

# Notes on advanced many body physics

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# Preface

These notes are part of the lectures held by Lara Benfatto during the PhD course in advanced many body physics (year 2018), University “Sapienza”, Rome.

Forgive me for any mistake, both grammatical and conceptual, that I may have introduced during the writing.

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# Chapter 1

## Introduction

If we must describe a system with many electrons and several states  $|k\rangle$ , it is convenient to define the creation and annihilation operators:

$$a_k^\dagger \quad a_k \quad (1.1)$$

If the system is composed by fermions (as electrons), these operators satisfy the anti-commutation rule:

$$\{a_k^\dagger, a_{k'}\} = \delta_{kk'} \quad (1.2)$$

If they are bosons we have the commutation rule:

$$[a_k^\dagger, a_{k'}] = \delta_{kk'} \quad (1.3)$$

We want to study the time propagation of the system. To do so it is convenient to split the Hamiltonian into two contributes: the non-interacting  $H_0$  and the interacting  $H_I$ .

$$H = H_0 + H_I \quad H_0 = \sum_k \xi_k a_k^\dagger a_k \quad (1.4)$$

As Eq. (1.4) shows, the non-interacting Hamiltonian is diagonalized by the the creation  $a_k^\dagger$  and annihilation  $a_k$  operators. These respectively destroy and create a particle in the  $|k\rangle$  state. It is possible to define a similar operator that annihilates or creates a particle in the  $\vec{r}$  position:

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_k e^{ikr} a_k \quad (1.5)$$

Thanks to Eq. (1.5) it is possible to redefine a second quantization version of the standard observables. For example, the density, defined as:

$$\rho = |\psi(\vec{r})|^2 \quad (1.6)$$

Can be rewritten in terms of the field operator in Eq. (1.5) as follows:

$$\rho(r) = \psi^\dagger(r)\psi(r) = \frac{1}{\Omega} \sum_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} a_{k'}^\dagger a_k = \frac{1}{\Omega} \sum_q e^{i\vec{q}\cdot\vec{r}} \rho_q \quad (1.7)$$

Any possible operator can be written in terms of creation and annihilation:

$$H_I = \frac{1}{2} \int dr dr' \rho(r) V(r - r') \rho(r') \quad (1.8)$$

This is a generic structure, for example the Coulomb interaction. If we do the same trick we can rewrite it as:

$$H_I = \frac{1}{2\Omega} \sum_q \rho_q^\dagger V(q) \rho_q = \frac{1}{2\Omega} \sum_q V(q) a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k \quad (1.9)$$

So the problem is that the interaction is usually quartic in the creation and annihilation operators, so we cannot solve it analytically. We must use some approximation.

## 1.1 Non interactive Green's functions

It is useful to learn something about the non interactive part of the Hamiltonian. We know exactly the eigenstates of the system:

$$\xi_k = \varepsilon_k - \mu = \frac{k^2}{2m} - \mu \quad (1.10)$$

Where  $\mu$  is the chemical potential, that fixes the Fermi level to zero.

We can introduce the Green's function:

$$G(r, t, r', t') = -i \langle \Phi_0 | T \tilde{\psi}(r, t) \tilde{\psi}(r', t') | \Phi_0 \rangle \quad (1.11)$$

Where  $|\Phi_0\rangle$  is the ground state of the system at  $T = 0$  K. It is the Fermi wavefunction: all the states with  $k < k_f$  are occupied, and for  $k > k_f$  are free. The tilde over the operators identifies the Heisenberg representation, so the time dependence is included in the operator, not in the wavefunction

$$\tilde{\psi}(r, t) = e^{iHt} \psi(r) e^{-iHt} \quad (1.12)$$

We assume that the chemical potential is already included in the Hamiltonian. So let's always assume that

$$H = H_0 - \mu N \quad (1.13)$$

We can always compute the time evolution of the operator in the Heisenberg picture:

$$\frac{\partial O}{\partial t} = [O(t), H] \quad (1.14)$$

This is true also for the interactive Hamiltonian, however we do not know how to solve the problem in that case.

For the moment, we can make the calculation in the momentum space, by computing the Heisenberg picture of the annihilation operator:

$$\tilde{a}_k(t) = e^{iH_0 t} a_k e^{-iH_0 t} \quad (1.15)$$

To compute the time evolution we must apply  $\tilde{a}_k(t)$  to a generic wavefunction  $|\Phi\rangle$ .

$$|\Phi\rangle = |\dots n_k \dots\rangle. \quad (1.16)$$

$$\tilde{a}_k(t) = e^{iH_0 t} a_k e^{-iH_0 t} = e^{it \sum_{k'} \xi_{k'} a_{k'}^\dagger a_{k'}} a_k e^{-it \sum_{k'} \xi_{k'} a_{k'}^\dagger a_{k'}} \quad (1.17)$$

All the terms with  $k \neq k'$  commutes with  $a_k$  so they annihilate each other with the two exponentials. We can compute the action of this on the state

$$\hat{n}_k = a_k^\dagger a_k \quad (1.18)$$

$$\hat{a}_k(t) |\Phi\rangle = e^{it \xi_k \hat{n}_k} a_k e^{-it \hat{n}_k} |\Phi_0\rangle = e^{-it \xi_k n_k} e^{it \xi_k \hat{n}_k} a_k |\dots n_k \dots\rangle \quad (1.19)$$

$$\hat{a}_k(t) |\Phi\rangle = e^{-it \xi_k n_k} e^{it \xi_k \hat{n}_k} |\dots n_k - 1 \dots\rangle = e^{-it \xi_k} |\dots n_k - 1 \dots\rangle \quad (1.20)$$

$$\tilde{a}_k(t) |\Phi\rangle = e^{-it \xi_k} a_k |\Phi\rangle \quad (1.21)$$

Now we have all the ingredients to compute the Greens functions. For  $t > 0$  we have:

$$G(k, t, k, 0) = -i \langle \Phi_0 | T \tilde{a}_k(t) \hat{a}_k^\dagger | \Phi_0 \rangle = -i \theta(k - k_f) \langle \Phi_0 | e^{-it \xi_k} a_k | 1_k \rangle \quad (1.22)$$

$$G(k, t, k, 0) = -i \theta(k - k_f) e^{-it \xi_k} \quad t > 0 \quad (1.23)$$

If I do the same with  $t < 0$  this means that  $k$  must be smaller than  $k_f$  ( we use the time order and we must first destroy the state):

$$G(k, t, k, 0) = i \theta(k_f - k) e^{it \xi_k} \quad t < 0 \quad (1.24)$$

The Green function is only a phase factor in the non interactive system. We can perform the Fourier transform. If  $k > k_f$  we have:

$$G(k, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G(\vec{k}, t) = -i \int_0^{\infty} e^{i\omega t} e^{-it \xi_k} = -i \int_0^{\infty} e^{i(\omega - \xi_k + i0^+) t} \quad (1.25)$$

If  $k > k_f$  then the green function is non zero only if  $t > 0$ . The  $0^+$  is the regularization to make the integral converge. It is possible to solve analytically the last integration.

$$G(k, \omega) = -i \left. \frac{e^{i(\omega - \xi_k + i0^+) t}}{i(\omega - \xi_k + i0^+)} \right|_0^{\infty} = \frac{1}{\omega - \xi_k + i0^+ \text{sign}(k - k_f)} \quad (1.26)$$

We use the sign because, if  $k < k_f$ , we get the same result with a  $-$  sign in the integral regularization factor. The last expression is valid for any  $k$ .

The Green function has singularities in specific positions in the complex plane, as reported in Figure 1.1.

The poles of the greens function represent the eigenstates of the system. What is the meaning of the Green function. We want to know how the states are evolving in time. We computed  $G(k, t)$ :

$$G(k, t) = -i \langle \Phi_0 | \hat{a}_k(t) a_k^\dagger(0) | \Phi_0 \rangle \quad (1.27)$$

Lets try to have an electron in the  $k$  state of the system:

$$a_k^\dagger |\Phi\rangle_0 \quad \Rightarrow \quad |\psi(t)\rangle = e^{-iHt} a_k^\dagger |\Phi\rangle_0 \quad (1.28)$$

Lets define a state that evolves, and then we add the electron:

$$|\psi'(t)\rangle = a_k^\dagger e^{-iHt} |\Phi_0\rangle \quad (1.29)$$



Figure 1.1: Poles of the Green's function in the complex plane.

The Green function is a . Since we have a system that is not interactive, the Green function is only a phase factor, means that the system preserve their coerence: the amplitude does not change. The typical Green function for a interactive system we have something as:

$$G(k, \omega) = \frac{z_k}{\omega - \xi_k + i\gamma_k} + G_{inch} \quad (1.30)$$

We have some spectral width  $z_k < 1$ , we have a non zero immaginary part, and a incoherent part. It is possible to show that when I switch on the interaciton I give finite lifetime to the states, if I look for the difference of the state how was evolving with or without the electron I have a exponential decay of their overlap:

$$G(k, t) \sim e^{-it\xi_k} z_k e^{-\gamma_k t} \quad (1.31)$$

The problem of the many body phiscis, the interaction is important ot determine the spectral weight and the lifetime  $\gamma_k$ .

## 1.2 Interactive Green function

We must introduce the interaction rapresentation. This is convenient when we have an Hamiltonian that can be splitted into a free and a interaction part. The states evolves with a Schrödinger like equation, with the interactive Hamiltonian only  $H_I$ :

$$i \frac{d|\psi_I(t)\rangle}{dt} = H_I(t) |\psi_I(t)\rangle \quad (1.32)$$

$$|\psi_I(t)\rangle = e^{iH_0 t} |\psi_s(t)\rangle = e^{iH_0 t} e^{-iH t} |\psi(0)\rangle \quad (1.33)$$

We have a evolution operator that is

$$U(t) = e^{iH_0 t} e^{-iH t} \quad (1.34)$$

The two Hamiltonians do not commute. We can define an operator  $S$  that evolves the system between time  $t'$  and  $t$ :

$$S(t, t') = U(t)U^\dagger(t') \quad (1.35)$$

$$S(t, t_0) = T \left\{ e^{-i \int_{t_0}^t dt' H_I(t')} \right\} \quad (1.36)$$



The  $T$  is the time ordering operator. We want to write the total green function of the system. What we can demonstrate is that the Green function can be written as:

$$G(r, t, r', t') = -i \frac{\langle \psi_0 | T S \psi(r, t) \psi^\dagger(r', t') | \psi_0 \rangle}{\langle \Phi_0 | S | P h i_0 \rangle} \quad (1.37)$$

Where we write the operator  $\psi$  without the tilde are evolving only with the non interactive hamiltonian.

$$S = S(-\infty, \infty) \quad (1.38)$$

This comes from the adiabatic theory, in which we imagine to turn on the interaction adiabatically from  $t = -\infty$ . In practice we try to make some approximation, depending on the interaction.

$$G^{-1}(k, \omega) = G_0^{-1}(k, \omega) - \Sigma(k, \omega) \quad (1.39)$$

Where we call  $\Sigma$  the self-energy. This is a kind of smooth function, close to the Fermi surface, so we can expand it. We care about the closeness to the Fermi level because only electrons in this states have the possibility to be thermally excited (otherwise they will find all the neighbour energies occupied). The self energy is in general a complex function, that can be divided in real  $\Sigma'$  and imaginary  $\Sigma''$  part:

$$\Sigma(k, \omega) = \Sigma'(k_f, 0) - \frac{\partial \Sigma'}{\partial \omega} \Big|_{\omega=0, k=k_f} \omega - \frac{\partial \Sigma'}{\partial k} \Big|_{k=k_f, \omega=0} (k - k_f) + i \Sigma''(k_f, 0) \quad (1.40)$$

$$G^{-1}(k, \omega) = \omega - \xi_k - \Sigma'(k_f, 0) - \frac{\partial \Sigma'}{\partial \omega} \Big|_{\omega=0, k=k_f} \omega - \frac{\partial \Sigma'}{\partial k} \Big|_{k=k_f, \omega=0} (k - k_f) + i \Sigma''(k_f, 0) \quad (1.41)$$

We can expand also the bare expression near to the fermi level:

$$\xi_k = \varepsilon_k - \mu = v_f(k - k_f) - \mu \quad (1.42)$$

$$G^{-1}(k, \omega) = \underbrace{\tilde{\mu}}_{z_k^{-1}} + \left( 1 - \frac{\partial \Sigma'}{\partial \omega} \Big|_{\omega=0, k=k_f} \right) \omega + \left( v_f - \frac{\partial \Sigma'}{\partial k} \Big|_{k=k_f, \omega=0} \right) (k - k_f) + i \Sigma''(k_f, 0) \quad (1.43)$$

Where we define  $\tilde{\mu} = \mu + \Sigma'(k_f, 0)$ . We can collect some terms:

$$G(k, \omega) = \frac{z_k}{\omega - \tilde{v}_f(k - k_f) + i \gamma_k} \quad \tilde{v}_f = \frac{v_f + \partial_k \Sigma'}{1 - \partial_\omega \Sigma} \quad \gamma_k = \frac{\Sigma''}{1 - \partial_\omega \Sigma} \quad (1.44)$$

The momentum dependence of the self energy gives us the modification on the fermi velocity, while the imaginary parts gives us the decoerence  $\gamma$ . For most of the system these approximation works. What it is possible to find out is that  $\gamma_k$  is usually something close to:

$$\gamma_k \sim \frac{(k - k_f)^2}{k_f} \quad (1.45)$$

As one approaches to the Fermi level, the states become well defined. We can call the states quasi-particles, because the decoherence they have in time gets smaller and smaller.

Lets restrict to  $k > k_f$ , in this case  $\gamma_k$  is a positive number:

$$G(k, t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \frac{z_k}{\omega - \tilde{\xi}_k + i\gamma_k} \quad (1.46)$$

We want to compute it for positive times. To perform this integral we can use the complex plane (Figure 1.2).

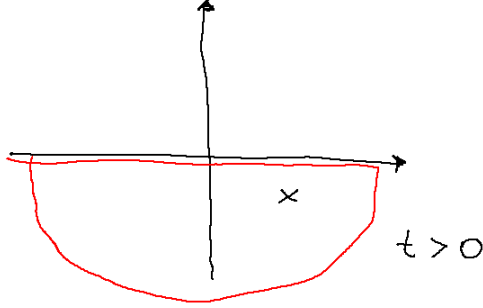


Figure 1.2: Integration path of the complex plane to perform the inverse Fourier transform of the interactive Green function.

We can use the residual theorem:

$$G(k, t) = \frac{1}{2\pi} \left[ 2\pi i z_k e^{-it(\tilde{\xi}_k - i\gamma_k)} \right] = i z_k e^{-it\tilde{x}_k} e^{-t\gamma_k} \quad (1.47)$$

So the real time Green function we have a total spectral width  $z_k$  smaller then 1, and we have a decoherence  $\gamma_k$ . How can we measure experimentally something light this. We usually use light. The typical way is the photoemission. We can define the spectral function as:

$$A(k, \omega) = -\frac{1}{\pi} \Im G_r(\omega, k) \quad (1.48)$$

Where  $G_r$  is the retarded Green function.

$$A(k, \omega) = -\frac{1}{\pi} \Im G_r(\omega, k) = \frac{1}{\pi} \frac{z_k \gamma_k}{(\omega - \hat{\xi}_k)^2 + \gamma_k^2} \quad (1.49)$$

This is a Lorentzian shape. If we take the parabolic system. Imagine to have a parabolic system.

Of course most of the most interesting system now are not fermi liquidis. Very often ARPES experiments can be used to extract the self energy.

### 1.3 Matsubara formalism

We defined the Matsubara function in real time:

$$G(k, \tau) = -\langle T a_k(\tau) a_k^\dagger(0) \rangle \quad (1.50)$$



Figure 1.3: Behaviour of the spectral function as the excitation gets closer to the Fermi surface.

We can compute them in the non interacting case, as done for  $T = 0$ .

$$a_k(\tau) = e^{\tau H_0} a_k e^{-\tau H_0} \quad H_0 = \sum_k \xi_k a_k^\dagger a_k \quad (1.51)$$

We proved that

$$a_k(t) = e^{iHt} a_k e^{-iHt} = e^{i\xi_k t} a_k \quad (1.52)$$

At imaginary time is exactly the same, and we can directly write the result:

$$a_k(\tau) = e^{-\tau \xi_k} a_k \quad (1.53)$$

We can compute explicitly the Green function.

$$G(k, \tau) = -\frac{1}{Z} \text{tr} \left[ e^{-\beta H_0} a_k(\tau) a_k^\dagger(0) \right] \quad \tau > 0 \quad (1.54)$$

$$Z = \text{tr} \left[ e^{-\beta H_0} \right] \quad (1.55)$$

$$G = -e^{-\tau \xi_k} \text{tr} \left[ e^{-\beta H_0} a_k a_k^\dagger \right] = e^{-\tau \xi_k} \text{tr} \left[ \frac{e^{-\beta H_0}}{Z} (1 - a_k^\dagger a_k) \right] \quad (1.56)$$

$$G = -e^{-\tau \xi_k} (1 - \langle n_k \rangle) = -e^{-\tau \xi_k} [1 - f(\xi_k)] \quad (1.57)$$

Where  $f$  is exactly the Fermi function. If we compute the same function for  $\tau < 0$  we get:

$$G(k, \tau) = e^{-\tau \xi_k} f(\xi_k) \quad (1.58)$$

We can compute the Fourier transform of the Matzubara function:

$$G(k, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G(k, \tau) = - \int_0^\beta d\tau e^{-\tau \xi_k} e^{-i\omega_n \tau} [1 - f(\xi_k)] = - [1 - f(\xi_k)] \frac{e^{(i\omega_n - \xi_k)\tau}}{i\omega_n - \xi_k} \Big|_0^\beta \quad (1.59)$$

Remember as  $\omega_n$  is defined for fermionic functions

$$G(k, i\omega_n) = \frac{[1 - f(\xi_k)] (e^{-\xi_k \beta} - 1)}{i\omega_n - \xi_k} = \frac{1}{1\omega_n - \xi_k} \quad (1.60)$$

It is possible to introduce the retarded Green's function, that has always the points in one points:

$$G_{ret}(k, \omega) = \frac{1}{\omega - \xi_k + i0^+ \text{sign}(k - k_f)} = G(k, i\omega_n \rightarrow \omega + i0^+) \quad (1.61)$$

In practice we will always use the finite temperature formalism, because it is possible to derive very easily the zero temperature.

