

I SUPERCONDUCTIVITY

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 [1]. 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 [2]. This started almost half a century of intensive theoretical research, which culminated in John Bardeen, Leon Cooper and J. Robert Schrieffer developing the microscopic theory now known as BCS theory [3]. 1986 and 1987: discovery of superconductivity with very high T_C found in cuprates [4, 5]. Cuprate superconductors are made up of layers of copper oxide and charge reservoirs in between. The specific charge reservoir layers determine the properties of the SC and varying them lead to a rich zoo of materials with high T_C [6].

Most current technical applications of superconductors rely on the fact that superconducting wires can carry much higher currents than ordinary wires and thus produce much larger magnetic fields. The largest commercial application to date is in magnetic resonance imaging, a medical technique using strong magnetic fields and field gradients [7]. Technical applications in research are much wider, ranging from strong superconducting magnets in the LHC [8] and other particle accelerators over detectors of single photons in astrophysics [9] to extremely sensitive measurement devices for magnetic fields [10].

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 is in twisted multilayer systems, first realized as twisted bilayer Graphene [11]. 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.

This chapter: introduction to the mean-field BCS theory in section I.3, GL-theory in section I.1 and

I.1 GINZBURG-LANDAU THEORY OF SUPERCONDUCTIVITY

Following [12, ch. 11].

ORDER PARAMETER Landau theory: phase transitions (e.g. iron becomes magnetic, water freezes, superfluidity/superconductivity) are associated with the development of an order parameter when the temperature drops below the transition temperature T_C .

$$|\psi| = \begin{cases} 0, & T > T_C \\ |\psi_0| > 0, & T < T_C \end{cases} \quad (\text{I.1})$$

Landau theory does not need microscopic expression for order parameter, it provides coarse-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.

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:

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

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

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

Minimum of free energy occurs for:

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

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:

$$\psi = \psi_1 + i\psi_2 = |\psi|e^{i\phi} \quad (\text{I.5})$$

The Landau free energy takes the form:

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

As before:

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

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:

$$f[\psi] = f[e^{ia}\psi] \quad (\text{I.8})$$

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.

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

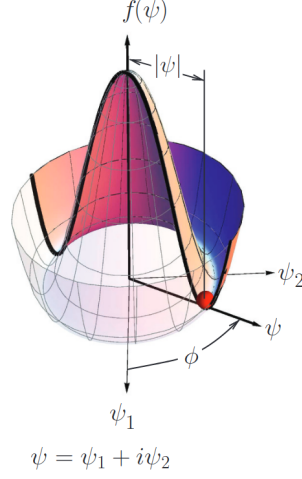


Figure I.1: Mexican hat potential

is twisted \rightarrow 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:

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

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

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

sets characteristic length scale of order-parameter fluctuations, where

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

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

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:

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

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:

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

Density operator is

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

so expectation value of that is the formula above.

Twist/gradient of phase determines superfluid velocity:

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

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 matter not a-priori self-evident from microscopic physics.

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

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

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

$$H = \int d^Dx \frac{\hbar^2}{2m}|\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \quad (\text{I.17})$$

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:

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

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

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

I dont know why that is. Can I support that somehow better?

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

$$\frac{\hbar^2 n_s}{2m} (\Delta\phi)^2 = \frac{mn_s}{2} \left(\frac{\hbar}{m} \Delta\phi\right)^2 \quad (\text{I.20})$$

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

$$\mathbf{v}_s = \frac{\hbar}{m} \Delta\phi \quad (\text{I.21})$$

(this is explained in detail later).

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

$$\hat{\psi}(x) |\psi\rangle = \psi(x) |\psi\rangle \quad (\text{I.22})$$

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 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:

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

So:

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

Phase rigidity and superflow

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

I.2 SUPERCONDUCTING LENGTH SCALES FROM THE CONSTRAINT OF FINITE-MOMENTUM PAIRING

From [13].

