necessarily obey the same symmetries of its Hamiltonian, i.e. for a symmetry operation that is described by a unitary operator U, the Hamiltonian commutes with U (which results in expectation values of the Hamiltonian being invariant under the symmetry operation) but the states $|\phi\rangle$ and $U|\phi\rangle$ are different. This phenomenon is called SSB (Sponteneous Symmetry Breaking) and the state $|\phi\rangle$ is said to be symmetry-broken.

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

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

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

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' [9]. 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 [10]. 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.



(a) (b)

Figure I.1: (*a*) *Landau free energy and* (*b*) *Mexican hat potential*

I.1.2 Landau and Ginzburg-Landau Theory

The free energy is a thermodynamic quantity:

$$F = E - TS \tag{I.2}$$

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:

$$F[\Psi] = \frac{r}{2}\Psi^2 + \frac{u}{4}\Psi^4 \,. \tag{I.3}$$

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

$$r = a(T - T_C) \,. \tag{I.4}$$

Figure I.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

Work over graphic for mexican hat potential two cases for the minima of the free energy F

$$\Psi = \begin{cases} 0 & T \geq T_C \\ \pm\sqrt{\frac{a(T_C-T)}{u}} & T < T_C \end{cases} , \tag{I.5}$$

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

$$|\Psi|^2 \propto T_C - T . \tag{I.6}$$

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

$$\Psi = \Psi_1 + \mathrm{i}\Psi_2 = |\Psi|e^{\mathrm{i}\phi} . \tag{I.7}$$

The Landau free energy then takes the form

$$F[\Psi] = r\Psi^*\Psi + \frac{u}{2}(\Psi^*\Psi)^2 = r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \tag{I.8}$$

with again

$$r = a(T_C - T) . \tag{I.9}$$

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

$$F[\Psi] = f[e^{\mathrm{i}\alpha}\Psi] . \tag{I.10}$$

This gives the so called 'Mexican hat' potential shown in fig. I.1b. In this potential, the order parameter can be rotated continuously from one broken-symmetry state to another.

In 1950, Ginzburg and Landau published their theory of superconductivity based on Landaus theory of phase transitions [10]. Where Landau theory as described above has an uniform order parameters, Ginzburg-Landau theory accounts for it being inhomogeneous, so an order parameter with spatially varying amplitude or direction. This in turn leads to the order parameter developing a fixed phase, which is the underlying mechanism of the superflow in superconductors.

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

$$F_{\mathrm{GL}}[\Psi, \Delta\Psi] = s|\Delta\Psi|^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4 \,, \tag{I.11}$$

where the gradient term $\Delta\Psi$ is added in comparison to Landau energy.

Work over paragraph

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

$$\Delta\psi = (\Delta|\psi| + \mathrm{i}\Delta\phi|\psi|)e^{\mathrm{i}\phi} \tag{I.12}$$

So:

$$f_{GL} = s|\psi|^2(\Delta\phi)^2 + \left[s(\Delta|\psi|)^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4\right] \tag{I.13}$$

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

$$\xi = \sqrt{\frac{s}{|r|}} = \xi_0 \left(1 - \frac{T}{T_C}\right)^{-\frac{1}{2}} \tag{I.14}$$

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

Phase rigidity and superflow

Twist/gradient of phase determines superfluid velocity:

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

We will derive this later in the chapter.

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

$$\frac{\hbar^2 n_s}{2m}(\Delta\phi)^2 = \frac{mn_s}{2}(\frac{\hbar}{m}\Delta\phi)^2 \tag{I.16}$$

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

$$\mathbf{v}_s = \frac{\hbar}{m}\Delta\phi \tag{I.17}$$

Phase rigidity and superflow

I.1.3 Superconducting Length Scales

Better introduction

From [6].

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:

$$\psi_{\mathbf{q}}(\mathbf{r}) = |\psi_{\mathbf{q}}|e^{i\mathbf{q}\mathbf{r}} \tag{I.18}$$

Then the free energy density is

$$f_{GL}[\psi_{\mathbf{q}}] = \alpha|\psi_{\mathbf{q}}|^2 + \frac{b}{2}|\psi_{\mathbf{q}}|^4 + \frac{\hbar^2 q^2}{2m^*}|\psi_{\mathbf{q}}|^2 \tag{I.19}$$