## 1.4 Response functions

We will introduce three different correlation functions. One is the product of two operator averaged:

$$S(t) = \langle A(t)A(0) \rangle \quad S(\omega) \quad (1.62)$$

$$\chi(t) = i\theta(t) \langle [A(t), A(0)] \rangle \quad \chi(\omega) \quad (1.63)$$

$$\chi(\tau) = \langle A(\tau)a(0) \rangle \quad \chi(i\omega_n) \quad (1.64)$$

The  $S$  wavefunction is the fluctuation, it can be related with the cross section, while  $\chi$  is connected with dissipation.

$$S(\omega) = 2\hbar(1 + n_b(\omega))\chi'(\omega) \quad (1.65)$$

We can do the linear response theory. If I put a perturbation in the system  $h(t)A$ , how does the system respond?

$$H_t = H - h(t)A \quad \langle A \rangle(t) = \int_{-\infty}^t \chi(t-t')h(t') \quad (1.66)$$

The interesting thing is that one can always do the calculation in the Matsubara frequencies, and then we can make the analytical continuation:

$$\chi(\omega) = \chi(i\omega_n \rightarrow \omega + 0^+) \quad (1.67)$$

We will write explicitly the three function and see how this holds. Why if a scattering experiment is connected with the fluctuation of the operator? Imagine that you want to probe the system:

$$H = H_s + H_{sp} \quad (1.68)$$

We can image that  $H_{sp}$  is a coupling Hamiltonian.

$$H_{sp} = gA_sA_p \quad (1.69)$$

where  $g$  is the coupling constant,  $A_s$  connected with the system, and  $A_p$  connected with the probe. The initial system will be a product of the system and the probe:

$$|i\rangle = |p_i\rangle |s_i\rangle \quad |f\rangle = |p_f\rangle |s_f\rangle \quad (1.70)$$

We can use the fermi golden rules. The matrix element is:

$$P_{i \rightarrow f} = \frac{2\pi}{\hbar} |V_{fi}|^w \delta(E_f - E_i - \omega) \quad (1.71)$$

We assume that we solved the state of the interacting system. We are just looking for the quantities connected with a scattering experiments:

$$V_{fi} = \langle f|H_{ps}|i\rangle = g \langle p_f|A_p|p_i\rangle \langle s_f|A_s|s_i\rangle \quad (1.72)$$

I have to assume that the initial state is a product between states of probe and system, but this is reasonable if they do not interact each other at  $t = -\infty$ .

$$P_{i \rightarrow f} = \frac{2\pi}{\hbar} g^2 |\langle p_f|A_g|p_i\rangle|^2 |\langle s_g|A_s|s_i\rangle|^2 \delta(E_f - E_i - \omega) \quad (1.73)$$

The first matrix element does not depend on the system, so the most interesting quantity is the other matrix element:

$$\sum_f |\langle s_f|A_s|s_i\rangle|^2 \delta(E_f - E_i - \omega) = \frac{1}{2\pi} \int dt e^{i\omega t} e^{-i(E_f - E_i)t} \langle s_i|A_s|s_f\rangle \langle s_f|A_s|s_i\rangle \quad (1.74)$$

We can include the phase factor with the system energy as the time evolution:

$$\int dt e^{i\omega t} \sum_f \langle s_i|e^{iH_s t} A_s e^{-iH_s t}|s_f\rangle \langle s_f|A_s|s_i\rangle \quad (1.75)$$

We have the heisenberg representation, we include the sum over all the final states:

$$\int dt e^{i\omega t} \underbrace{\langle s_i|A(t)A(0)|s_i\rangle}_{S(t)} \quad (1.76)$$

If we are a  $T = 0$  the initial state of the system is the ground state, otherwise we have to sum over all  $s_i$  with the boltzmann factor. Therefore, the cross section of the scattering experiment is related with the correlation of the system

$$\frac{d^2\sigma}{d\Omega d\omega} = \int dt e^{i\omega t} S(t) = S(\omega) \quad (1.77)$$

We can now compute the  $\chi$  function explicitly

$$\chi(t) = i\theta(t) \sum_{nm} e^{-\beta E_m - F} \langle m|e^{iHt} A e^{-iHt}|n\rangle \langle n|A|m\rangle - e^{-\beta(E_m - F)} \langle m|A|n\rangle \langle n|e^{iHt} A e^{-iHt}|m\rangle \quad (1.78)$$

$$\chi(t) = i\theta(t) \sum_{mn} e^{-\beta(E_m - F)} \left[ \langle m|A|n\rangle n|A|m e^{i(E_m - E_n)t} - e^{i(E_n - E_m)t} \langle m|A|n\rangle \langle n|A|m\rangle \right] \quad (1.79)$$

$$\chi(t) = i\theta(t) \sum_{mn} |\langle m|A|n\rangle|^2 e^{\beta F} (e^{-\beta E_m} e^{-\beta E_n}) e^{i(E_m - E_n)t} \quad (1.80)$$

We want to compute the fourier transform. We have to regularize the integral in the upper imaginary plane.

$$\chi(\omega) = \int_{-\infty}^{\infty} \chi(t) r^{i\omega t} \sim \int_0^{\infty} dt e^{i\omega t} e^{i\alpha t} \quad \alpha = E_m - E_n \quad (1.81)$$

To regularize the integral we must write:

$$\chi(\omega) = \lim_{\varepsilon \rightarrow 0^+} \chi(\omega + i\varepsilon) \quad (1.82)$$

$$\chi(\omega) \sim \frac{e^{i\omega\alpha+i0^+}}{i(\omega + \alpha + i0^+)} \Big|_0^\infty = \frac{i}{\omega + \alpha + i\delta} \quad (1.83)$$

If we apply this to the Eq. (1.80) we get:

$$\chi(\omega) = \sum_{mn} e^{\beta F} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\omega + E_m - E_n + i0^+} |\langle m|A|n\rangle|^2 \quad (1.84)$$

If we take the imaginary part:

$$\frac{1}{\omega + i0^+} = P \frac{1}{\omega} - i\pi\delta(\omega) \quad (1.85)$$

$$\chi''(\omega) = \pi \sum_{mn} e^{\beta F} [e^{-\beta E_m} - e^{-\beta E_n}] \delta(\omega + E_m - E_n) |\langle m|A|n\rangle|^2 \quad (1.86)$$

$$\chi''(\omega) = \pi(1 - e^{-\beta\omega}) \sum_{mn} e^{\beta(E_m - F)} \delta(\omega + E_m - E_n) |\langle m|A|n\rangle|^2 \quad (1.87)$$

If you want to dissipate we need to have the energy induce some transition in the system. It is possible to prove that this absorption is related with the fluctuation:

$$S(t) = \langle A(t)A(0) \rangle = \sum_{mn} e^{-\beta(E_m - F)} \langle m|A(t)|n\rangle \langle n|A|0\rangle \quad (1.88)$$

$$S(t) = \sum_{mn} e^{-\beta(E_m - F)} e^{i(E_m - E_n)t} \left| \langle m|A|n\rangle \right|^2 \quad (1.89)$$

$$S(\omega) = \text{int}_{-\infty}^{\infty} S(t) = \sum_{mn} 2\pi e^{-\beta(E_m - F)} |\langle n|A|m\rangle|^2 \delta(\omega + E_m - E_n) \quad (1.90)$$

We get immediatly that:

$$S(\omega) = 2[1 + n_B(\omega)] \chi''(\omega) \quad (1.91)$$

Flucuation of the system are connected to dissipation. This is generically true. Lets prove the last relation. We can compute the real frequency response function with the Matzubara frequencies.

$$\chi(\tau) = \langle T_\tau A(\tau)A(0) \rangle_{\tau>0} = \langle A(\tau)A(0) \rangle = \sum_{nm} e^{-\beta(E_m - F)} \langle m|e^{\tau H} A e^{-\tau H}|n\rangle \langle n|A|m\rangle \quad (1.92)$$

$$\chi(\tau) = \sum_{mn} e^{-\beta(E_m - F)} e^{\tau(E_m - E_n)} |\langle m|A|n\rangle|^2 \quad (1.93)$$

We have the Fourier transform. We use  $\Omega$  for bosonic matzubara frequencies and  $\omega$  for the fermionic frequencies.

$$\int_0^\beta d\tau e^{i\Omega_m \tau} e^{\tau\alpha} = \frac{e^{i\Omega_m \tau} e^{\tau\alpha}}{i\Omega_m + \alpha} \Big|_0^\beta = \frac{e^{\beta\alpha} - 1}{i\Omega_m + \alpha} \quad (1.94)$$

This means that:

$$\chi(\Omega) = \sum_{mn} e^{-\beta(E_m - F)} \frac{e^{\beta(E_m - E_n)} - 1}{i\Omega + E_m - E_n} |\langle m|A|n\rangle|^2 \quad (1.95)$$

$$\chi(\Omega) = \sum_{mn} e^{\beta F} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{i\Omega + E_m - E_n} |\langle m|A|n\rangle|^2 \quad (1.96)$$

It is now pretty clear that:

$$\chi(\omega) = \chi(i\omega_n \rightarrow \omega + 0^+) \quad (1.97)$$

### 1.4.1 Linear response

We can define a new hamiltonaian

$$H_t = H - h(t)A \quad (1.98)$$

We can derive how a third observable  $B$  respond to the system after the perturbation:

$$\langle B \rangle(t) - \langle B \rangle(0) = \int_{-\infty}^t dt' h(t') \chi_{BA}(t-t') \quad (1.99)$$

This function is exactly the one computed so far. Once we have an hamiltonian that is time dependent.

$$\langle B \rangle(t) \stackrel{?}{=} e^{-\beta(H-hA)} B \quad (1.100)$$

$$\langle B \rangle(t = -\infty) = \text{tr} [e^{-\beta H} B] = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n|B|n\rangle \quad (1.101)$$

We hope that we can switch on adiabatically the system. We decouple the statistical weight of the states from the problem.

$$\langle \psi_n(t)|B|\psi_n(t)\rangle \quad i \frac{d|\psi_n(t)\rangle}{dt} = H_t |\psi_n(t)\rangle \quad (1.102)$$

So we do the thermal averages with time evolving vector of the system.

$$\langle B \rangle(t) = \text{tr} [\rho(t)B] \quad (1.103)$$

$$\rho(t) = \sum_n c_n |\psi_n(t)\rangle \langle \psi_n(t)| \quad (1.104)$$

We try to solve this equation. We can show easily that the  $\rho$  matrix satisfy:

$$i\hbar \frac{\partial \rho}{\partial t} = [H_t, \rho] \quad (1.105)$$

We can use linear response theory:

$$\rho = \rho_0 + f(t) \quad \rho_0 = \frac{e^{-\beta H}}{Z} \quad (1.106)$$

So the only time dependent term is  $f(t)$ :

$$i \frac{\partial f}{\partial t} = [H - hA, \rho_0 + f(t)] \quad (1.107)$$

We can compute the commutator:

$$\frac{\partial f}{\partial t} = -h[A, \rho_0] + [H, f(t)] + O(\hbar^2) \quad (1.108)$$

It is possible to solve this equation:

$$f(t) = i \int_{-\infty}^t dt' e^{-iH(t-t')} [A, \rho_0] h(t') e^{iH(t-t')} \quad (1.109)$$

We can get the response function:

$$\langle B \rangle(t) - \langle B \rangle(t) = \text{tr} [f(t)B] = i \int_{-\infty}^t dt' \text{tr} \left[ e^{-iH(t-t')} [A, \rho_0] e^{iH(t-t')} B \right] h(t') \quad (1.110)$$

This is is just:

$$\text{tr} [A\rho B - \rho AB] = \text{tr} [\rho BA - \rho AB] \quad (1.111)$$

$$i \int_{-\infty}^t dt' \text{tr} [\rho_0 [B(t), A(t')] h(t')] = \int_{-\infty}^t dt' \chi_{BA}(t-t') h(t') \quad (1.112)$$

As we have that:

$$\chi_{BA}(t) = i\theta(t) \langle [B(t), A(0)] \rangle \quad (1.113)$$

The response function appears always, and it is the quantity that we want to prove. Usually  $A$  and  $B$  are operators that will be connected with two fermionic operator (bosonic). In ARPES, this is a single particle operator, so it is fermionic. We will look at ARPES more carefully, and then we will look and some typical example like density-density and current-current response. This can be used to derive the drude formula, which is pretty nice.

## 1.4.2 Density bubble

We compute now the density response function. The perturbation is:

$$\int V(x, t) \rho(x, t) dx \quad (1.114)$$

We want to compute the Matsubara response:

$$\chi_{\rho\rho}(x, \tau) = \langle T\sigma(\beta, 0)\psi^\dagger(r, 1\tau)\psi(r, \tau)\psi^\dagger(0, 0)\psi(0, 0) \rangle \quad (1.115)$$

We have to establish what is the quantity we want to compute. This is solve by linear response theory: the correlation function. But can we really compute the correlation function for an interactive system? We must compute  $\sigma$  matrix. For a non interactive system we already know that:

$$\sigma(\beta, 0) = 1 \quad (1.116)$$

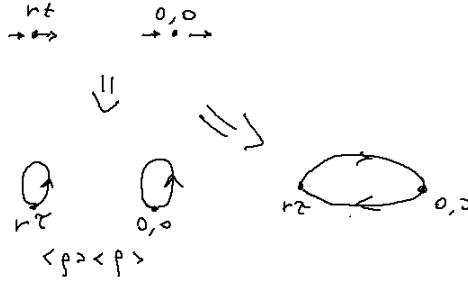
$$\chi_{\rho\rho}^0 = \langle \psi^\dagger(r, \tau)\psi(r, \tau)\psi^\dagger(0, 0)\psi(0, 0) \rangle \quad (1.117)$$

The Wick's theorem tells us that we have two vertex in  $r\tau$  and  $0, 0$ ). We have a creation and annihilation. We want to decompose this product into products of one body operators (that are the Green's functions).

$$G(r, \tau) = -\langle T\psi(r, \tau)\psi^\dagger(0, 0) \rangle \quad (1.118)$$

We have two possible contractions:





The only contraction that matters is:

$$\chi_{\rho\rho}^0 = -G(r, \tau)G(-r, -\tau) \quad (1.119)$$

Now we want to transform this quantity in Matsubara space. We can perform the Fourier transform:

$$\chi_{\rho\rho}(q, i\Omega_m) = - \int dr \int d\tau e^{-i\vec{q}\cdot\vec{r}} e^{i\Omega_m\tau} G(r, \tau)G(-r, -\tau) \quad (1.120)$$

We Fourier Transform the Green's functions:

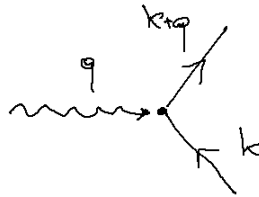
$$\chi_{\rho\rho}(q, i\Omega_m) = \int d^4x e^{-i\vec{q}\cdot\vec{x}} \sum_{kk'} G(k)G(k') e^{ikx} e^{-ik'x} \quad (1.121)$$

The integral over the  $x$  variable gives the usual conservation over the 4-momentum:

$$-q + k - k' = 0 \quad (1.122)$$

$$\chi_{\rho\rho}^0(q, i\Omega_m) = - \sum_k G(k)G(k+q) \quad (1.123)$$

When we must do the calculation in real life, we always use the momentum space. Doing the Fourier transform we have only to take care on the momentum.



In the interactive terms, this bubble is decorated with the interaction. We now compute the bare function, the leading term in the perturbation theory. We can now do the analytical continuation:

$$\chi_{\rho\rho}^0(i\Omega_m, q) = -\frac{T}{\Omega} \sum_{k, i\omega_n} G(ik, i\omega_m)G(kq, i\omega_n + i\Omega_m) \quad (1.124)$$

We can do the Matsubara sum. We have the Matsubara frequencies for fermions:

$$i\omega_n = (2n + 1)\pi T \quad (1.125)$$

We have to sum over all possible state. If we take the fermi function we have that a all the poles of the fermi function are exactly in the same of the Matsubara fermionic frequencies:

$$f(z) = \frac{1}{e^{\beta z} + 1} \quad e^{\beta z} = -1 \quad (1.126)$$

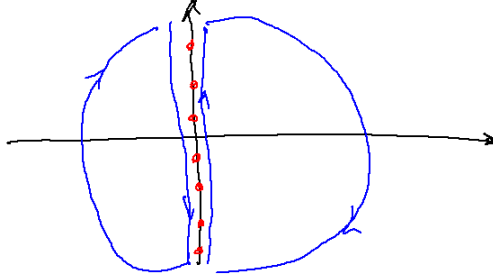
We can compute the residual of the fermi functions:

$$f(i\omega_n) = \lim_{z \rightarrow i\omega_n} \frac{1}{\beta e^{\beta z}} = -\frac{1}{\beta} \quad (1.127)$$

This means that the Matsubara sum can be pefrommed as:

$$T \sum_{i\omega_n} F(i\omega_n) = -\frac{1}{2\pi i} \int F(z) f(z) dz \quad (1.128)$$

Where the path on the complex plane goes around



It is possible to deform the integration path as shown in figure, in this way we have only to take into account the poles of the  $F(z)$  function not overlapping the imaginary axes. We can rewrite as:

$$T \sum_{i\omega_n} F(i\omega_n) = \sum_{Res F(z)} F(z) f(z) \quad (1.129)$$

In practice we have:

$$G(k, i\omega_m) = \oint dz f(z) \frac{1}{z - \xi_k} \frac{1}{z + i\Omega_m - \xi_{k+q}} \quad (1.130)$$

We have two poles:

$$-\frac{1}{\Omega} \sum_k \left[ \frac{f(\xi_k)}{\xi_k + i\Omega_m - \xi_{k+q}} + \frac{f(\xi_{k+q} - i\Omega_m)}{\xi_k + q - i\Omega_m - \xi_k} \right] \quad (1.131)$$

The Fermi function is periodic in the bosonic matsubara frequencies:

$$\chi_{\rho\rho}^0(q, i\Omega_m) = \frac{1}{\Omega} \sum_k \frac{f(\xi_{k+q}) - f(\xi_k)}{i\Omega_m + \xi_k - \xi_{k+q}} \quad (1.132)$$

