I Superconductivity

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

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

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

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

There are many textbooks covering these topics which can be referenced for a more detailed treatment, such as refs. [1–4].

I.1 Ginzburg-Landau Theory of Superconductivity

For this review, follow chapter 11 in ref. [1].

More extensive introduction

Order parameter

Work over paragraph

Similarly to a magnetically ordered state, the SC state is characterized by [5, 6]

Introduce spontaneous symmetry breaking

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

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

Intuitive understanding why that is?

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:

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

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:

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

Minimum of free energy occurs for:

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

Make graphic for Landau free energy

Make graphic for Landau OP and BCS OP

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

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

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

The Landau free energy takes the form:

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

As before:

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

Make my own graphic for mexican hat potential

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

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

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

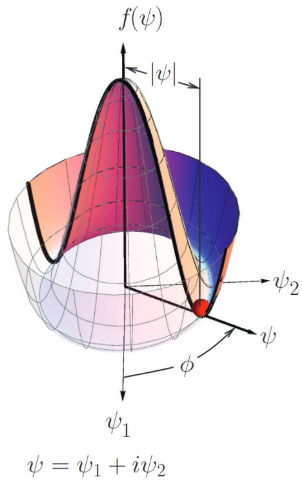

Figure I.1: *Mexican hat potential*

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

Ginzburg-Landau theory

Work over paragraph

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

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

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

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

sets characteristic length scale of order-parameter fluctuations, where

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

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

Work over paragraph

COMPLEX ORDER AND SUPERFLOW

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

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

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:

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

Density operator is

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

so expectation value of that is the formula above.

Twist/gradient of phase determines superfluid velocity:

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

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):

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

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

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

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:

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

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

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

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 $\frac{m}{2}v^2$):

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

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

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

(this is explained in detail later).

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

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

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

Better introduction

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:

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

So:

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

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

I.1.1 Superconducting length scales

From [7].

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:

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

Then the free energy density is

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

Stationary point of the system:

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

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

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

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

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

Specifically: take

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

with **Q** such that

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

The Cooper pair [8, 9]

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

I.2 Bardeen-Coooper-Schrieffer Theory

First phenomenological description of SC: Fritz London in 1937 [10]. He was motivated by the discovery of the Meissner effect in 1933 [11], 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 [6]: GL interpreted this wave function as a complex order parameter as explained in section I.1.

Following [1, ch. 14].

I.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 [12]. Description is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [13]. 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 [12]. BCS-Hamiltonian:

$$H_{\mathrm{BCS}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{I.32}$$

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

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

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. 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: for one in establishing the

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

What is explained by phononic pairing?

I.2.2 Attractive Hubbard Model

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

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [14], Kanamori [15] and Gutzweiler [16].

$$H_{\mathrm{int}} = U \sum_{i} c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{I.34}$$

where $U > 0$.

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Besides
[17]
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 [18]. 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

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

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).

Order of operators? -> also in all other 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. [1]. 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.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

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

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

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

$$\begin{aligned}
H_{\text{int}} &= -\sum_{i,\alpha} U_\alpha c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} && \text{(I.38)} \\
&= -\sum_{i,\alpha} U_\alpha \left(d^\dagger_{i,\alpha} + \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \right) \left(e_{i,\alpha} + \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle \right) && \text{(I.39)} \\
&= -\sum_{i,\alpha} U_\alpha (d_{i,\alpha} e_{i,\alpha} + d_{i,\alpha} \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle + e_{i,\alpha} \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle && \text{(I.40)} \\
&+ \langle c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} \rangle \langle c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \rangle) && \text{(I.41)}
\end{aligned}$$

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

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

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

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

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

with the expectation values

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

General multi-band mean field theory theory

Mean field with finite momentum

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

Fourier transformation:

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

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

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

Mean-field approximation:

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

with

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

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

This gives the BCS mean field Hamiltonian:

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

with Nambu spinor

Nambu spinor

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

we have:

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

with

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

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

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

How to solve mean field theory self-consistently

Finite momentum To include finite momentum, take the ansatz of a Fulde-Ferrel (FF) type pairing [19]:

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

How to include finite momentum

I.3 Dynamical Mean-Field Theory

I.3.1 Green's Function Formalism

Following [3]

Work over the paragraph

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

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

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

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:

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

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

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

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

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

Define Fourier-transform:

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

Can define the spectral function from this:

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

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:

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

Show GFs can be related to observables

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

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

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

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 $C_{AB}(\tau, 0)$:

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

with time-ordering operator in imaginary time:

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

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

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

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

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

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

with fermionic/bosonic Matsubara frequencies

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

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

How to resolve ambiguity at borders of integral

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

So in particular the extrapolation of the Matsubara GF to zero is proportional to the density of states at the chemical potential. Gapped: density is zero (Matsubara GF goes to 0), metal: density is finite (Matsubara GF goes to finite value) [3, p. 8.3.4].

single-particle Matsubara GF

I.3.2 Perturbation theory, Dyson equation

equations of motion for Matsubara GF

Short introduction to diagrams

Self energy

Dyson equation

Dyson equation:

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

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:

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

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{I.75}$$

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 [20].

Most general non-interacting electronic Hamiltonian in second quantization:

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

with lattice coordinates i, j and spin σ.

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

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

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

The Dyson equation

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

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!).