Stationary point of the system:

$$\frac{\delta f_{GL}}{\delta \psi^*_{\mathbf{q}}} = 2\psi_{\mathbf{q}}\left[\alpha(1-\xi^2 q^2) + b|\psi_{\mathbf{q}}|^2\right] = 0 \tag{I.20}$$

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

$$|\psi_{\mathbf{q}}|^2 = |\psi_0|^2(1-\xi(T)^2 q^2) \tag{I.21}$$

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

$$\xi(T) = \xi_0(1-\frac{T}{T_C})^{-\frac{1}{2}} \tag{I.22}$$

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

Make graphic for Landau OP and BCS OP with q

The Cooper pair [11, 12]

I.2 Bardeen-Coooper-Schrieffer Theory

It took nearly 50 years after the first discovery of superconductivity in mercury by Heike Kamerlingh Onnes in 1911 [13] for the first microscopic description of this phenomenon to be published in 1957 by John Bardeen, Leon Cooper and J. Robert Schrieffer [14]. This BCS (Bardeen-Cooper-Schrieffer) theory is one of the great successes in physics history.

The BCS description of superconductivity is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [15]. The origin of the attractive interaction $V_{\mathbf{k},\mathbf{k}'}$, which Bardeen, Cooper and Schrieffer identified as a retarded electron-phonon interaction [14].

There exist many textbooks tackling BCS theory from different angles, such as chapter 14 in refs. [1, 2]. This section gives an introduction to the relevant physics of BCS theory as originally proposed, then derives the

Better introduction

I.2.1 BCS Hamiltonian

Work over paragraph

BCS-Hamiltonian:

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{I.23}$$

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

$$\Delta = -\frac{U}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -U \langle c_{-\mathbf{r}=0\downarrow} c_{\mathbf{r}=\mathbf{0}\uparrow} \rangle \simeq U\Psi\,. \tag{I.24}$$

More about mean field theory in section I.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 [16, 17] and the band gap measured by Giaever in 1960 [18]. 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 [19].

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

I.2.2 Multiband BCS Mean Field Theory

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [20], Kanamori [21] and Gutzweiler [22].

$$H_{\text{int}} = U \sum_{i} c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{I.25}$$

where $U > 0$.

Besides

[23]

Some relevance of the repulsive Hubbard model

This simple Hubbard model can be extended in a multitude of ways to model a variety of physical system. In this work: extension to multiple orbitals (i.e. atoms in the unit cell for lattice systems) and an attractive interaction, i.e. a negative U. Physical motivation for taking a negative-U Hubbard model: electrons can experience a local attraction interaction, for example through electrons coupling with phononic degrees of freedom or with electronic excitations that can be described as bosons [24]. 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

$$H_{\text{int}} = -\sum_{i,\alpha} U_{\alpha} c^{\dagger}_{i,\alpha,\uparrow} c^{\dagger}_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{I.26}$$

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. [1]. The review follows [25]. A more intuitive way based on ref. [3] discussed here looks at the operators and which one are small.

Look at interaction term eq. (I.26). 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

deviations with small deltas

$$d_{i,\alpha} = c^{\dagger}_{i,\alpha,\uparrow} c^{\dagger}_{i,\alpha,\downarrow} - \langle c^{\dagger}_{i,\alpha,\uparrow} c^{\dagger}_{i,\alpha,\downarrow} \rangle \tag{I.27}$$

$$e_{i,\alpha} = c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \tag{I.28}$$

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

$$H_{\text{int}} = -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \tag{I.29}$$

$$= -\sum_{i,\alpha} U_\alpha \left(d^\dagger_{i,\alpha} + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle\right)\left(e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle\right) \tag{I.30}$$

$$= -\sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle \tag{I.31}$$

$$+ \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle) \tag{I.32}$$

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

$$H_{\text{int}} \approx -\sum_{i,\alpha} U_\alpha \left(d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle\right) \tag{I.33}$$

$$= -\sum_{i,\alpha} U_\alpha (c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle + c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle \tag{I.34}$$

$$- \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow}\rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle) \tag{I.35}$$

$$= \sum_{i,\alpha} (\Delta_{i,\alpha} c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} + \Delta^*_{i,\alpha} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} - \frac{|\Delta_{i,\alpha}|^2}{U_\alpha}) \tag{I.36}$$

with the expectation value

$$\Delta_{i,\alpha} = -U_\alpha \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow}\rangle \tag{I.37}$$

which is called the superconducting gap. Using the Fourier transform

$$c_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{i\alpha}} c_{\mathbf{k}\alpha\sigma} \tag{I.38}$$

can write

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

$$H_{\text{MF}} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha,\mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{I.39}$$