Now we just have to make the analytical continuation. We can compute the real part:

$$\chi'(q, \omega) = \frac{1}{\Omega} \sum_k \frac{f(\xi_{k+q}) - f(\xi_k)}{\omega + \xi_k - \xi_{k+q}} \quad (1.133)$$

If we compute it for  $q = 0$  we have zero:

$$\chi'(q = 0; \omega) = 0 \quad (1.134)$$

$$\lim_{q \rightarrow 0} \chi'(q, \omega = 0) = \frac{1}{\Omega} \sum_k \frac{\partial f}{\partial \xi_k} \rightarrow N_F \quad (1.135)$$

### 1.4.3 Photoemission

The only case where the response function is not a bouble is the photoemission. It is in principle something extremely complicated. There are a given number of approximations. We assume that the electron does not loose energy during the travel inside the sample, and to be emitted only pay the extraction energy to pass from the surface of the material to the free space. With this approximation we can compute it as:

$$P_{fi} = M_{fi} |\langle m | c_{k\sigma} | n \rangle|^2 \delta(E_m - E_n - \omega) \quad (1.136)$$

$M_{fi}$  is something that crucially depends on polarization and the crystal structure and must be characterized for any kind of systems. We have to some over all possible initial states.

$$G_{<}(k, \omega) = \sum_{mn} e^{-\beta E_n} |\langle m | c_{k\sigma} | n \rangle|^2 2\pi \delta(E_m - E_n - \omega) \quad (1.137)$$

We can also define the Green's function for the inverse photoemission:

$$G_{>}(k, \omega) = \sum_{mn} e^{-\beta E_m} |\langle m | c_{k\sigma}^\dagger | n \rangle|^2 2\pi \delta(E_m - E_n + \omega) \quad (1.138)$$

You can define the Fourier transform of these two Green's functions:

$$\langle c_{k\sigma}(t) c_{k\sigma}^\dagger(0) \rangle = \sum_{mn} e^{-\beta(E_n - F)} \langle n | e^{iHt} c_{k\sigma} e^{-iHt} | m \rangle \langle m | c_{k\sigma}^\dagger | n \rangle \quad (1.139)$$

$$\sum_{nm} e^{-\beta(E_n - F)} e^{i(E_n - E_m)t} |\langle n | c_{k\sigma}^\dagger | m \rangle|^2 \quad (1.140)$$

If we can introduce a Delta function for the complex exponential

$$\int d\omega \delta(\omega - E_n + E_m) e^{i\omega t} \sum_{nm} e^{-\beta(E_n - F)} |\langle n | c_{k\sigma}^\dagger | m \rangle|^2 = \int \frac{d\omega}{2\pi} G_{>}(k, \omega) e^{i\omega t} \quad (1.141)$$

We can define the retarded Green's function and the Spectral function

$$A(k, \omega) = -\frac{1}{\pi} \Im G_R(\omega + i\delta) = (1 + e^{-\beta\omega}) \frac{G_{>}(k, \omega)}{2\pi} = (1 + e^{\beta\omega}) \frac{G_{<}(k, \omega)}{2\pi} \quad (1.142)$$

Therefore, the intensity is of the probe is:

$$I(k, \omega) \propto G_{<}(k, \omega) = 2\pi f(\omega) A(k, \omega) \quad (1.143)$$

$$I_{inv}(k, \omega) \propto G_{>}(k, \omega) = 2\pi [1 - f(\omega)] A(k, \omega) \quad (1.144)$$

If we define the retarded Green's function we can see that:

$$G_r(t) = -i\theta(t) \langle \{c_k(t), c_k^\dagger(0)\} \rangle \quad (1.145)$$

Then the greens function that obtain this quantity is:

$$G(k, \tau) = -\langle T c_{k\sigma}(\tau) c_{k\sigma}^\dagger(0) \rangle \quad (1.146)$$

This can be proven by using the Lemman rappresentation.

Apart from photoemission where we compute only the single fermions operators, all the other responce theory are product of fermionic operators.

## 1.5 Optical conductivity

### DRUDE THEORY

The only assumption in the Drude theory is a damping in the propagation of the electron:

$$\frac{dp}{dt} = -\frac{p}{\tau} - eE(t) \quad (1.147)$$

The final conducibility is:

$$\sigma(\omega) = \frac{ne^2\tau}{1 + i\omega} \quad (1.148)$$

We can explain very well why drude works so well form metals in the Sommerfeld approach.

We can use the minimal substitution to insert the gauge field:

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c} \vec{A} \quad (1.149)$$

where  $e$  is the negative charge of the electron (with the minus sign  $e = -1.6 \times 10^{-19}$  C).

$$H = \frac{1}{2m} \int dx c^\dagger(x) \left( -i\vec{\nabla} - \frac{e}{c} \vec{A} \right)^2 c(x) = H_0(\vec{A} = 0) - \int \vec{J}_p(x) \cdot \vec{A} + \underbrace{\frac{1}{2} e^2 A^2 \frac{n}{m}}_{\frac{1}{2} \sum_i e^2 A_i^2(x) \tau_i(x)} \quad (1.150)$$

This is by definition the diamagnetic tensor. In any case we will make the continuum case.

$$H = \frac{1}{2m} \int dx c^\dagger(x) \left( -i\vec{\nabla} - \frac{e}{c} \vec{A} \right) (-i\nabla c - eAc) \quad (1.151)$$

Now we put the speed of light  $c = 1$

$$\frac{1}{2m} \int dx c^\dagger(x) \left[ -\nabla^2 c + ie\vec{\nabla} \cdot \vec{A} c + ie\vec{A} \cdot \vec{\nabla} c + e^2 A^2 c \right] \quad (1.152)$$

We can integrate by part.

$$\int c^\dagger(c)(\nabla A)c(x) = - \int \nabla c^\dagger A c - \int c^\dagger A \nabla c \quad (1.153)$$

$$\frac{1}{2m} \int dx [-c^\dagger \nabla^2 c + ie(\nabla c^\dagger)cA - ieA(c^\dagger \nabla c) + e^2 A^2 c] \quad (1.154)$$

We have derived the correct expression. So the current is given by two terms. The paramagnetic current is therefore:

$$\vec{J}_p = - \left. \frac{\partial H}{\partial A} \right|_{A=0} = -i \frac{e}{2m} \int dx (\nabla c^\dagger c A - c^\dagger \nabla c) \quad (1.155)$$

The last term is:

$$H = H_0 - \vec{j}_p \cdot \vec{A} - \frac{e^2}{2m} A^2 n \quad (1.156)$$

Therefore the current is:

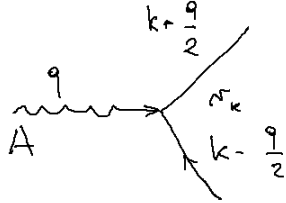
$$\vec{j} = - \frac{\partial H}{\partial A} = \vec{j}_p - \frac{e^2 \vec{A} n}{m} \quad (1.157)$$

When we will do the Fourier transform of the current operator we will have:

$$\vec{j}_p(q) = e \sum_k \frac{k}{m} c_{k-\frac{q}{2}}^\dagger c_{k+\frac{q}{2}} = e \sum_k \vec{v}_k c_{k-\frac{q}{2}}^\dagger c_{k+\frac{q}{2}} \quad (1.158)$$

$$\vec{v}_k = \frac{\partial \epsilon_k}{\partial \vec{k}} \quad (1.159)$$

This means that the vertex of the Feynman theory are



We can now make the linear response theory. One can derive a generalized quadridimensional current:

$$J_\mu(q) = e K_{\mu\nu}(q) A_\nu(q) \quad (1.160)$$

Where

$$K_{\mu\nu}(q, i\Omega_n) = -\frac{n}{m} \delta_{\mu\nu} (1 - \delta_{\mu 0}) + \Pi_{\mu\nu}(q, i\Omega_m) \quad (1.161)$$

The first term is the diamagnetic term, that is only present for the current component ( $\mu \neq 0$ ) plus the response function:

$$\Pi_{\mu\nu}(q, i\Omega_m) = \int d\tau e^{i\Omega_m \tau} \langle T j_\mu(\rho, \tau) j_\nu(-q, 0) \rangle \quad (1.162)$$

Now it is possible to define the optical conductivity.

$$\sigma_x(\omega) = e^2 \frac{K_{xx}(q=0, \omega + i\delta)}{i(\omega + i\delta)} \quad (1.163)$$

If we now compute the real part of the optical conductivity using this formula:

$$\sigma'(\omega) = e^2 \pi \delta(\omega) \left[ \frac{n}{m} - \Re \Pi_{xx}(q=0, \omega) \right] + e^2 \frac{\Im \Pi_{xx}(q=0, \omega)}{\omega} \quad (1.164)$$

In a compleately unrealistic case it is equivalent to assume that you have not any scattering event. The states have no chance to decay. For this very compleately unrealistic case, for this systems we have the  $\Pi_x x(q=0) = 0$ , therefore we have only the delta function. If we have interaction the term inside the Box brakets is zero. However, it is usefull to write it in this way because we can write a sum rule:

$$\int_{-\infty}^{\infty} d\omega \Re \sigma(\omega) = \frac{\pi e^2 n}{m} - \pi e^2 \Pi_{xx}(0) + e^2 \int d\omega \frac{\Im \Pi_{xx}(\omega)}{\omega} \quad (1.165)$$

Lets try now to do the calculations for electrons having some form of interactions. Lets write explicely the bare bouble approximation for the  $\Pi$  matrix. We will do the same as before, considering the velocity in the vertex. The bare bouble approximation is:

$$\Pi(q, i\Omega_m) = -\frac{2T}{N} \sum_{k, i\omega_n} v_k^2 G(k + \frac{q}{2}, i\omega_n + i\Omega_m) G(k - \frac{q}{2}, i\omega_n) \quad (1.166)$$

The two in front of the expression comes from the spin. We want to do the calculation for in the most general interacting case. We can just write that:

$$G(k, i\omega_n) = \int dz \frac{A(k, z)}{i\omega_n - z} \quad (1.167)$$

$$A(k, z) = -\frac{1}{\pi} \Im G(i\omega_n \rightarrow z + i0^+) \quad (1.168)$$

In the case of non interactive system we have:  $A(k, z) = \delta(z - \xi_k)$ , in the case of a non interactive system we have:

$$A(k, z) = \frac{1}{\pi} \frac{\Gamma}{(z - \xi_k)^2 + \Gamma^2} \quad (1.169)$$

Therefore, the interaction is encoded in the spectral function  $A(k, z)$ . We are considering a very simple basic approximation where  $\Gamma$  is not dependent by the frequency. We can use the spectral representation for the Greens Functions:

$$\Pi(q, i\Omega_m) = -\frac{2T}{N} \sum_{q, i\omega_m} \int dz dz' \frac{A(k + \frac{q}{2}, z)}{i\omega_n + i\Omega_m - z} \frac{A(k - \frac{q}{2}, z')}{i\omega_n - z'} \quad (1.170)$$

Now we can use exactly the same rule as the Matzubara sum.

$$\Pi(q \rightarrow 0, i\Omega_m) = -\frac{2}{N} \sum_k v_k^2 \int dz dz' A(k, z) A(k, z') \frac{f(z) - f(z')}{i\Omega_m + z - z'} \quad (1.171)$$

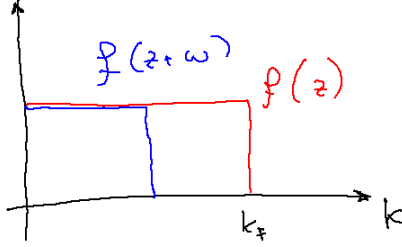
We have to make the analytical continuation, and take the imaginary part divided by  $\omega$ :

$$i\Omega_m \rightarrow \omega + i\delta \quad (1.172)$$

$$\Pi(q \rightarrow 0, \omega + i\delta) = -\frac{2}{N} \sum_k v_k^2 \int dz dz' A(k, z) A(k, z') \frac{f(z) - f(z')}{\omega + z - z' - i\delta} \quad (1.173)$$

Then I want to take the imaginary part to have the  $\sigma'$  function that gives us a delta function that gets rid on the  $z'$  integration:

$$\sigma'(\omega) = -\frac{2\pi e^2}{N} \sum_k \int dz v_k^2 A(k, z + \omega) A(k, z) \frac{f(z + \omega) - f(z)}{\omega} \quad (1.174)$$



The difference between the two fermi function is very easy to compute, as shown in the figure:

$$\sigma'(\omega) = \frac{2\pi e^2}{N} \sum_i \left(\frac{k}{m}\right)^2 \int_{\mu-\omega}^{\mu} dz \frac{A(k, z + \omega) A(k, z)}{\omega} \quad (1.175)$$

We can assume that the quantities are constant around the fermi levels:

$$\sigma'(\omega) = -i\pi e^2 N_f \frac{v_f^2}{D} \int_{\mu-\omega}^{\mu} \frac{dz}{\omega} \int d\xi A(\xi) A(\xi + \omega) \quad (1.176)$$

If we want to make an optical conductivity we have to make a transition between an occupied and an unoccupied state. We want to make an optical transition at  $q = 0$ . If the states are all perfectly defined, we have no possibility to have a  $q = 0$  transition. If we start to broden the system, then it is possible to do particle-hole transition because we can have an overlap between empti and occupied states: Luckily the integral of two Lorentzian function can be done analytically, and it is again a Lorentzian with twice its amplitude as the original one.

$$\int d\xi A(\xi) A(\xi + \omega) = \frac{4\Gamma}{\pi} \frac{1}{\omega^2 + (2\Gamma)^2} \quad (1.177)$$

What we get is:

$$\sigma(\omega) = \frac{2\pi e^2 N_f v_f^2}{D} \frac{4\Gamma}{\pi} \frac{1}{\omega^2 + (2\Gamma)^2} \quad (1.178)$$

This formula can just be rewritten in this way:

$$\sigma(\omega) = \frac{e^2 n \tau}{m} \frac{1}{1 + (\omega \tau)^2} \quad \tau = \frac{1}{2\Gamma} \quad (1.179)$$

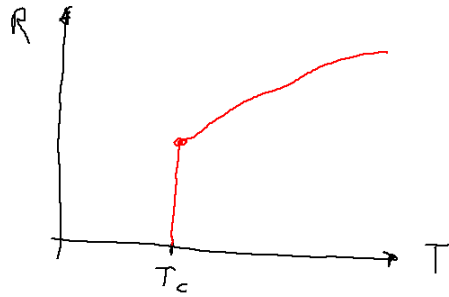
Now what we get is that the Drude formula is correct in this picture. We can have in the general case in which  $\Gamma$  can depend itself on the frequency. There are other process that interaction are called vertex correction in which the interactive Green function can interact. They can in part included into the scattering rate. Boltzmann theory is a very elegant way to encode empirically some of the vertex corrections. Computing optical response remains very difficult. For Fermi liquids one can more or less resolve this kind of approximation.



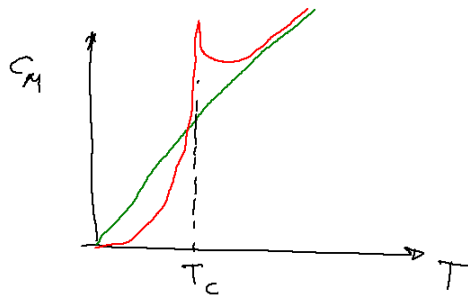
## Chapter 2

# Superconductivity

Superconductive phenomena was discovered in 1909. This was a result in a technological improvement in low temperature cryogenic. The resistivity was seen drop to zero.



The main characteristics are zero resistivity  $R = 0$ , that means infinite conductivity  $\sigma = \infty$ . Below the superconductive temperature even if the electron has finite lifetime the conductivity gain a  $\delta(\omega)$  factor.



From specific heat experiment an exponential decayment was observed. This is a mark of a electronic GAP in the system. THE most remarkable effect is the Meissner effect. This is a second order phase transition, there is a spontaneous symmetry breaking. The broken symmetry is completly not evident.

For magnetic systems it is evident the breaking symmetry (spin alignment). The Heisenberg hamiltonian is invariant under spin rotation. Below the broken symmetry, the ground state is no more invariant under the symmetry operation. This is the reason why it took so much to have a microscopic theory. It is a very important theory BCS, it is able to answer in a mean-field approach most of the questions.

We will first describe the BCS theory.

## 2.1 Bardeen-Cooper-Schriffer

This is substantially a Bose-Einstein condensation for cooper pairs. If we have electrons with  $\omega < \omega_D$  and  $k \approx k_f$  they can have an attraction between them. Typilcally the energy between electrons is given by Coulomb interaction. How we can get rid of this repulsion? In the metal the Coulomb Interaction is screened by electrons and phonons:

$$V(q, \omega) = \frac{4\pi e^2}{q^2 \varepsilon(q, \omega)} \quad (2.1)$$

The electric constat can be derived into electronic and lattice contribution:

$$\varepsilon(q, \omega) = \varepsilon_{el} + \varepsilon_{ph} - 1 \quad (2.2)$$

We will take the electronic dielectric constant in the static limit and the lectronic dielectric constant in the pure dynamic limit (Adiabatic approximation). If we take an energy close to the fermi levels.