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 length scales ξ_0, λ_L through analysis of the momentum and temperature-dependent OP. Constrain for FF-type pairing:

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

Finish up the discussion of Niklas paper

I.3 MEAN-FIELD THEORY OF SUPERCONDUCTIVITY

Clear up nomenclature: BCS theory? BdG theory? Mean field theory?

I.3.1 BCS THEORY

Following [12, ch. 14].

First phenomenological description of SC: Fritz London in 1937 [14]. This description is based on a one-particle wave function $\phi(x)$

Finish up London theory

Microscopic description of SC: 1957 by John Bardeen, his postdoc Leon Cooper and the graduate in the group, J. Robert Schrieffer [3]. Description is based on the fact that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [15]

Better explanation microscopic OP

BCS theory gave a microscopic explanation for the wavefunction used in the phenomenological London theory. Furthermore, it is the order parameter in the developing GL-theory of phase transitions [16]. As explained in section I.1, finite order parameter carry a superflow.

The BCS-Hamiltonian is:

$$H_{BCS} = \quad (\text{I.26})$$

BCS Hamiltonian

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

What is explained by phononic pairing?

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

How can BCS theory be taken as a mean-field theory?

Some relevance of the repulsive Hubbard model

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

Define: what exactly are orbitals in this context?

I.3.2 MEAN FIELD-THEORY ON THE ATTRACTIVE HUBBARD MODEL

The Hubbard model is the simplest model for interacting electron systems. It goes back to works by Hubbard [17], Kanamori [18] and Gutzweiler [19].

$$H_{\text{int}} = U \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow} c_{i,\uparrow} \quad (\text{I.27})$$

where $U > 0$.

Besides

[20]

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 (on the honeycomb lattice) 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 [21]. The form of the interaction term is then:

$$H_{\text{int}} = -U \sum_{i,\alpha} c_{i,\alpha,\uparrow}^\dagger c_{i,\alpha,\downarrow}^\dagger c_{i,\alpha,\downarrow} c_{i,\alpha,\uparrow} \quad (\text{I.28})$$

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.

MULTI-BAND BCS THEORY ON THE HUBBARD MODEL Fourier transformation:

$$H_{\text{int}} = -\frac{1}{N^2} \sum_{\alpha, \mathbf{k}_1, 2, 3, 4} U_\alpha e^{i(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_3) \cdot \mathbf{r}_{i\alpha}} c_{\mathbf{k}_1\alpha\uparrow}^\dagger c_{\mathbf{k}_3\alpha\downarrow}^\dagger c_{\mathbf{k}_2\alpha\downarrow} c_{\mathbf{k}_4\alpha\uparrow} \quad (\text{I.29})$$

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

$$H_{int} = - \sum_{\alpha, \mathbf{k}, \mathbf{k}'} U_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \quad (\text{I.30})$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha, \mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^{*} c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{I.31})$$

with

$$\Delta_{\alpha} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \quad (\text{I.32})$$

$$\Delta_{\alpha}^{*} = -U_{\alpha} \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\alpha\uparrow}^{\dagger} c_{-\mathbf{k}'\alpha\downarrow}^{\dagger} \rangle \quad (\text{I.33})$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c_{\mathbf{k}\alpha\sigma}^{\dagger} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha, \mathbf{k}} (\Delta_{\alpha} c_{\mathbf{k}\alpha\uparrow}^{\dagger} c_{-\mathbf{k}\alpha\downarrow}^{\dagger} + \Delta_{\alpha}^{*} c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (\text{I.34})$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c_{1,-\mathbf{k}\downarrow}^{\dagger} \\ c_{2,-\mathbf{k}\downarrow}^{\dagger} \\ c_{3,-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \quad (\text{I.35})$$

we have:

$$H_{MF} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \quad (\text{I.36})$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^{\dagger} & -H_{0,\downarrow}^{*}(-\mathbf{k}) + \mu \end{pmatrix} \quad (\text{I.37})$$

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

SELF-CONSISTENT SOLUTION

FINITE MOMENTUM

General multi-band
mean field theory
theory

How to solve mean
field theory self-
consistently

How to include fi-
nite momentum