To include finite momentum, take the ansatz of a Fulde-Ferrel (FF) type pairing [26]:

How to include finite momentum, rewrite equations

$$\Delta \tag{I.40}$$

The Hamiltonian in eq. (I.39) can be writen as

Get the rem terms here

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}} \mathbf{C}^{\dagger}_{\mathbf{k}} H_{\mathrm{BdG}}(\mathbf{k}) \mathbf{C}_{\mathbf{k}} \tag{I.41}$$

$$C_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}1\uparrow} & c_{\mathbf{k}2\uparrow} & \cdots & c_{\mathbf{k}n_{\mathrm{orb}}\uparrow} & c^{\dagger}_{-\mathbf{k}1\downarrow} & c^{\dagger}_{-\mathbf{k}2\downarrow} & \cdots & c^{\dagger}_{-\mathbf{k}n_{\mathrm{orb}}\downarrow} \end{pmatrix}^{T} \tag{I.42}$$

with the so-called Bogoliubov-de-Gennes matrix

$$H_{\mathrm{BdG}}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^{\dagger} & -H^{*}_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{I.43}$$

General multi-band mean field theory theory

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

Formula for OP using the Bogoliubov operators

$$\Delta_\alpha = -U \tag{I.44}$$

Write indeces everywhere without comma

I.3 Dynamical Mean-Field Theory (DMFT)

How to solve mean field theory self-consistently

I.3.1 Green's Function Formalism

SC current in BCS

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

Following [3]

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

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

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{r}\sigma}(t), c^{\dagger}_{\mathbf{r}\sigma}(t')\}\rangle \tag{I.45}$$

Give an introduction

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:

Work over the paragraph

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t-t') \tag{I.46}$$

Slim down to relevant information

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

$$G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) = -\mathrm{i}\Theta(t)\,\langle\{c_{\mathbf{r}\sigma}(t), c^{\dagger}_{\mathbf{r}\sigma}(0)\}\rangle \tag{I.47}$$

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

$$G^R(\mathbf{k},\sigma,\sigma' t) = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma'}(0)\}\rangle \tag{I.48}$$

Define Fourier-transform:

$$G^R(\mathbf{k},\sigma,\sigma',\omega) = \int_{-\infty}^{\infty} \mathrm{d}t G^R(\mathbf{k},\sigma,\sigma' t) \tag{I.49}$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma,\omega) = -2\Im G^R(\mathbf{k}\sigma,\omega) \tag{I.50}$$

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:

$$A_0(\mathbf{k}\sigma,\omega) = 2\pi\delta(\omega-\epsilon_{\mathbf{k}\sigma}) \tag{I.51}$$

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

Show GFs can be related to observables

Introduction Matsubara GF: finite temperatures

$$t \to -\mathrm{i}\tau \tag{I.52}$$

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 $\mathcal{C}_{AB}(\tau,0)$:

$$\mathcal{C}_{AB}(\tau,0) = -\left\langle T_\tau(A(\tau)B(0))\right\rangle \tag{I.53}$$

with time-ordering operator in imaginary time:

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau-\tau')A(\tau)B(\tau') \pm \Theta(\tau'-\tau)B(\tau')A(\tau) \tag{I.54}$$

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

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

$$-\beta < \tau < \beta \tag{I.55}$$

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

$$\mathcal{C}_{AB}(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{I.56}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{I.57}$$

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:

$$C^R_{AB}(\omega) = C_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{I.58}$$

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

single-particle Matsubara 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) [3, p. 8.3.4].

I.3.2 Self Energy

Short introduction to diagrams

Self energy

Dyson equation

Dyson equation:

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \xi_{\mathbf{k}-\Sigma_\sigma(\mathbf{k},\mathrm{i}\omega_n)}} \tag{I.59}$$

I.3.3 Nambu-Gorkov GF

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

Introduction following [1, ch. 14.7]

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{I.60}$$

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{I.61}$$

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

Sources for these?

How to get quasiparticle weight?

I.3.4 DMFT

Following [27].

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \tag{I.62}$$

with lattice coordinates i, j and spin σ.

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

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)} \tag{I.63}$$

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

The Dyson equation

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \left(G_0(\mathbf{k}, \mathrm{i}\omega_n) - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)\right)^{-1} \tag{I.64}$$

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!).