In general the dyelectric constant can be related either to the compressibility function or the conducibility:

$$\varepsilon = 1 + \frac{4\pi\chi_{\rho\rho}(q, \omega)}{q^2} = 1 + \frac{4\pi i\sigma(q, \omega)}{\omega} \quad (2.3)$$

$$\chi_{\rho\rho}(\omega = 0, q \rightarrow 0) = N_f \quad (2.4)$$

$$\sigma(q = 0, \omega) = \frac{ne^2\tau}{m(1 - i\omega\tau)} \quad (2.5)$$

The real part of the conductivity is:

$$\varepsilon' = 1 + \frac{4\pi\sigma''}{\omega} = 1 - \frac{4\pi\tau ne^2\tau}{m\omega [1 + (\omega\tau)^2]} \xrightarrow{\omega\tau \gg 1} 1 - \frac{4\pi ne^2}{m\omega^2} = 1 - \frac{\omega_p^2}{\omega^2} \quad (2.6)$$

This is the dielectric function in the dynamic limit. Taking this two relation under consideration we can estimate the complete dyelectric function. The electronic dielectric function is the Thomas-Fermi screening:

$$\varepsilon_{el}(\omega = 0, q) = 1 + \frac{4\pi N_f}{q^2} = 1 + \frac{k_s^2}{q^2} \quad (2.7)$$

We can take the one of Ions just replacing the mass of the electrons to the one of the ions:

$$\Omega_q^2 = \frac{4\pi n_{lat}(Ze)^2}{M} \quad \varepsilon_{ph}(\omega, q = 0) = 1 - \frac{\Omega_q^2}{\omega^2} \quad (2.8)$$

We can now write the total dielectric function to get the complete dielectric response:

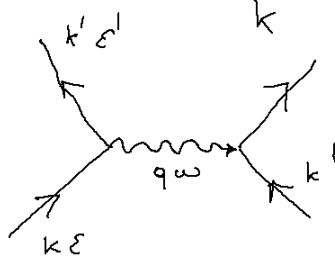
$$\varepsilon(q, \omega) = 1 + \frac{k_s^2}{q^2} - 1 + 1 - \frac{\Omega_q^2}{\omega^2} = \frac{q^2 + k_s^2}{q^2} - \frac{\Omega_p^2}{\omega^2} \quad (2.9)$$

$$\varepsilon(q, \omega) = -\frac{q^2 + k_s^2}{q^2 \omega^2} \left[ \omega^2 - \frac{q^2 \Omega_p^2}{q^2 + k_s^2} \right] = \frac{q^2 + k_s^2}{q^2 \omega^2} (\omega^2 - \omega_q^2) \quad (2.10)$$

Then the total potential can be written as:

$$V(q, \omega) = \frac{4\pi e^2}{q^2 + k_s^2} \left[ 1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2} \right] \quad (2.11)$$

If we have  $\omega < \omega_q \sim \omega_D$  we have  $V < 0$ . So we can have an attractive potential between electrons mediated by phonons.



It is possible redo this by describing it as the electron-phonon interaction:

$$H_{e-p} = \sum_{k,q} g(q) \left[ a_q + q_{-q}^\dagger \right] \left[ c_{k+q}^\dagger c_k \right] \quad (2.12)$$

$$H_{e-p} = \sum_{k,q} g(q) \left[ a_q + q_{-q}^\dagger \right] \rho(q) \quad (2.13)$$

This is just the second quantization version of what we described. We have the bare interaction between electrons plus the electron phonons:

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + H_{e-p} + \sum_k \omega_q a_q^\dagger a_q \quad (2.14)$$

It is possible to integrate out the phonon degrees of freedom, we end up with an effective hamiltonian between electrons, that is

$$H = H_0 - U \sum_k \rho^\dagger(q) \rho(q) \quad (2.15)$$

So there is an interaction between electrons mediated by phonons that is attractive. We analyze the BCS model, that is an effective model of interacting electrons with attraction in the Cooper channel.

## 2.2 BCS model

The BCS Hamiltonian is:

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \frac{g}{\Omega} \sum_{kk'} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger c_{k'\downarrow} c_{k'\uparrow} \quad (2.16)$$

We already ordered the fermionic creation and annihilation operators. This is an interactive model, we do not know how to solve it exactly. We use the meanfield approximation (Hartree-Fock). We define the superconductive order parameter is:

$$\Delta_0 = \frac{g}{\Omega} \sum_k \langle c_{k\uparrow} c_{k\downarrow} \rangle \quad A = \sum_k |\xi_k| < \omega_D c_{k\downarrow} c_{k\uparrow} \quad (2.17)$$

We can rewrite our model in a mean-field Hartree-Fock (acting on a single slater-determinant):

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \Delta_0 \sum_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger - \Delta_0^\dagger \sum_k c_{-k\downarrow} c_{k\uparrow} + \frac{|\Delta_0|^2 \Omega}{g} \quad (2.18)$$

$$H = \sum_k \xi_k c_{k\sigma}^\dagger c_{k\sigma} = \sum_k \xi_k \left[ 1 - c_{k\downarrow} c_{k\downarrow}^\dagger \right] \quad (2.19)$$

If we introduce a spinor:

$$\psi_k = c_{k\uparrow} c_{-k\downarrow}^\dagger \quad (2.20)$$

It is possible to rewrite the HF hamiltonian as:

$$H = \sum_k \psi_k^\dagger \hat{H} \psi_k + \sum_k \xi_k + \frac{\Delta_0^2 \Omega}{g} \quad (2.21)$$

$$\hat{H} = \begin{pmatrix} \xi_k & \Delta_0 \\ \Delta_0 & -\xi_{-k} \end{pmatrix} \quad (2.22)$$

Let us assume that  $\Delta_0$  is a real quantity, so we do not care about complex conjugate. Now we have the Hamiltonian written as a quadratic model. We can diagonalize the new diagonal problem. Then we have a free order parameter  $\Delta_0$ , that must be minimized on the solution of the Hartree-Fock. This is the self consistent equation of the Hartree-Fock theory, that will result in the self consistent gap equation:

$$\begin{pmatrix} \xi_k - \lambda & \Delta_0 \\ \Delta_0 & -\xi_k - \lambda \end{pmatrix} = (\xi_k - \lambda)(-\xi_k - \lambda) - \Delta_0^2 \quad (2.23)$$

The eigenvalues are:

$$\lambda = \pm \sqrt{\xi_k^2 + \Delta_0^2} = \pm E_k \quad (2.24)$$

Now we can write the partition function as:

$$Z = \prod_{k\alpha} (1 + e^{-\beta \varepsilon_{k\alpha}}) \quad (2.25)$$

This formula is usually used to derive the partition function for the Fermi gas. In fact we can label the states telling how many electrons we have in any state:

$$\prod_{n_{k\alpha}} \sum_{k_\alpha} \langle n_{k\alpha} | e^{-\beta H} | n_{k\alpha} \rangle = \prod_{n_{k\alpha}} (1 + e^{-\beta \varepsilon_{k\alpha}}) \quad (2.26)$$

So we have for the partition function

$$Z = \prod_k (1 + e^{-\beta E_k})(1 + e^{\beta E_k}) \quad (2.27)$$

We can obtain the free energy:

$$F = -k_b T \ln Z = -k_b T \sum_k [\ln(1 + e^{-\beta E_k}) + \ln(1 + e^{\beta E_k})] + \sum_k \xi_k + \frac{\Delta_0^2 \Omega}{g} \quad (2.28)$$

Where we must add the constant factor of the energies. We can get the self-consistent equation, we have to minimize the free energy respect the order parameter:

$$\frac{\partial F}{\partial \Delta_0} = 0 \quad (2.29)$$

$$\frac{\partial F}{\partial \Delta_0} = -T \sum_k \frac{e^{-\beta E_k}}{1 - e^{-\beta E_k}} \left( -\beta \frac{\Delta_0}{E_k} \right) - T \sum_k \frac{e^{\beta E_k}}{1 + e^{\beta E_k}} \left( \beta \frac{\Delta_0}{E_k} \right) + \frac{2\Delta_0 \Omega}{g} = 0 \quad (2.30)$$

$$\frac{\partial F}{\partial \Delta_0} = - \sum_k \frac{\Delta_0}{E_k} \left[ \frac{-e^{-\beta E_k/2}}{e^{\beta E_k/2} + e^{-\beta E_k/2}} + \frac{e^{\beta E_k/2}}{e^{\beta E_k/2} + e^{-\beta E_k/2}} \right] + \frac{2\Delta_0 \Omega}{g} = 0 \quad (2.31)$$

$$\Delta_0 = \frac{g\Delta_0}{2\Omega} \sum_k \frac{1}{E_k} \tanh \left( \frac{\beta E_k}{2} \right) \quad (2.32)$$

This equation has always the solution  $\Delta_0 = 0$ . This is the case, because if  $g < 0$  (repulsion) then no way to form cuper pairs. If I have interaction on the system, this interaction promotes system in the cooper pair:

$$\Delta_0 = \sum_k \langle c_{k\uparrow} c_{-k\downarrow} \rangle \quad (2.33)$$

If it is not energetically favorable to do this,  $\Delta_0 = 0$  we recover the Fermi level. What are electrons doing in the superconductive state? This information is encoded in the eigenvector of the Hamiltonian we diagonalized.

We can compute the number of particle by deriving the free energy respect to the chemical potential:

$$n = -\frac{1}{\Omega} \frac{\partial F}{\partial \mu} = \frac{1}{\Omega} \sum_k \left( 1 - \frac{\xi_k}{E_k} \tanh \frac{\beta E_k}{2} \right) \quad (2.34)$$

Therefore the density of state is not given any more by the Fermi function. If we want to work at fixed number of particle, this is an equation on the chemical potential. In practice we have to solve two coupled equations, one for the Gap and one for the chemical potential.

## 2.3 Self consistent Gap equation

Lets try to solve the Gap equation at zero temperature first, then the hyperbolic tangent is 1.

$$1 = \frac{g}{2} \int d\xi N(\xi) \frac{1}{\sqrt{\xi^2 + \Delta^2}} \quad (2.35)$$

We want to study only the region close to the Fermi surface, and energies up to  $\omega_D$ :

$$1 = gN_0 \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_0^2}} = gN_0 \ln \left[ \frac{\omega_D}{\Delta_0} + \sqrt{\left(\frac{\omega_D}{\Delta_0}\right)^2 + 1} \right] \quad (2.36)$$

Usually we have  $\Delta_0 \ll \omega_D$ :

$$1 \approx gN_0 \ln \frac{2\omega_D}{\Delta_0} \quad (2.37)$$

Therefore we solve the equation for the Gap:

$$\Delta_0 = 2\omega_D e^{-\frac{1}{gN_0}} \quad (2.38)$$

This is a quite remarkable equation. Regardless as small as  $g$  can be, I will always form a bounded state. This means that we can always tends to form a a bound state. As the coupling is decreases we have smaller  $\Delta_0$ . If you increase the energy of the bosonic  $\omega$ . People tried to work on  $g$  and the density of states to increase exponentially the GAP. Also other kind of fluctuations, like spin fluctuations, that can form a superconductive glue. The validity of BCS theory goes far behind where its defined. Of course, a lot of caveat and modifications can be included, as the retarded interaction, and superconductivity must be modified in the Eliashberg theory.

We can derive again the equation for  $T_c$  by chosing  $\Delta_0(T) \rightarrow 0$ :

$$1 = gN_0 \int_0^{\omega_D} d\xi \frac{1}{\xi} \tanh \frac{\beta_c \xi}{2} \quad (2.39)$$

We are solving the GAP equation at finite themperature, but with the gap equal to zero. When  $\beta\xi \rightarrow 0$  the integral is regular, if  $\beta\xi \rightarrow \infty$  the integral diverges close to zero. Then we can get rid of he divergence:

$$1 \sim gN_0 \int_{2T_c}^{\omega_D} \frac{1}{\xi} d\xi = 2N_0 \ln \frac{\omega_d}{2T_c} \quad (2.40)$$

Therefore we can estimate the  $T_c$ :

$$T_c \sim \omega_D e^{-\frac{1}{\beta N_0}} \quad (2.41)$$

We can also solve exactly the integral, therefore we have:

$$T_c = \frac{2e^\gamma}{\pi} \omega_d e^{-\frac{1}{gN_0}} \quad (2.42)$$

$$\Delta_0 = 1.76 \cdot T_c \quad (2.43)$$

## 2.4 BCS ground state: the Cooper pairs

We want to compute the Eigenvectors of the original mean-field hamiltonian:

$$\vec{v} = \begin{pmatrix} a \\ b \end{pmatrix} \quad (2.44)$$

$$\begin{cases} (\xi_k - E_k)a + \Delta_0 b = 0 \\ a^2 + b^2 = 1 \end{cases} \quad (2.45)$$

$$b = -\frac{\xi - E_k}{\Delta_0} a \quad (2.46)$$

$$a^2 \left[ 1 + \frac{(\xi_k - E_k)^2}{\Delta_0^2} \right] = 1 \quad (2.47)$$

$$a^2 = \frac{\Delta_0^2}{\Delta_0^2 + \xi^2 + E^2 - 2\xi E} = \frac{\Delta_0^2}{2E^2 - 2\xi E} = \frac{\Delta_0^2}{2E(E - \xi)} \quad (2.48)$$

$$a = \frac{\Delta_0}{\sqrt{2E}\sqrt{E - \xi}} = \frac{\sqrt{E^2 - \xi^2}}{\sqrt{2E}\sqrt{E - \xi}} = \sqrt{\frac{1}{2} \left( 1 + \frac{\xi}{E} \right)} = u_k \quad (2.49)$$

Now it is trivial to get  $b$  as  $a^2 + b^2 = 1$ :

$$b = \sqrt{\frac{1}{2} \left( 1 - \frac{\xi}{E} \right)} = v_k \quad (2.50)$$

It is possible to do the same. We have the new operator that can be written like:

$$U_k = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \quad (2.51)$$

Then we have

$$\hat{H}U_k = U_k\Lambda \quad \Lambda = \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \quad (2.52)$$

Once that we have this transformation we know what are the operators that diagonalizes our Hamiltonian.

$$H = \sum_k \psi_k^\dagger \hat{H} \psi_k = \sum_k \psi_k^\dagger U_k \Lambda U_k^\dagger \psi_k = \sum_k \phi_k^\dagger \Lambda \phi_k \quad (2.53)$$

Then we have a new spinor that is diagonalizing the problem as:

$$\phi_k = U_k^\dagger \psi_k \quad \psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}^\dagger \end{pmatrix} \quad (2.54)$$

$$\phi_k = \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^\dagger \end{pmatrix} \quad (2.55)$$

Then we can get the new fermionic excitation of the system:

$$\gamma_{k\uparrow} = u_k c_{k\uparrow} + v_k c_{-k\downarrow}^\dagger \quad (2.56)$$

$$\gamma_{-k\downarrow}^\dagger = -v_k c_{k\uparrow} + u_k c_{-k\downarrow}^\dagger \quad (2.57)$$

So these are the transformation that diagonalizes the BCS ground state. It is possible to prove that actually the Bogoliogov operators  $\gamma$  are actually creation and annihilation operators.

$$\gamma_{k\uparrow}|BCS\rangle = 0 \quad (2.58)$$

$$\gamma_{k\uparrow}^\dagger|BCS\rangle = |E_k\rangle \quad (2.59)$$

It means that the BCS ground state contains simulataneously double occupied and empty states. This means that the number of the particle in the ground state is not fixed. The superconductive ground state is the quantum mechanical phase of the electrons. This is a compleately new concept. We have a macroscopic condensation of the macroscopical phase of electrons.

We can write the Hartree-Fock BCS theory as:

$$H = \sum_k E_k \left( \gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} - \gamma_{-k\downarrow} \gamma_{-k\downarrow}^\dagger \right) \quad (2.60)$$

I can use a anticommutation operator to write it as:

$$H = \sum_{k\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} - \underbrace{\sum_k E_k}_{E_g} \quad (2.61)$$

Then we have a non interactive Hamiltonian of the  $\gamma^\dagger$  created excitation. The mean field BCS hamiltonian can be diagonalized through the Bogoliogov transformation. This introduces the fermionic creation and annihilation operators  $\gamma_{k\sigma}^\dagger$  and  $\gamma_{k\sigma}$ .

Then the Hamiltonian can be rewritten as:

$$H = \sum_{k\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + E_g \quad (2.62)$$

Here  $E_k$  are all positive numbers:

$$E_k = \sqrt{\xi_k^2 + \Delta_0^2} \quad (2.63)$$

The occupatoin number of the new fermionic excitations:

$$f(E_k) = \frac{1}{e^{\beta E_k} + 1} \xrightarrow{T \rightarrow 0} 0 \quad (2.64)$$

So the ground state has no fermionic excitations: it is the bogolonc vacuum state. We must build a wave function that satisfy the property:

$$\gamma_{k\sigma}|BCS\rangle = 0 \quad (2.65)$$

It is possible to show that the Fermi level does not satisfy this characteristic (in fact it is not the Ground state):

$$|FS\rangle = \prod_{k\sigma}^{k < k_f} a_{k\sigma}^\dagger |0\rangle \quad (2.66)$$



The ground state BCS can be, instead, written as:

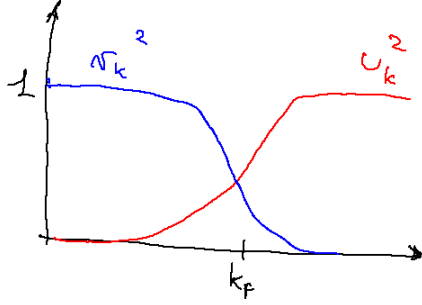
$$|BCS\rangle = \prod_k \left( u_k + v_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger \right) |0\rangle \quad (2.67)$$

We will use the property:

$$[A, BC] = \{A, B\} C - B \{A, C\} \quad (2.68)$$

$$|BCS\rangle = \prod_{k'} \left( u_{k'} + v_{k'} c_{-k'\downarrow}^\dagger c_{k'\uparrow}^\dagger \right) |0\rangle \quad (2.69)$$

We can write  $u_k$  and  $v_k$ :



Since  $u_k$  and  $v_k$  depends on  $k$  only close to the fermi see, the difference between BCS and the fermi level are only in a very tiny region close to the Fermi surface.

$$\gamma_{k\uparrow} |BCS\rangle = \prod_{k \neq k'} \left( u_{k'} + v_{k'} c_{-k'\downarrow}^\dagger c_{k'\uparrow}^\dagger \right) \gamma_{k\uparrow} \left( u_k + v_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger \right) |0\rangle \quad (2.70)$$

$$\gamma_{k\uparrow} v_k |0\rangle = v_k c_{-k\downarrow} |0\rangle \quad (2.71)$$

$$v_k \gamma_{k\uparrow} c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger |0\rangle = v_k \left( u_k c_{k\uparrow} + v_k c_{-k\downarrow}^\dagger \right) c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger |0\rangle = -v_k u_k c_{-k\downarrow}^\dagger |0\rangle \quad (2.72)$$

Therefore their sum gives zero. The application the destruction Bogoligov operator I get zero. The BCS state is a very crazy state. It is the superposition of a vacuum and double occupied state. We can also write the BCS ground state as:

$$|BCS\rangle \propto \prod_k \left( 1 + \frac{v_k}{u_k} \overbrace{c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger}^{b^\dagger} \right) |0\rangle \quad (2.73)$$

$$b^\dagger = \sum_k \alpha_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger \quad (2.74)$$

I can rewrite the bcs using an exponential notation:

$$|BCS\rangle = \prod_k e^{\sum_k \alpha_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger} |0\rangle = e^{b^\dagger} |0\rangle \quad (2.75)$$

Therefore the BCS state, we have the condensation of this operator  $b^\dagger$ . This is a coherent state. It is possible to write the exponential:

$$e^{b^\dagger} |0\rangle = \sum_k \frac{1}{n!} (b^\dagger)^n |0\rangle = \sum_k \frac{1}{n!} |n\rangle \quad (2.76)$$

The BCS state is a superposition of a Cooper pairs. The BCS ground state has no defined particle, because we are summing on all possible number of pairs. This is not well defined. However this is very relative.

$$N = 2 \sum_k v_k^2 \quad (2.77)$$

However, the average value has a finite variance:

$$\langle N^2 \rangle - \langle N \rangle^2 = 2 \sum_k u_k v_k \quad (2.78)$$

Therefore, since there is an undefined variable  $N$ , for the indetermination principle another conjugate quantity that is perfectly defined, that is the phase. What is the range dimension in which we find a difference between the the fermi level and the BCS level? This is of the order of the superconductive gap:

$$v_k(k - k_f) \sim \Delta_0 \quad \delta k \sim \frac{\Delta_0}{v_f} \quad (2.79)$$

Since we have a correlation length of the order of how the Cooper pair usually go:

$$\xi \sim \frac{1}{\delta k} \sim \frac{v_f}{\Delta_0} = \frac{mv_f^2}{\Delta_0 mv_f} = \frac{E_f \lambda_f}{\Delta_0} \quad (2.80)$$

This is a much bigger size than the fermi length. Usually we have  $\Delta_0 \ll E_f$ , therefore the Cooper pair is much larger than the typical electronic scale. This is the reason why mean-field theories works so well for BCS. When we go in unconventional superconductors, we have higher temperatures, with smaller fermi energy, so the mean-field theories do not hold any more.

## 2.5 Green's function on BCS

We can now couple the Green function formalism in the BCS theory. We can compute the spectral function in a superconductive state. We can start again by our Hamiltonian:

$$U = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \quad HU = U\Lambda \quad (2.81)$$

$$\Lambda = \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \quad (2.82)$$

We can compute the Green function, The Green's function can be defined as:

$$\mathbf{G}^{-1} = i\omega \mathbf{I} - \mathbf{H}_{HF} \quad (2.83)$$

$$\mathbf{G}^{-1} = i\omega\mathbf{I} - \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\dagger = \mathbf{U}(i\omega - \mathbf{\Lambda})\mathbf{U}^\dagger \quad (2.84)$$

We can invert the matrix easily:

$$\mathbf{G} = \mathbf{U} \begin{pmatrix} \frac{1}{i\omega - E} & 0 \\ 0 & \frac{1}{i\omega + E} \end{pmatrix} \mathbf{U}^\dagger \quad (2.85)$$

$$\mathbf{G} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \frac{1}{i\omega - E} & 0 \\ 0 & \frac{1}{i\omega + E} \end{pmatrix} \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \quad (2.86)$$

$$\mathbf{G} = \begin{pmatrix} \frac{u^2}{i\omega - E} + \frac{v^2}{i\omega + E} & \frac{uv}{i\omega - E} - \frac{uv}{i\omega + E} \\ \frac{vu}{i\omega - E} - \frac{vu}{i\omega + E} & \frac{v^2}{i\omega - E} + \frac{u^2}{i\omega + E} \end{pmatrix} \quad (2.87)$$

We introduced operators that has as components  $c_{k\uparrow}$  and  $c_{-k\downarrow}^\dagger$ . The first element is:

$$G(k, \omega) = -\langle T c_{k\uparrow} c_{k\uparrow}^\dagger \rangle \quad (2.88)$$

Then we can rewrite the matrix as:

$$\mathbf{G} = \begin{pmatrix} G(k, i\omega_n) & \mathcal{F}(k, i\omega_n) \\ \mathcal{F}^*(k, i\omega_n) & G(-k, -i\omega_n) \end{pmatrix} \quad (2.89)$$

Where  $\mathcal{F}$  is the so called anomalous Green function. The green function is the sum of two poles, one in  $E$  and the other in  $-E$ . Then we have the anhomalous:

$$\mathcal{F}(k, i\omega_n) = \langle c_{k\uparrow} c_{-k\downarrow} \rangle \quad (2.90)$$

Then we can compute the spectral function:

$$G(k, i\omega_n) = \frac{u^2}{i\omega - E} + \frac{v^2}{i\omega + E} \quad (2.91)$$

$$\Im G(k, i\omega_n \rightarrow 0^+) = A(k, i\omega_n) = u_k \delta(\omega - E) + v_k^2 \delta(\omega + E) \quad (2.92)$$

We started with a system with a parabolic band. We are mixing  $\xi_k$  with  $-\xi_{-k}$

The spectral function tell us that close to the fermi surface we can see occupied both the states on the top and on the bottom band. We can see in a photoemission experiment we see the pick growing over the  $k$  fermi position. The real information on the electronic state are encoded in the spectral function, that is where actually sits the electrons.

## 2.6 Ginzburg-Landau

The BCS theory has been done fifty years after, the first propose to understand the Meissner effect was the London theory. The Drude model is a classical theory for conduction, and it follows from the force plus a scattering term:

$$m \frac{d\vec{v}}{dt} = -e\vec{E} + \frac{\vec{v}}{\tau} \quad (2.93)$$

The London theory starts from the hypothesis as  $\tau \rightarrow \infty$ . Let us suppose hat only a  $n_s$  part of the electrons condensate in this non resistivity status:

$$\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} \quad (2.94)$$

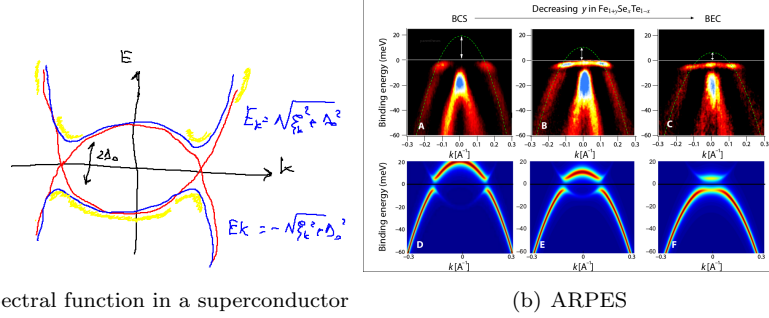


Figure 2.1: In red the two parabolic dispersion  $E_k$  and  $-E_k$  for  $\Delta = 0$ . In blue the superconductive dispersion with  $\Delta \neq 0$ . In yellow I report the spectral function, where the electronic states have more weight in the density of states. The experimental figure for a system of holes is also reported, here the ARPES band (top left) is compared with the theoretical spectral function (bottom left).

$$m \frac{d\vec{v}_s}{dt} = -\frac{m}{n_s e} \frac{d\vec{j}}{dt} = -e\vec{E} = \frac{e}{c} \frac{\partial \vec{A}}{\partial t} \quad (2.95)$$

Therefore we get:

$$\frac{d}{dt} \left( \vec{A} + \frac{mc}{n_s e^2} \vec{j} \right) = 0 \quad (2.96)$$

The London hypothesis is that:

$$\vec{A} + \frac{mc}{n_s e^2} \vec{j} = 0 \quad (2.97)$$

This is not only the solution of Eq. (2.96), but it is a much stronger assumption. This is a gauge fixed relation, so we must chose the Coulomb Gauge:

$$\vec{\nabla} \cdot \vec{A} = 0 \quad (2.98)$$

From this assumption we can derive the Meissner effect:

$$\vec{j} = \frac{c}{4\pi} \vec{\nabla} \times \vec{h} \quad \vec{h} = \vec{\nabla} \times \vec{A} \quad (2.99)$$

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{h}) = \frac{4\pi}{c} \vec{\nabla} \times \vec{j} = -\frac{n_s e^2 4\pi}{mc^2} \vec{\nabla} \times \vec{A} \quad (2.100)$$

$$-\nabla^2 \vec{h} = -\frac{n_s e^2 4\pi}{mc^2} \vec{h} \quad (2.101)$$

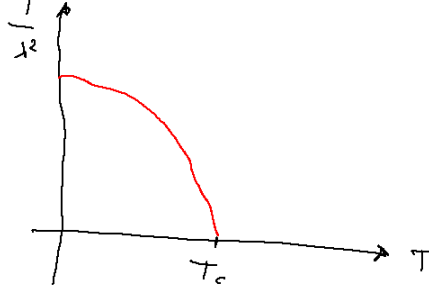
$$\vec{\nabla}^2 \vec{h} = \frac{1}{\lambda^2} \vec{h} \quad (2.102)$$

The London assumption Eq. (2.97) has the Meissner effect as a direct consequence: let us assume a system with an interface between vacuum and a superconductor. If we have a linear system, the magnetic field can depend only on the  $z$  variable. From the second Maxwell equation we get:

$$\vec{\nabla} \cdot \text{vech} = 0 \quad h_z = \text{const} \quad (2.103)$$

$$\partial_z^2 h = \frac{1}{\lambda^2} h_x \quad h_x(z) = h_x(0)e^{-\frac{z}{\lambda}} \quad (2.104)$$

Therefore the magnetic field penetrates only in a length of the order of  $\lambda$ . In a superconductor  $\lambda$  is a function of the temperature. Therefore, the number



of electrons condensated in the superconductive states  $n_s$  are a fraction of the system, according to the second order phase transition theory. If we compute the current, there is a region close to the surface of supercurrent that inhibits the magnetic field to penetrate inside the material.

We can use the Feynman theory. Let us write a free Hamiltonian:

$$H = \frac{p^2}{2m} \quad \vec{p} \rightarrow \vec{p} - \frac{q}{c} \vec{A} \quad (2.105)$$

If we substitute this inside the Hamiltonian, we get the energy of the system as:

$$E = \int dx \psi^\dagger(x) \left[ \frac{1}{2m} \left( -i\hbar\nabla - \frac{q}{c} \vec{A} \right)^2 \right] \psi(x) \quad (2.106)$$

$$\vec{j} = \frac{\partial E}{\partial \vec{A}} = \frac{\hbar q}{2m} [\psi^* \nabla \psi - (\nabla \psi^*) \psi] - \frac{q^2}{mc} \vec{A} \psi^* \psi \quad (2.107)$$

Usually the first part of this function is the paramagnetic function. If  $\vec{A} = 0$  the current is zero. If we have a  $\psi_0$  wavefunction, then the current must be zero:

$$\psi_0 \nabla_0^\psi - (\nabla_0^* \psi_0) \psi_0 = 0 \quad (2.108)$$

Lets turn on the superconductivity and a gauge magnetic field. Let us suppose that the superconductor remains equal in the presence of the magnetic field. This is the superconductor rigidity. The if  $\psi$  remains equal to  $\psi_0$ , than we have only the diamagnetic function:

$$\vec{j} = -\frac{q^2}{mc} \vec{A} |\psi|^2 = -\frac{qn}{mc} \vec{A} \quad (2.109)$$

This is the London hypothesis. So the quantum version of the London hypothesis is that the wavefunction is rigid. The new wavefunction when we add a perturbation is:

$$|\psi(A)\rangle = |\psi_0\rangle + \sum_{n \neq 0} \frac{\langle n | H | 0 \rangle}{E_n - E_0} |n\rangle \quad (2.110)$$

Then since we are opening a gap, the wavefunction remains almost still, because  $E_n - E_0 > \Delta$ . The problem of the superconductor is that the opening of a gap generate a superconductive behaviour and not an isolant system. The interesting thing of this formalis is that we start observing that the superconductor is rigid, and does not respond to the gauge field. The order is the creation of the cooper pairs, then the rigidity is a consequence of the macroscopic phase. The London equation is really phenomenological, just Maxwell equation. We can take a generic model for free electrons:

$$K = \frac{1}{2m} \int dx c^\dagger(x) \left( -i\hbar \vec{\nabla} \right)^2 C(x) \quad (2.111)$$

We first notice that this model is invariant under global phase transformations.

$$C(x) = e^{i\theta} C(x) \quad (2.112)$$

We can use the minimal substitution to add a magnetic field

$$H = \frac{1}{2m} \int dx \left[ c^\dagger(x) \left( -i\hbar \vec{\nabla} - \frac{q}{c} \vec{A} \right)^2 C(x) + \frac{1}{2\pi} (\nabla \times A)^2 \right] \quad (2.113)$$

The minimal substitution assure us tha this guarantees that we get the correct equation of motion. When we couple with a gauge field we get a model that is invariant under the local phase transformation:

$$C(x) \rightarrow e^{i\theta(x)} C(x) \quad (2.114)$$

This occurs because also the gauge field is defined up to a gradient function:

$$\vec{A} \rightarrow \vec{A} + \vec{\nabla} \chi \quad (2.115)$$

We can substitute the new phase shifted  $C$  we get:

$$C^\dagger(x) \left( -i\hbar \nabla - \frac{q}{c} \vec{A} + \hbar \nabla \theta \right)^2 C(x) + \frac{1}{8\pi} (\nabla \times A)^2 \quad (2.116)$$

If we change the gauge of the  $\vec{A}$  field we get:

$$- \frac{q}{c} \nabla \chi + \hbar \nabla \theta = 0 \quad (2.117)$$

$$\chi = \frac{\hbar c}{q} \theta(x) \quad (2.118)$$

What are we learning? There is something very interesting. What is a phase transformation in electrons? This means apply a unitary operator like:

$$U = e^{-i \int dx \theta(x) c^\dagger(x) c(x)} \quad (2.119)$$

In fact we have:

$$U c^\dagger(x) U^\dagger = e^{-i\theta(x)} c^\dagger(x) \quad (2.120)$$

When  $\theta(x)$  is a constant,  $U$  is very simple:

$$U = e^{-i\theta_0 \hat{N}} \quad (2.121)$$

The original model was invariant under the action with  $U$ , or in other words:

$$[H, U] = 0 \quad [H, \hat{N}] = 0 \quad (2.122)$$

Therefore the invariance under the global phase transformation is the conservation of the charge (the number of electrons).

We can describe the superconductor case with the Ginzburg Landau. We can write the free energy of the system in an expansion in the order parameter near to the critical temperature.

$$Z = Z_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*}|\hbar\nabla\psi|^2 \quad (2.123)$$

We know that the order parameter is a complex number:

$$\psi = \psi_0 e^{i\theta_0} \quad (2.124)$$

The model needs to have the correct symmetries.  $\alpha$  is a quantity which change sign near the transition:

$$\alpha = \alpha'(T - T_c) \quad (2.125)$$

FIGURE 1

Then we want to understand the minimum of the energy:

$$\frac{\partial F}{\partial \psi_0} = 2\alpha\psi_0 + 2\beta\psi_0^3 = 0 \quad (2.126)$$

$$\psi_0^2 = -\frac{\alpha}{\beta} \quad (2.127)$$

In the non trivial minimum we have a lower energy state with broken symmetry (finite value of the order parameter).

Now we can try to make fluctuations in the amplitude or in the phase.

$$\psi = \psi_0 + \Delta \quad (2.128)$$

This is an amplitude fluctuation. The energy is

$$\psi^2 = \psi_0^2 + 2\Delta\psi_0 + \Delta^2 \quad (2.129)$$

$$\psi^4 = \psi_0^4 + 6\Delta^2\psi_0^2 + 4\Delta\psi_0^3 + O(\Delta^3) \quad (2.130)$$

$$\alpha\psi_0^2 + 2\alpha\psi_0\Delta + \frac{\beta}{2}\psi_0^4 + 2\beta\Delta^2\psi_0^2 + 2\beta\Delta\psi_0^3 \quad (2.131)$$

The linear term cancel out (I'm in the minimum).

$$F = F_{GS} + (\alpha + 2\beta\psi_0^2)\Delta^2 \quad (2.132)$$

If I use the self-consistent equation for the non trivial minimum of  $\psi_0$  we get:

$$\alpha + 2\beta\psi_0^2 = -\alpha \quad (2.133)$$

Therefore we have the free energy as:

$$F(\Delta) = F_{GS} + |\alpha|\Delta^2 \quad (2.134)$$

This amplitude fluctuation is also called the Higgs fluctuation, because this is a massive excitation.

We can try to do a phase transformation in space. This is not just as turning around the mexican hat, because we have a different phase for each point in the space:

$$\psi(x) = \psi_0 e^{i\theta(x)} \quad \nabla\psi = i\nabla\theta\psi(x) \quad (2.135)$$

We have some energy that comes from the gradient term:

$$F = F_{gs} + \frac{\hbar\psi_0^2}{2m^*}(\nabla\theta)^2 \quad (2.136)$$

Elasticity in the solid is the response for rigidity. Atoms are in fixed position. Connected to order there is rigidity. The rigidity is the fact tha deforming the lattice cost an energy that cost quadratically cost energy:

$$H = k(\nabla u(x))^2 \quad (2.137)$$

In superconductor is exactly in the same way, we must pay an energy to do a phase deformation, this is a manifestation on phase rigidity. This is the superconductor stiffness. The ground state has one fixed value of the phase. The signature of the original symmetry is the fact that I have infinite ground states connected by a change of the phase. The phase fluctuation is massless (Goston mode). In the contex of particle physics we cam write equation of motion:

$$(\square + m^2)\phi(x) = 0 \quad (2.138)$$

This is the Klein-Gordon equation, in frequency is:

$$-\omega^2 + q^2 + m^2 = 0 \quad \omega^2 = m^2 + q^2 \quad (2.139)$$

So a massive particle has a finite mass. The equation for the gauge field is:

$$\square A^\mu = 0 \quad \omega = q \quad (2.140)$$

Therefore photo is massless. In the LandauGinzburg we have no time, but we can look to the energy. Even if the Higgs field is constant, we have to pay some energy:

$$\delta F = |\alpha|\Delta^2 \quad (2.141)$$

For the phase field, if I make a fluctuation, I have:

$$\delta F = q^2\theta(q)^2 \quad (2.142)$$

Therefore  $\omega \propto q$  for the phase fluctuation. In particle physics to get a mass, you must have a term in the lagrangian  $m^2\phi^2$ . This is exactly what happens in the Higgs mode in the Landau-Ginzburg. Indeed we are talking about bosonic collective excitation, so the Dirac equation is not involved. We can have space amplitude fluctuation where we have:

$$\delta F = |\alpha|\Delta^2 + A(\nabla\Delta(x))^2 \quad (2.143)$$

Then it is clear the analogy with the Higgs mode. In all the Landau Ginzburg approach what we are studing is actually the GAP  $\psi = \langle c_{k\uparrow}c_{-k\downarrow} \rangle$ . When we will write down the gauge field in the superconductive state we will see that the photon acquires mass, this is a manifestation of the  $U(1)$  symmetry breaking. Getting a therm like  $m^2 A^2$  in the Hamiltonian we will see that the system will acquire a rigidity.



## 2.7 Coupling with the Gauge field

The Ginzburg-Landau we can write as

$$Z = Z_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m} \left| \left( -i\hbar\nabla + \frac{e^*}{c}A \right) \psi \right|^2 \quad (2.144)$$

Then we can do a local phase transformation:

$$C(x) \rightarrow C(x)e^{i\eta(x)} \quad (2.145)$$

Since the order parameter is done by two electrons we have:

$$\psi \rightarrow \psi e^{2i\eta} \quad (2.146)$$

$$\left( -i\hbar\nabla + 2\hbar\nabla\eta + \frac{e^*}{c}A + \frac{e^*}{c}\nabla\chi \right) \quad (2.147)$$

When we write the relation for  $\chi$  and  $\eta$  for the gauge transformation we have to impose that:

$$e^* = 2e \quad (2.148)$$

The value of the mass is arbitrary, because we can redefine the change of the order parameter up to a constant. But the value of the charge is not, because this fix the gauge invariance!

We can again make a phase transformation for the order parameter as:

$$\psi(x) = \psi_0 e^{i\theta(x)} \quad (2.149)$$

$$F = F_{GS} + \frac{\psi_0^2}{2m^*} \left( \hbar\nabla\theta + \frac{2e}{c}\vec{A} \right)^2 + \frac{(\nabla \times A)^2}{8\pi} \quad (2.150)$$

This is the very important message, fluctuation of the phase are directly connected with the gauge. We can fix the gauge to delete the  $\nabla\theta$  term, then we have:

$$F = F_{GS} + \frac{2\psi_0^2 e^2}{c^2 m^*} A^2 + \frac{(\nabla \times A)^2}{8\pi} \quad (2.151)$$

So we are generate a phase term in the energy that is nothing else than a mass term for the gauge field. The Goston mode is couple in the gauge field in such a way that we can eliminate the freedom on the gauge field, that gives a mass in the gauge field. This is why the presence of the Higgs that gives a mass in the particle. The reason why this mechanism is called Anderson-Higgs. The original idea was proposed by Anderson.

We can derive the equation of the gauge field from the free energy:

$$\frac{\partial F}{\partial A} = 0 \quad (2.152)$$

$$\delta F = \frac{2\psi_0^2 e^2}{m^* c^2} 2(A\delta A) + \frac{2}{8\pi} (\nabla \times A) (\nabla \times \delta A) \quad (2.153)$$

Lets integrate the last term by part (we have omitted the integral on the space).

$$\nabla(A \times B) = (\nabla \times A) \cdot B - A \cdot (\nabla \times B) \quad (2.154)$$

Therefore:

$$\int \frac{2}{8\pi} (\nabla \times A) (\nabla \times \delta A) = \int \frac{2}{8\pi} \delta A [\nabla \times \nabla \times A] - \int \nabla [(\nabla \times A) \times \delta A] \quad (2.155)$$

The last integral is a surface term, that goes to zero.

$$\int dx \left[ \frac{4\psi_0 e^2}{n^* c^2} A + \frac{1}{4\pi} \nabla \times \nabla \times A \right] \delta A = 0 \quad (2.156)$$

$$\nabla^2 A = \frac{16\pi\psi_0^2 e^2}{m^* c^2} \vec{A} \quad \frac{1}{\lambda^2} \vec{A} \quad (2.157)$$

This is exactly the London equation for the penetration depth. if we take  $m^* = 2m$  and  $\psi_0^2 = \frac{n_s}{2}$ , taking into account that we are considering Cooper pairs. Then we have a mass term:

$$\nabla^2 A = m^2 A \quad (2.158)$$

## 2.8 Flux quantization

Let us imagine to have a superconductive ring in an external magnetic field.

$$F = F_{gs} + \frac{n_s}{4m} \left( \nabla\theta + \frac{2e}{c} \vec{A} \right) \quad (2.159)$$

If we want to derive the current we must just derive the free energy:

$$\vec{J} = \frac{\partial Z}{\partial \vec{A}} = \frac{en_s}{2m} \left( \nabla\theta + \frac{2e}{c} \vec{A} \right) \quad (2.160)$$

If I make the circuitation of  $J$  along the superconductive ring, this must be zero (the current does not penetrate further the penetration length, as the magnetic field):

$$\oint \vec{J} \cdot d\vec{l} = 0 \quad (2.161)$$

$$\oint \vec{J} \cdot d\vec{l} = \int \hbar \nabla\theta \cdot d\vec{l} + \frac{2e}{c} \oint ds (\nabla \times A) \quad (2.162)$$

$$0 = \hbar \Delta\theta + \frac{2e}{c} \Phi(B) = 0 \quad (2.163)$$

Then, since the phase can only acquire a multiple of  $2\pi$ , this means that:

$$\Phi_n(B) = -\frac{\hbar c}{2e} 2\pi n = n\Phi_0 \quad (2.164)$$

Just doing this measurement, we knew that the order parameter is actually related by  $2e$ , then it is composed by couples of electrons.

## 2.9 Superconductive microscopic current

We now are going to see that the microscopic BCS theory can really justify the London equation. We saw that the number of particles is not conserved ( $\delta N \neq 0$ ), this is a consequence of the phase condensation.

How we implement Gauge invariance if we are compute current into the Kubo formalism? What we have seen is that, in general, the current is composed by a paramagnetic part and a non diamagnetic part.

$$\vec{J} = \vec{J}_p - \frac{ne^2}{m} \vec{A} \quad (2.165)$$

We have

$$H_0 \rightarrow H_0 - \vec{j}_p \cdot \vec{A} + \frac{ne^2}{m} A^2 \quad (2.166)$$

We have that the current will be given by a response function:

$$J_\mu = \left( \Pi_{\mu\nu} - \frac{ne^2}{m} \delta_{\mu\nu} \right) A^\nu = K_{\mu\nu} A^\nu \quad (2.167)$$

We have essentially to compute the correlation current current function:

$$\Pi_{\mu\nu} = \langle J_p^\mu J_p^\nu \rangle \quad (2.168)$$

A theory is gauge invariant if we want to conserve charge, and make transformation of the gauge field:

$$\rho + \nabla \times \vec{J} = 0 \quad (2.169)$$

Charge conservation can be rewritten in quadridimensional space as:

$$q^\mu J_\mu = 0 \quad (2.170)$$

This means that:

$$q^\mu K_{\mu\nu} = 0 \quad (2.171)$$

This means that we can make a gauge transformation:

$$\vec{A} \rightarrow \vec{A} + \nabla \chi \quad A^0 \rightarrow A^0 + \partial_t \chi \quad (2.172)$$

Therefore, we get:

$$A^\mu \rightarrow A^\mu + q^\mu \chi \quad (2.173)$$

The result must be unchanged, whatever is  $\chi$ . This becomes with:

$$K^{\mu\nu} q_\nu = 0 \quad (2.174)$$

Whenever we do some approximation to compute  $K_{\mu\nu}$  we must always check the consistence with gauge invariance and charge conservation. The BCS approximation it does not satisfy all these relations. In particular the response to the longitudinal field are not conserved, but likely they are not physical quantities. If I take a longitudinal field, this does not produce no electric nor magnetic field, therefore no physical quantity is actually done. However, the presence of a violation of the gauge invariance traduces that the BCS approximation violates charge conservation. This is the reason why, in the BCS approximation,  $\delta N \neq 0$ .

### 2.9.1 Current current response

We want to compute the response to of the superconductor using the Kubo formula, in the superconductive state, in order to see what happen to the superconductor, opening the gap in a way to derive the diamagnetic response.

$$\vec{j} = \frac{1}{N} \sum_k \vec{v}_k c_{k-\frac{q}{2},\sigma}^\dagger c_{k+\frac{1}{2},\sigma} \quad (2.175)$$

This is always the description of the velocity. Let's now rewrite the current in terms of the Nambu spinors:

$$\psi = (c_{k\uparrow} \ c_{-k\downarrow}) \quad (2.176)$$

So the current can be described as a matrix multiplication:

$$\vec{j} = \frac{1}{n} \sum_k \vec{v}_k c_{-\frac{q}{2}\uparrow}^\dagger c_{k+\frac{q}{2}\uparrow} - \frac{1}{n} \sum_k \vec{v}_{-k} c_{-k+\frac{1}{2}\downarrow} c_{-k-\frac{q}{2}\downarrow}^\dagger \quad (2.177)$$

Since the velocity is an odd function, then we have

$$\vec{j} = \frac{1}{n} \sum_k \vec{v}_k c_{-\frac{q}{2}\uparrow}^\dagger c_{k+\frac{q}{2}\uparrow} + \frac{1}{N} \sum_k \vec{v}_k c_{-k+\frac{1}{2}\downarrow} c_{-k-\frac{q}{2}\downarrow}^\dagger = \frac{1}{N} \sum_k \psi_{k-\frac{q}{2}}^\dagger v_k \sigma_0 \psi_{k+\frac{q}{2}} \quad (2.178)$$

Also the density can be written in terms of the Nambu operators:

$$\rho = \frac{1}{N} \sum_k c_{k-q,\sigma}^\dagger c_{k,\sigma} = \frac{1}{N} \sum_k \psi_{k-q}^\dagger \sigma_z \psi_k \quad (2.179)$$

Now we know how to compute the correlation function in the superconductive state. We introduced the matrix  $U$ , which is the one that diagonalized the BCS Hamiltonian

$$\hat{G} = U(i\omega - \Lambda)^{-1} U^\dagger \quad (2.180)$$

$$U = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \quad (2.181)$$

$$(i\omega - \Lambda)^{-1} = \begin{pmatrix} \frac{1}{i\omega - E_k} & 0 \\ 0 & \frac{1}{i\omega + E_k} \end{pmatrix} \quad (2.182)$$

$$J_\mu(q) = e^2 K_{\mu\nu}(q) A_\nu(q) \quad (2.183)$$

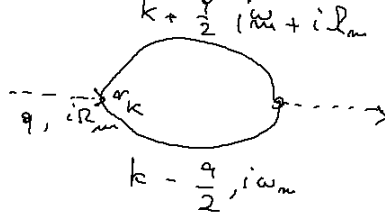
$$K_{xx} = -\langle j_{xx} \rangle + \Lambda_{JJ}^{xx} = -\frac{n}{m} + \Lambda_{jj}^{xx} \quad (2.184)$$

When we compute the correlation function for free electrons we have the bouble:

$$\Lambda_{jj}^{xx}(q, i\Omega) = -\frac{2\pi}{N} \sum_{k, i\omega} v_k^2 G(k + \frac{q}{2}, i\omega_n + i\Omega_m) G(k - \frac{q}{2}, i\omega_n) \quad (2.185)$$

We can do the same as the bouble computation. Here we do not put the 2 because the Nambu spinors takes into account the spin multiplicity:

$$\Lambda_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum \text{tr} \left[ G(k - \frac{q}{2}, i\omega_n) \sigma_0 v_k G(k + \frac{q}{2}, i\omega_n + i\Omega_m) v_k \sigma_0 \right] \quad (2.186)$$



We use  $\sigma_0$  because it is the vertex of the current current operator. We replace for each  $G$  the superconductive structure:

$$\Lambda_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum v_k^2 \text{tr} \left[ U (i\omega - \Lambda)^{-1} U^\dagger \sigma_0 U' (i\omega + i\Omega - \Lambda')^{-1} U'^\dagger \sigma_0 v_k \sigma_0 \right] \quad (2.187)$$

Where  $U'$  is the Bogoliugov matrix at  $k + \frac{q}{2}$ , whether  $U$  is at  $k - \frac{q}{2}$

Since we have the diagonal matrix we have:

$$\Lambda_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum v_k^2 \text{tr} \left[ (i\omega - \Lambda)^{-1} U U^\dagger \sigma_0 (i\omega + i\Omega - \Lambda')^{-1} U'^\dagger U' \sigma_0 v_k \sigma_0 \right] \quad (2.188)$$

$$U^\dagger U' = \begin{pmatrix} u & v \\ -vu & v \end{pmatrix} \begin{pmatrix} u' & -v' \\ v' & u' \end{pmatrix} = \begin{pmatrix} uu' + vv' & -uv' + vu' \\ -vu' + uv' & vv' + uu' \end{pmatrix} \quad (2.189)$$

$$U^\dagger U' = \begin{pmatrix} uu' + vv' & uv' - vu' \\ vu' - uv' & vv' + uu' \end{pmatrix} \quad (2.190)$$

We have

$$\Lambda_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum v_k^2 \text{tr} \left[ \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \begin{pmatrix} \frac{1}{i\omega + i\Omega - E'} & 0 \\ 0 & \frac{1}{i\omega + i\Omega + E'} \end{pmatrix} \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} \frac{1}{i\omega - E} & 0 \\ 0 & \frac{1}{i\omega + E} \end{pmatrix} \right] \quad (2.191)$$

$$\Lambda_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum v_k^2 \text{tr} \left[ \begin{pmatrix} \frac{a}{i\omega + i\Omega - E'} & \frac{b}{i\omega + i\Omega + E'} \\ -\frac{b}{i\omega + i\Omega - E'} & \frac{a}{i\omega + i\Omega + E'} \end{pmatrix} \begin{pmatrix} \frac{a}{i\omega - E} & -\frac{b}{i\omega + E} \\ \frac{b}{i\omega - E} & \frac{a}{i\omega + E} \end{pmatrix} \right] \quad (2.192)$$

$$-\frac{T}{N} \sum v_k^2 \frac{a^2}{i\omega + i\Omega - E'} \frac{1}{i\omega - E} + \frac{b^2}{(i\omega + i\Omega + E')(i\omega - E)} + \frac{b^2}{(i\omega + i\Omega - E')(i\omega + E)} + \frac{aq^2}{(i\omega + i\Omega + E')(i\omega + E)} \quad (2.193)$$

Summing over the maztubara sum:

$$\text{Lambda}_{jj}^{xx}(q, i\Omega_m) = -\frac{T}{N} \sum v_k^2 a^2 \left[ \frac{f(E')}{E' - i\Omega - E} + \frac{f(E)}{-E + i\Omega - E'} + \frac{f(-E')}{-E' - i\Omega + E} + \frac{f(-E)}{E + i\Omega + E'} \right] + \quad (2.194)$$

$$+ b^2 \left[ \frac{f(-E')}{-E' - i\Omega - E} + \frac{f(E)}{E + i\Omega + E'} + \frac{f(E')}{E' - i\Omega + E} + \frac{f(-E)}{-E + i\Omega - E'} \right] \quad (2.195)$$

$$-\sum_k a^2 \left[ \frac{f(-E) - f(-E')}{i\Omega + E' - E} + \frac{f(E) - f(E')}{i\Omega + E - E'} \right] - \sum_k b^2 \left[ \frac{f(E) - f(-E')}{i\Omega + E + E'} + \frac{f(-E) - f(E')}{i\Omega - E - E'} \right] \quad (2.196)$$

This structure is very general,  $a$  and  $b$  are what change for each response. The structure is always the same. Depending of the function we are computing one of  $a$  or  $b$  is zero. We can compute now the terms  $a^2$  and  $b^2$

$$a^2 = (uu' + vv')^2 \quad (2.197)$$

$$u^2 = \frac{1}{2} \left(1 + \frac{\xi}{E}\right) \quad v^2 = \frac{1}{2} \left(1 - \frac{\xi}{E}\right) \quad (2.198)$$

$$a^2 = u^2 u'^2 + v^2 v'^2 + 2uvu'v' = \frac{1}{4} \left(1 + \frac{\xi}{E}\right) \left(1 + \frac{\xi}{E'}\right) + \frac{1}{4} \left(1 - \frac{\xi}{E'}\right) \left(1 - \frac{\xi}{E}\right) + \frac{2\xi\xi'}{4EE'} \quad (2.199)$$

$$a^2 = \frac{1}{2} \left(1 + \frac{\xi\xi'}{EE'}\right) + \frac{1}{2} \frac{\Delta\Delta'}{EE'} \quad (2.200)$$

$$a^2 = \frac{1}{2} \left(1 + \frac{\xi\xi' + \Delta\Delta'}{EE'}\right) \quad (2.201)$$

$$b^2 = u^2 v'^2 + v^2 u'^2 - 2uvu'v' = \frac{1}{2} \left(1 - \frac{\xi\xi' + \Delta\Delta'}{EE'}\right) \quad (2.202)$$

For  $q \rightarrow 0$  we get a very simple expression. In our case we have  $a^2 = 1$  and  $b^2 = 0$ . This is true for this specific response function. The only things we need to know are the  $a$  and  $b$  variables. In particular, if we are interest in the limit for  $q \rightarrow 0$  and  $i\Omega = 0$ :

$$\Lambda_{jj}^{xx} = (q = 0, i\Omega = 0) = - \sum_k v_k^2 \frac{\partial f}{\partial E} \quad (2.203)$$

We implemented the fact that the spectrum of our quasiparticle representation is very difficult.

$$K'_{xx} = -\frac{n}{m} + \Lambda_{jj}^{xx} \quad (2.204)$$

$$K_{xx}(i\Omega = 0, q \rightarrow 0) = -\frac{n}{m} \sum_k \left(-\frac{\partial f}{\partial E}\right) v_k^2 \quad (2.205)$$

The Meissner effect was the fact that the current is proportional to the gauge field:

$$\vec{J}(x) = -\frac{n_s e^2}{mc} \vec{A}(x) = -\frac{1}{4\pi\lambda^2} \vec{A}(x) \quad (2.206)$$

In real space we have:

$$\vec{J}(q) = -\frac{n_s e^2}{m} \vec{A}(\vec{q}) \quad (2.207)$$

This is the Coulomb gauge.

$$\vec{\nabla} \cdot \vec{A} = 0 \quad q_x A_x(\vec{q}) + q_y A_y(\vec{q}) = 0 \quad (2.208)$$

In particular we are making the limit  $\vec{q}$  going to zero. Of course it depends on how we do the limits:

$$q_y = 0 \quad q_x A_x(q_x, q_y = 0) = 0 \quad A_x = 0 \quad (2.209)$$

To have a non zero x component we must take the reverse limits:

$$q_x = 0 \quad q_y \rightarrow 0 \quad (2.210)$$

$$J_x(q \rightarrow 0) = -\frac{n_s e^2}{mc} A_x(q_x = 0, q_y \rightarrow 0) \quad (2.211)$$

Now lets take our responce function

$$J_x(q \rightarrow 0) = K_x x(q_x = 0, q_y \rightarrow 0, \Omega = 0) A_x \quad (2.212)$$

For the point of view of the BCS function we do not see any difference on the order of the limit  $q \rightarrow 0$ . Then we can compute the superfluid density:

$$\frac{n_s}{m} = \frac{n}{m} - \sum_k v_k^2 \left( -\frac{\partial f}{\partial E} \right) \quad (2.213)$$

Now lets take the limit  $T \rightarrow 0$ :

$$T \rightarrow 0 \quad -\frac{\partial f}{\partial E} = \delta(E) \quad (2.214)$$

$$E_k = \sqrt{\xi_k^2 + \Delta^2} \quad (2.215)$$

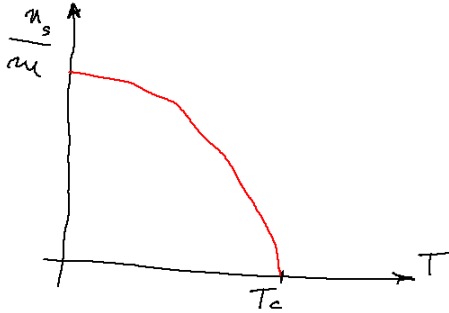
There is now way to satisfy the delta.

$$\frac{n_s}{m} \stackrel{T \rightarrow 0}{=} \frac{n}{m} \quad (2.216)$$

What happens to the superconductor, the paramagnetic state complicitly suppress paramagnetism, and the responce is purely diamagnetic. Indeed, we may realize that, when we go back to  $T_c$  and the gap closes, we have the paramagnetic responce as:

$$\sum_k v_k^2 \frac{\partial f}{\partial \xi_k} = \sum_k v_k \frac{d}{dk} f(\xi_k) = -\sum_k \frac{dv_k}{dk} f(\xi_k) = -\frac{1}{m} \sum_k f(\xi_k) = -\frac{n}{m} \quad (2.217)$$

Now we have no more diamagnetic responce. We are suppressing completely the diamagnetic limit, however closing the gap we recover. This function is a function of the temperature, and we get somethign as:



We can characterize the sperconducting by the appearence of a superfluid responce. This is the quantity that must be different from zero to give rise a superconductive behaviour.

If now we take the finite temperature behaviour we have the spectrum of the quasiparticles:

$$E_k = \sqrt{\xi_k^2 + \Delta^2} \quad (2.218)$$

Then the decay is approximate as:

$$e^{-\beta\Delta} \quad (2.219)$$

We can also have a power law, when we approach to  $T_c$  we can have also other type of excitation as phase fluctuations.

## 2.10 Phase fluctuations and gauge invariance breaking of BCS

The response function should satisfy some very important relations.

$$q_\mu K^{\mu\nu} = 0 \quad K^{\mu\nu} q_\nu = 0 \quad (2.220)$$

$$\omega K^{0i} + q_j K^{ji} = 0 \quad (2.221)$$

Let us take a static properties  $\omega = 0$  and  $q \rightarrow 0$ . In this case the response function becomes diagonal so:

$$q_x K_{xx}(\omega = 0, q \rightarrow 0) = 0 \quad (2.222)$$

To be more specific, this must be taken in the longitudinal limit.

$$K_{xx}(\omega = 0, q_y = 0, q_x \rightarrow 0) = 0 \quad (2.223)$$

This is the longitudinal limit. The vanishing of the response function in the longitudinal limit is the requirement of the Gauge invariance. Now, we can take the response function of BCS approximation. This is the correct response for the transfer. Our BCS response function does not satisfy this requirement, it violates gauge invariance and charge conservation. This is exactly what we expect, since the number of particles is not well defined in BCS (so the charge). This is a consequence of the phase condensation of the BCS wavefunction. We can recover the correct response by adding to the bare bubble the phase fluctuations. We can show this in the Ginzburg-Landau model. We have:

$$Z = \frac{n_s}{8m} (\nabla\theta)^2 \rightarrow \frac{n_s}{8m} (\vec{\nabla}\theta - \partial\vec{A})^2 \quad (2.224)$$

We can write an action to the dynamical case:

$$S = \frac{1}{8} \sum_k \vartheta(q) \vartheta(-q) q^\alpha q^\beta K_{BCS}^{\alpha\beta}(q) \quad (2.225)$$

If we take the  $q \rightarrow 0$  of the action we recover the static  $Z$  limit. So it is an extension of the dynamical Ginzburg-Landau. We can use the minimal substitution, to have the effect of a finite magnetic field:

$$S(A) = -\frac{1}{8} \sum_k [(iq^\alpha\theta + 2eA^\alpha)(-iq^\beta\theta + 2eA^\beta)] K_{BCS}^{\alpha\beta}(q) \quad (2.226)$$



$$S(A) = \frac{1}{8} \sum_q e^2 K_{BCS}^{\alpha\beta} A_\alpha(q) A_\beta(-q) + S_\theta + S_{\theta A} \quad (2.227)$$

This is an action. Then the partition function of the system will be:

$$Z = \int D[\theta] e^{-S_\theta[\theta]} \quad (2.228)$$

$$Z[A] = \int D[\theta] e^{-S(\nabla\theta+A)} = e^{-S[A]} \quad (2.229)$$

We can now compute the full electromagnetic response as the second derivative of the action respect to  $A$ :

$$\Pi_{\alpha\beta} = \left. \frac{\partial^2 S}{\partial A_\alpha(q) \partial A_\beta(-q)} \right|_{A=0} \quad (2.230)$$

If we do not include the coupling to the phase, we obtain simply the BCS response. If we have the fluctuation, we understand immediatly that the term  $S_{\theta A}$  gives a contribution to the response function. The phase is really coupled with the Gauge field.

$$Z = \int D[\theta] e^{-\theta^2 q^2 + q\theta A} \quad (2.231)$$

We can perform this integral analytically ( $q \rightarrow 0$ ):

$$S_\theta + S_{\theta A} = \frac{1}{8} \sum_q q^2 K_{BCS} \theta_q^2 + 4e_i \theta(q) \vec{q} \cdot \vec{A} K \quad (2.232)$$

$$\frac{1}{8} \sum_q q^2 \left[ \theta_q + 2e^i \frac{\vec{q} \cdot \vec{A}}{q^2} \right] K_{BCS} - \frac{1}{8} \sum_q AK_{BCS} \frac{(\vec{q} \cdot \vec{A})^2}{q^2} \quad (2.233)$$

The integration in  $\theta$  can be done explicity, we realize that the full response function is:

$$S_A = \frac{1}{2} e^2 K_{BCS} A^2 - \frac{1}{2} e^2 K_{BCS} \frac{(\vec{q} \cdot \vec{A})^2}{q^2} \quad (2.234)$$

This is the goal, because we can write the total response taking into account for all the phase fluctuations

$$\Pi_{xx} = K_{BCS} - \frac{q_x^2 K_{BCS}}{q_x^2 + q_y^2} \quad (2.235)$$

Now if we take the transverse limit:

$$\Pi_{xx}(q_x = 0, q_y \rightarrow 0) = K_{BCS} = \frac{n_s}{m} \quad (2.236)$$

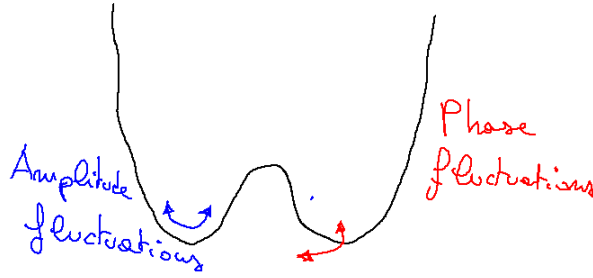
So the BCS approximation is correct in the transverse limit. When I take the longitudinal limit, then we have:

$$\Pi_{xx}(q_x \rightarrow 0, q_y = 0) = K_{BCS} - K_{BCS} = 0 \quad (2.237)$$

Then we are satisfying the gauge invariance equations. This is also physical, because only letting the phase to fluctuate we can conserve the number of particle. On the other hand BCS theory gives the correct response. The BCS theory

reproduces correctly the experimental results. The only problem is when we have disorder because disorder can couple longitudinal and transverse response, and BCS theory gives wrong results. This issue was discussed by Shrieffer in the first time. BCS theory is a bare bouble, you have to dress the bouble with all the processes with the vertex correction. What shrieffer showed is the vertex correction has a pole that describe the phase mode.

## 2.11 Amplitude and phase fluctuation in BCS approach



To use the Green function formalism it is convenient to write all the formulas in the Nambu notation. We must define the amplitude and phase excitations from the creation operators. The definitio of current and density are straight-forward. However, phase and amplitude are defined only for superconductors. We can define the operator:

$$\phi(q) = \sum_{k\sigma} c_{-k+\frac{q}{2},\downarrow} c_{k-\frac{q}{2},\downarrow} - \Delta_0 \quad (2.238)$$

$$A(q) = \phi(q) + \phi^\dagger(q) \quad (2.239)$$

If we have the superconductor order parameter that is constant we have:

$$\psi = \Delta e^{i\theta} \quad \Delta \approx \Delta \cos \theta = \psi^\dagger + \psi = \quad (2.240)$$

If we have take

$$i(\psi^\dagger - \psi) = \Delta \sin \theta \approx \Delta_0 \theta \quad (2.241)$$

Then the phase iperator can be defined as:

$$\theta(q) = i [\phi(q) - \phi^\dagger(q)] \quad (2.242)$$

Using this definition, we can rewrite the amplitude as:

$$A(q) = \sum_k \psi_{k+\frac{q}{2}}^\dagger \sigma_1 \psi_{k-\frac{q}{2}} \quad (2.243)$$

$$\theta(q) = \sum_k \psi_{k+\frac{q}{2}}^\dagger \sigma_2 \psi_{k-\frac{q}{2}} \quad (2.244)$$

If we take the green function:

$$G^{-1} = \begin{pmatrix} i\omega_n - \xi_k & \Delta \\ \Delta^* & i\omega + \xi_k \end{pmatrix} \approx \begin{pmatrix} i\omega - \xi_k & \Delta' + i\Delta'' \\ \Delta' - i\Delta'' & i\omega + \xi_k \end{pmatrix} \quad (2.245)$$

It is clear that the phase fluctuation change the imaginary part of the green function, while the amplitude the real part of the order parameter  $\Delta$  through the  $\sigma$  Pauli matrices.

We want to compute the correlation function. The interaction in the BCS equation can be written as:

$$H_I = -U \sum \phi^\dagger(q)\phi(q) \quad (2.246)$$

The BCS hamiltonian is the:

$$H_{BCS} = -U \phi^\dagger(0)\phi(0) = -U \sum_{kk'} c_{-k\downarrow} c_{k\uparrow} c_{k'\uparrow}^\dagger c_{-k\downarrow}^\dagger \quad (2.247)$$

The interaction we are taking is going behound the BCS theory, because we are adding the interaction at  $q \neq 0$ . So we are going beond the ground state of the BCS theory computed with mean-field. Electrons can also have bosonic collective excitations. What is the energy and momento that we have to put and trasmit to the system. Collective excitations are exactly the same as the metal.

Let me write the interaction in the way:

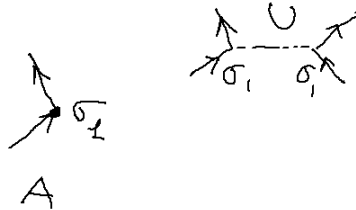
$$H_I = -U \sum_{\rho} [A^\dagger(q)A(q) - \theta^\dagger(q)\theta(q)] \quad (2.248)$$

We want to compute the correlation function for the amplitude:

$$\langle T A^\dagger(q)A(q) \rangle = \langle T A^\dagger(q)A(q) e^{-\beta H_I} \rangle = \quad (2.249)$$

$$\langle A^\dagger(q)A(q) \rangle - \beta \langle A^\dagger(q)A(q)H_I \rangle + \dots \quad (2.250)$$

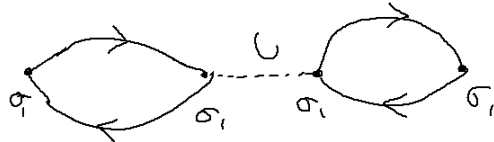
The first term is



The first term we have a bouble:

The bouble is simply:

$$\chi_0 = G(k - \frac{q}{2})\sigma_1 G(k + \frac{q}{2})\sigma_1 \quad (2.251)$$

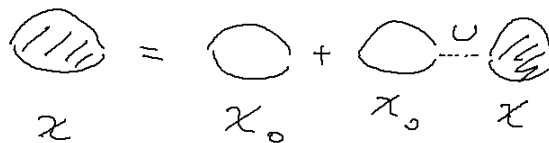


The second term we have:  
 The second term can be called as:

$$\chi_0 U \chi_0 \tag{2.252}$$

The other terms can be summed and the total susceptibility is:

$$\chi = \chi_0 + \chi_0 U \chi \tag{2.253}$$



We are not taking all the possible diagrams, because we are neglecting vertex correction. This is the RPA (Random Phase Approximation) resummation. We can solve RPA by:

$$\chi = \frac{\chi_0}{1 - U\chi_0} \tag{2.254}$$

We can have a denominator that goes to zero. We can get resonance in the frequencies, therefore RPA is able to describe the modes. We neglected the  $\theta$

terms, because the boucle between  $A$  and  $\theta$  do not talk each other. This is a particular case for BCS superconductors.

We must compute the  $\chi_0$  susceptibility:

$$\chi_{\Delta\Delta}^0 = \frac{T}{V} \sum_{ki\omega_n} \text{tr} [G_0(k, i\omega_n) \sigma_1 G_0(k+q, i\omega = i\Omega) \sigma_1] \quad (2.255)$$

The other is:

$$\chi_{\theta\theta}^0 = \frac{T}{V} \sum_{ki\omega_n} \text{tr} [G_0(k, i\omega_n) \sigma_2 G_0(k+q, i\omega = i\Omega) \sigma_2] \quad (2.256)$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (2.257)$$

$$G = U (i\omega - \Lambda)^{-1} U^\dagger = \begin{pmatrix} u_k & -v_k \end{pmatrix} \quad (2.258)$$

Inside the trace we:

$$\text{tr} [i\omega - \Lambda)^{-1} U^\dagger \sigma_1 U' (i\omega + i\Omega - \Lambda')^{-1} U^\dagger \sigma_1 U] \quad (2.259)$$

$$U^\dagger \sigma_1 U' = \begin{pmatrix} u & v \\ -v & u \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u' & -v' \\ v' & u' \end{pmatrix} = \begin{pmatrix} u & v \\ -v & u \end{pmatrix} \begin{pmatrix} v' & u' \\ u' & -v' \end{pmatrix} = \begin{pmatrix} uv' + u'v & -vv' + uu' \\ uu' - vv' & -uv' - vu' \end{pmatrix} \quad (2.260)$$

$$a = u'v + uv' \quad b = uu' - vv' \quad (2.261)$$

$$a^2 = u'^2 v^2 + u^2 v'^2 + 2u'uv'v \quad b^2 = u^2 u'^2 + v^2 v'^2 - 2uu'vv' \quad (2.262)$$

$$a^2 = \frac{1}{4} \left(1 + \frac{\xi'}{E'}\right) \left(1 - \frac{\xi}{E}\right) + \frac{1}{4} \left(1 + \frac{\xi}{E}\right) \left(1 - \frac{\xi'}{E'}\right) + \frac{\Delta\Delta'}{2EE'} = \frac{1}{2} - \frac{1}{2} \frac{\xi\xi'}{EE'} + \frac{1}{2} \frac{\Delta\Delta'}{EE'} = \frac{1}{2} \left(1 - \frac{\xi\xi' - \Delta\Delta'}{EE'}\right) \quad (2.263)$$

We can go to the final full expression, the same computed for the current:

$$\chi_{\Delta\Delta}^0 = \frac{T}{N} \sum_k \frac{1}{2} \left(1 - \frac{\xi\xi' - \Delta^2}{EE'}\right) [f(E') - f(E)] \left[ \frac{1}{E' - E - i\Omega} + \frac{1}{E' - E + i\Omega} \right] \quad (2.264)$$

$$+ \frac{1}{2} \left(1 + \frac{\xi\xi' - \Delta^2}{EE'}\right) [f(E') - f(-E)] \left[ \frac{1}{E' + E - i\Omega} + \frac{1}{E' + E + i\Omega} \right] \quad (2.265)$$

$$\Delta\chi_{\Delta\Delta} = \frac{\chi_{\Delta\Delta}^0}{\frac{2}{U} + \chi_{\Delta\Delta}^0} \quad (2.266)$$

The 2 and the + in the denominators comes from how we defined the greens functions.

We can start to do the limit:

$$\chi_{\Delta\Delta}^0(q \rightarrow 0, i\Omega) = -\frac{1}{N} \sum_k \frac{\xi^2}{E^2} \tanh \frac{\beta E}{2} \left[ \frac{1}{2E - i\Omega} + \frac{1}{2E + i\Omega} \right] \quad (2.267)$$

This is a complex function. We want to see what happens for  $\omega$  and  $q$  going to zero. If we have the behaviour of a typical massive mode, we get a finite quantity. If we have zero mass, we get an infinite response.

So we consider the denominator of the  $\chi_{\Delta\Delta}$

$$\frac{2}{U} + \chi_{\Delta\Delta}^0(q=0, \omega=0) = \frac{2}{U} - \frac{1}{N} \sum_k \frac{\xi^2}{E^3} \tanh\left(\frac{\beta E}{2}\right) \quad (2.268)$$

The self consistent gap equation between  $U$  and  $E_k$ :

$$\frac{2}{U} + \chi_{\Delta\Delta}^0(q=0, \omega=0) = \frac{1}{N} \sum_k \frac{1}{E_k} \tanh\frac{\beta E_k}{2} - \sum_k \frac{\xi^2}{E^3} \tanh\frac{\beta E_k}{2} = \frac{1}{N} \sum_k \tanh\frac{E_k \beta}{2} \frac{\Delta^2}{E_k^3} \quad (2.269)$$

In the limit  $T = 0$  we get:

$$\frac{2}{U} + \chi_{\Delta\Delta}^0(q=0, \omega=0) \stackrel{T=0}{=} \frac{1}{N} \sum_k \frac{\Delta^2}{E_k^3} \neq 0 \quad (2.270)$$

$$\frac{2}{U} + \chi_{\Delta\Delta}^0(q=0, \omega=0) \stackrel{T=T_c}{=} 0 \quad (2.271)$$

The mass of the Higgs mode is different from zero only in the superconductive state. We can write the  $a^2$  and  $b^2$  value also for the phase fluctuations:

$$a^2 = \frac{1}{2} \left(1 - \frac{\xi\xi' + \Delta\Delta'}{EE'}\right) \quad b^2 = \frac{1}{2} \left(1 - \frac{\xi\xi' + \Delta\Delta'}{EE'}\right) \quad (2.272)$$

We have:

$$\frac{2}{U} + \chi_{\theta\theta}^0(q=0, \omega=0) = \frac{2}{U} - \frac{1}{N} \sum_k \tanh\frac{\beta E_k}{2} \frac{1}{E_k} \quad (2.273)$$

If we now use the self consistent equation we have:

$$\frac{2}{U} + \chi_{\theta\theta}^0(q=0, \omega=0) = 0 \quad (2.274)$$

This is exactly the Goston mode for the transition, so it is massless. We have linked the Ginzburg-Landau theory with BCS, because we considered the excitations of the Mexican hat.

Is the Higgs mode a relativistic mode (at finite frequency)? The Green's function of the electron is:

$$G = \frac{1}{i\omega_n - \xi} \quad (2.275)$$

The spectrum of the electron is:

$$A(k, \omega) = \delta(\omega - \xi_k) \quad (2.276)$$

If we take the phonons:

$$G(q, \omega) = \frac{1}{i\omega_n - \omega_0} \quad (2.277)$$

If we want to know the spectrum of the Higgs fluctuations we have:

$$A_{\Delta\Delta}(k, \omega) = -\frac{1}{\pi} \Im \chi_{\Delta\Delta}(k, \omega) \quad (2.278)$$

The Higgs mode has no a pick around the finite mass. We can compute the same for  $q \rightarrow 0$  but finite frequency:

$$\frac{2}{N} + \chi_{\Delta\Delta}^0(\omega, q = 0) = \frac{1}{n} \sum_k \frac{1}{E_k} \tanh \frac{\beta E_k}{2} - \frac{1}{N} \sum_k \tanh \frac{\beta E_k}{2} \frac{\xi^2}{E^2} \frac{4E}{4E^2 - \omega^2} \quad (2.279)$$

$$\frac{2}{N} + \chi_{\Delta\Delta}^0(\omega, q = 0) = \frac{1}{N} \sum_k \frac{1}{E_k} \tanh \frac{\beta E_k}{2} \left[ 1 - \frac{4\xi^2}{4E^2 - \omega^2} \right] = \frac{1}{N} (4\Delta^2 - \omega^2) \sum_k \tanh \frac{\beta E_k}{2} \frac{1}{E(4E^2 - \omega^2)} \quad (2.280)$$

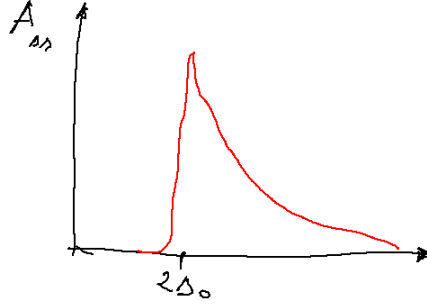
This means that this guy has the structure:

$$\frac{2}{N} + \chi_{\Delta\Delta}^0(\omega, q = 0) = (4\Delta^2 - \omega^2) F(\omega) \quad (2.281)$$

If  $F$  is regular when  $\omega = 2\Delta$  then I have the excitation. However,  $F(\omega)$  diverges at that values as:

$$F(\omega) \sim \frac{1}{\sqrt{4\Delta^2 - \omega^2}} \quad (2.282)$$

Then we have a Higgs mode that has a divergence at  $2\Delta$ . This is very strange behaviour, we have a long tail around the excitation.



The problem of the superconductor is that the Higgs has the same mass as the single particle excitations that completely cover it. Higgs mode is not visible, because it is scalar, it does not couple with current or density.

## Chapter 3

# Berezinsky-Konsterlitz-Touless

In the original formulation the transition was studied from classical spin model.

$$H = -J \sum_{ij} \vec{s}_i \cdot \vec{s}_j \quad (3.1)$$

Below some transition temperature the spins are aligned, if we look at the average value of the spin, this is aligned in some direction.

$$\langle \vec{s}_i \rangle = \vec{m} \quad (3.2)$$

The correlation of the spin this is a typical correlation length:

$$\langle \vec{s}_i \cdot \vec{s}_j \rangle = M_0^2 + e^{-r_{ij}/\xi} \quad T < T_c \quad (3.3)$$

This is the 3d model. To understand the problem in 2D we now consider the xy model. We fix the length of the spins to 1. So the interaction becomes:

$$H = -J \sum_{ij} \cos(\theta_i - \theta_j) \quad (3.4)$$

What happens now to this model? Is it possible to have a transition. We are talking about classical spins. The spin can be written with a modulus and a phase:

$$\vec{S} = S e^{i\theta} \quad (3.5)$$

This is analogous with the order parameters of superconductors:

$$\Delta = |\Delta| e^{i\theta} \quad (3.6)$$

This analogy is even more profound, if the spins are more or less ordered and we can expand the cosine:

$$H \approx \frac{J}{2} \int d^3r (\Delta\theta(r))^2 \quad (3.7)$$



This expression recalls the one that we derive the Ginzburg Landau model for phase fluctuations. If we identify  $J$  with:

$$J = \frac{n_s e^2}{4m} \quad (3.8)$$

This describes the universality class of the physical interpretations. The problem of being in two dimensions is the fact that phase fluctuations (the Goldstone mode) are dangerous. Phase fluctuations cost too much, and the system tries to remain in the disordered phase. This is what is stated in the Mermin-Wagner theorem. We can consider in general the Hamiltonian:

$$H = \frac{1}{2\Omega} \sum_q G(q) |u_q|^2 \quad u_q = u_{-q}^* \quad (3.9)$$

This is exactly the form of our Hamiltonian in  $q$  space.  $u_q$  is a general Fourier transform of the variable of our model. In our case it will be  $\theta_q$ . We want to compute the thermodynamic averages.

$$\mathcal{Z} = \int \mathcal{D}[u] e^{-\beta H[u]} = \prod_q \int \frac{du_q du_q^*}{2\pi} e^{-\beta H} \quad (3.10)$$

This integral can be restricted only to the positive  $q$  because we know that  $u_q = u_{-q}^*$ .

$$\int \frac{du_q du_q^*}{2\pi} e^{-a u_q u_q^*} = \frac{1}{a} \quad (3.11)$$

The average value of  $u^2$  is:

$$\int \frac{du_q du_q^*}{2\pi} u_q u_q^* e^{-a u_q u_q^*} = \frac{1}{a^2} \quad (3.12)$$

Now we can compute the partition function over this Gaussian Hamiltonian.

$$\mathcal{Z} = \prod_{q>0} \int \frac{du_q du_q^*}{2\pi} e^{-\frac{\beta}{\Omega} G(q) u_q u_q^*} = \prod_{q>0} \frac{\Omega}{\beta G(q)} \quad (3.13)$$

In the same way we can compute the correlation function:

$$\langle u_q u_{q'} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[u] u_q u_{q'} e^{-\beta H[u]} = \frac{1}{\mathcal{Z}} \delta_{q+q'} \prod_{q'' \neq q} \frac{\Omega}{\beta G(q'')} \left[ \frac{\Omega}{\beta G(q)} \right] = \frac{\Omega}{\beta G(q)} \delta_{q+q'} \quad (3.14)$$

In a Gaussian model the correlation function is the inverse of the Hamiltonian coupling. Now we can discuss a more profound property.

$$\langle e^{iR(r)} \rangle = e^{-\frac{1}{2} \langle [R(r)]^2 \rangle} \quad (3.15)$$

Where the  $R(r)$  function is linear in our Gaussian variable.

$$R(r) = \frac{1}{\Omega} \sum_q u_q C_{-q}(r) \quad (3.16)$$

The only non zero result is for  $q' = -q$ . This is a very well known property. If we have a quadratic model, we know how to compute the averages.

$$\langle e^{iR(r)} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[u] e^{i\frac{1}{r} \sum_q u_q C_q(r)} e^{-\beta H[u]} = \frac{1}{\mathcal{Z}} \int \mathcal{D}[u] e^{-\frac{\beta}{\Omega}} \left[ \sum_{q>0} G(q) u_q u_q^* + \frac{i}{\Omega} \sum_{q>0} (u_q C_{-q} + u_{-q} C_q) \right] \quad (3.17)$$

We can rewrite it as:

$$\frac{1}{\mathcal{Z}} \int \mathcal{D}u \exp \left[ \underbrace{-\frac{\beta}{r} \sum_q G(q) \left( u_q + i \frac{C_q}{2\beta G(q)} \right) \left( u_q - i \frac{C_{-q}}{2\beta G(q)} \right)}_{\mathcal{Z}} \right] \exp \left( -\frac{1}{4\Omega} \sum_{q>0} \frac{C_q C_{-q}}{\beta G(q)} \right) \quad (3.18)$$

SO the result is:

$$\langle e^{iR(r)} \rangle = e^{-\frac{T}{2\Omega} \sum_q \frac{C_q C_{-q}}{G(q)}} \quad (3.19)$$

We must then prove that:

$$\langle [R(r)]^2 \rangle = \left\langle \frac{1}{\Omega^2} \sum_{qq'} u_q C_{-q} u_q' C_{-q'}(r) \right\rangle = \frac{T}{\Omega} \sum_q \frac{C_{-q}(r) C_q(r)}{G(q)} \quad (3.20)$$

If I have the Gaussian model we can analytically compute the correlation functions of gaussian models. All the properties will depend on the form of the gaussian propagator as a function of the momenta.

To have a finite magnetization we need to have a finite magnetization:

$$\langle \vec{S} \rangle \neq 0 \quad S = S e^{i\theta} \quad (3.21)$$

So what we want to compute is:

$$\langle S \rangle = \langle e^{i\theta(r)} \rangle \quad (3.22)$$

We can do this integral explicitly in the quadratic case:

$$C_q(r) = e^{iqr} \quad (3.23)$$

We can use the equation we derived:

$$\langle S \rangle = e^{-\frac{T}{2} \sum_q \frac{1}{Jq^2}} \quad (3.24)$$

This integral is:

$$\sum_q \frac{1}{Jq^2} = \frac{1}{J} \int \frac{d^2q}{(2\pi)^2} \frac{1}{q^2} = \frac{1}{J} \int_{1/L}^{1/a} \frac{dq}{2\pi} \frac{1}{q} = \frac{1}{2\pi J} \ln \frac{L}{a} \quad (3.25)$$

If the integral was in 3D i wuold not have this divergence in the thermodynamic limit. We are not worried by ultraviolet divergences are cutoff by the lattice space. But infrared divergences that is with the system size  $L$ .

$$\langle S \rangle = e^{-\frac{T}{4\pi J} \ln \frac{L}{a}} = \left( \frac{a}{L} \right)^{\frac{T}{4\pi J}} \xrightarrow{L \rightarrow \infty} 0 \quad (3.26)$$

The presence of the phase mode, that is massless in the long wavelength limit, implise that the order parameter goes to zero in two dimension. The presence of

the Goston mode forbids the breaking of the continuous symmetry. The Mermin-Wagner theorem states that we cannot brake the continuous symmetry in two dimension. An ordinary phase transition is not possible in the thermodynamic limit. This limitation is not so serious for finite systems because they have a finite size. If we try to plug a numbers we understand that the limitation is not so serious. For superconductor we can use:

$$S = 0.01 \quad a \sim 10 \text{ nm} \quad \frac{T}{4\pi J} = \frac{1}{8} \quad (3.27)$$

Then  $L$  to have the order parameter vanishing should be:

$$L = 10 \times 10^5 \text{ km} \quad (3.28)$$

Therefore, we see phase transitions in two dimensional system that are usually very small. But we can take the correlation function:

$$\langle S_i S_j \rangle = \langle e^{i\theta(q)} e^{-i\theta(0)} \rangle = e^{-\frac{1}{2} \sum_q \langle [\theta(r) - \theta(0)]^2 \rangle} \quad (3.29)$$

$$\sum_q \langle [\theta(r) - \theta(0)]^2 \rangle = \frac{T}{\Omega} \beta \sum_q \frac{(e^{iqr} - 1)(e^{-iqr} - 1)}{Jq^2} = \frac{T}{\Omega} \sum_q \frac{2 - 2 \cos q \cdot r}{Jq^2} \quad (3.30)$$

The problem is when  $qr \gg 1$  in this integral

$$\frac{T}{2\pi} \int_{\frac{1}{r}}^{1/a} dq \frac{1}{Jq} = \frac{T}{\pi J} \ln \frac{r}{a} \quad (3.31)$$

This a very similar result

$$\langle S_i S_j \rangle = e^{-\frac{T}{2\pi J} \ln ra} = \left( \frac{a}{r} \right)^{\frac{T}{2\pi J}} \quad (3.32)$$

Then the correlation goes to zero with a power low. The way in which correlation function goes to zero the system is quasi-long range ordered. It is true that in principle the Goston mode should forbid ordering, in practice the correlation function decays correlation. If we use the full cosine formula, we discover that the correlation function in the high temperature phase we have a correlation function that decays as an exponential. So we have actually a phase transition.

$$\langle S_i S_j \rangle \sim e^{-r_{ij}/\xi} \quad \text{high } T \quad (3.33)$$

You cannot go smooth from a powerlow behaviour and an exponential decayment, so there must be a phase transition at a finite temperature. The transition is driven by the presence of an excitation that we have not included so far. We have the continius system that generate goston modes. But the model has another symmetry:  $\theta_i + 2\pi$  leaves the system unchanged. To this syummetry we can include the presence of an additional excitation that are topological excitations that are the vortices. This transition came out from the fact that we are dealing with a cosine model, that is not analytically integrable.

### 3.1 Vortex excitation

We can take an analytical solution so that:

$$\vec{S} = \begin{pmatrix} \cos(\theta_0 + \theta_v) \\ \sin(\theta_0 + \theta_v) \end{pmatrix} \quad (3.34)$$

$$\theta_v(r) = \arctan \frac{y - y_0}{x - x_0} \quad (3.35)$$

We can compute the configuration of the spins if we are going around the vortex.

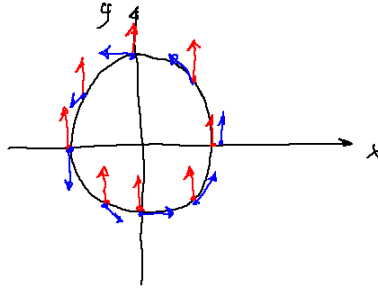


Figure 3.1: Vortex excitation.

Let us compute the gradient:

$$\vec{\nabla}\theta_v = \begin{pmatrix} -\frac{y-y_0}{(r-r_0)^2} \\ \frac{x-x_0}{(r-r_0)^2} \end{pmatrix} = \frac{1}{r} \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} = \frac{1}{r} \hat{dl} \quad (3.36)$$

That means that if we try to compute the circulation of the theta we have:

$$\oint \vec{\nabla}\theta \cdot d\vec{l} = \frac{1}{r} \int_0^{2\pi} d\theta r = 2\pi \quad (3.37)$$

We are accumulating the  $2\pi$  phase while we circulate around the vortex. We can compute the energy cost of the vortex:

$$E = \frac{J}{2} \int d^2r (\nabla\theta_v)^2 \quad (3.38)$$

$$(\nabla\theta_v)^2 = \frac{1}{r^2} \quad (3.39)$$

$$E = \frac{2\pi J}{2} \int_a^L dr \frac{1}{r} = \pi J \ln \frac{L}{a} \quad (3.40)$$

Its energetic cost is again logarithmic. However, at finite temperature, I have the balance between energy and entropy:

$$F = E - TS \quad (3.41)$$

So we must compute the entropy of the vortex:

$$S = \ln \# = \ln \frac{L^2}{a^2} \quad (3.42)$$

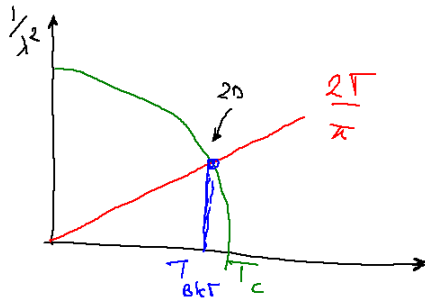
The entropy always goes logarithmic with the system size. However here also the energy increases logarithmic.

$$F = (\pi T - 2T) \ln \frac{L}{2} \quad (3.43)$$

Then will exist a temperature where entropic gain in free energy to generate a vortex is greater than its energetic cost. Then we found the transition temperature:

$$T_c \approx \frac{\pi J}{2} \quad (3.44)$$

The temperature is directly connected with the stiffness  $J$ . Then when the  $T > T_c$  vortices proliferate. If we have two vortices with opposite vorticity are like charges that interact with a logarithmic potential. If they are bounded together the system is ordered, if they are unbounded, they proliferate and we have disorder. What characterizes superconductors, what really characterizes the superconductive behaviour is the stiffness. The Kosterlitz-Toules describes a state with zero stiffness that goes in a state with finite stiffness.



This discontinuous jump there are two manifestation of this jump. One is this discussed, and the other one is the current:

$$I \sim V^a \quad (3.45)$$

Where  $a$  goes from 1 to 2 discontinuous. This is very difficult to see by experiments. We should see signatures that are not the usual one. For example. People did these experiments on superfluid helium.