# Notes on advanced many body physics

Lorenzo Monacelli

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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.

Lorenzo Monacelli

# **Contents**



## <span id="page-4-0"></span>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:

$$
a_k^{\dagger} \qquad a_k \tag{1.1}
$$

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

$$
\left\{a_k^{\dagger}, a_{k'}\right\} = \delta_{kk'} \tag{1.2}
$$

If they are bosons we have the commutation rule:

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

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  $H_I$ .

<span id="page-4-1"></span>
$$
H = H_0 + H_I \qquad H_0 = \sum_k \xi_k a_k^\dagger a_k \tag{1.4}
$$

As Eq. [\(1.4\)](#page-4-1) 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:

<span id="page-4-2"></span>
$$
\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{k} e^{ikr} a_k \tag{1.5}
$$

Thanks to Eq. [\(1.5\)](#page-4-2) it is possible to redefine a second quantization version of the standard observables. For example, the density, defined as:

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

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

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

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

$$
H_{I} = \frac{1}{2} dr dr' \rho(r) V(r - r') \rho(r')
$$
\n(1.8)

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

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

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

#### <span id="page-5-0"></span>1.1 Non interactive Green's functions

It usefull to learn something about the non interactive part of the Hamitlonian. We know exactly the egienstates of the system:

$$
\xi_k = \varepsilon_k - \mu = \frac{k^2}{2m} - \mu \tag{1.10}
$$

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

We can introduce the Green's function:

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

Where  $|\Phi_0\rangle$  is the groud 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 identify the Heisenberg representation, so the time dependence is included in the operator, not in the wave-fucntion

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

We assume that the chemical potential is already included in the Hamiltonian. So lets always assume taht

$$
H = H_0 - \mu N \tag{1.13}
$$

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

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

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:

$$
\tilde{a}_k(t) = e^{iH_0t} a_k e^{-iH_0t} \tag{1.15}
$$

To compute the time evolution we must apply  $\tilde{a_k}(t)$  to a generic wave-function  $|\Phi\rangle$ .

$$
|\Phi\rangle = |\cdots n_k \cdots\rangle. \tag{1.16}
$$

$$
\tilde{a}_k(t) = e^{iH_0t} a_k e^{-iH_0t} = e^{it \sum_{k'} \xi_{k'} a_{k'}^\dagger a_{k'}} a_k e^{-it \sum_{k'} \xi_{k'} a_{k'}^\dagger a_{k'}} \tag{1.17}
$$

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

$$
\hat{n}_k = a_k^{\dagger} a_k \tag{1.18}
$$

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

$$
\hat{a}_k(t) \left| \Phi \right\rangle = e^{-it\xi_k n_k} e^{it\xi_k \hat{n}_k} \left| \cdots n_k - 1 \cdots \right\rangle = e^{-it\xi_k} \left| \cdots n_k - 1 \cdots \right\rangle \tag{1.20}
$$

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

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

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

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

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

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

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:

$$
G(k,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G(\vec{k},t) = -i \int_{0}^{\infty} e^{i\omega t} e^{-it\xi_k} = -i \int_{0}^{\infty} e^{i(\omega - \xi_k + i0^+)} (1.25)
$$

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.

$$
G(k,\omega) = -i \left. \frac{e^{i(\omega - \xi_k + i0^+)} }{i(\omega - \xi_k + 0^+)} \right|_0^\infty = \frac{1}{\omega - \xi_k + i0^+ \operatorname{sign}(k - k_f)}
$$
(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 secific positions in the complex plane, as reported in Figure [1.1.](#page-7-1)

The poiles 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  $G(k, t)$ :

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

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

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

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

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



<span id="page-7-1"></span>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:

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

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

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

#### <span id="page-7-0"></span>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  $H_I$ :

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

$$
|\psi_I(t)\rangle = e^{iH_0t} |\psi_s(t)\rangle = e^{iH_0t} e^{-iHt} |\psi(0)\rangle
$$
\n(1.33)

We have a evolution operator that is

$$
U(t) = e^{iH_0t}e^{-iHt}
$$
\n(1.34)

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

$$
S(t, t') = U(t)U^{\dagger}(t')
$$
\n(1.35)

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

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

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

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

$$
S = S(-\infty, \infty) \tag{1.38}
$$

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.

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

$$
\Sigma(k,\omega) = \Sigma'(k_f,0) - \left. \frac{\partial \Sigma'}{\partial \omega} \right|_{\omega=0 \, k=k_f} \omega - \left. \frac{\partial \Sigma'}{\partial k} \right|_{k=k_f} \omega = 0} (k-k_f) + i\Sigma''(k_f,0)
$$
\n(1.40)

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

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

$$
\xi_k = \varepsilon_k - \mu = v_f(k - k_f) - \mu \tag{1.42}
$$

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

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

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

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:

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

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:

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

We want to compute it for positive times. To perform this integarl we can use the complex plane (Figure [1.2\)](#page-9-1).



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

<span id="page-9-1"></span>We can use the residual theorem:

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

So the real time Green function we have a total spetral 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:

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

Where  $G_r$  is the retarded Green function.

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

### <span id="page-9-0"></span>1.3 Matzubara formalism

We defined the Matzubara funcion in real time:

$$
G(k,\tau) = -\langle Ta_k(\tau)a_k^{\dagger}(0)\rangle
$$
 (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  $T = 0$ .

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

We proved that

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

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

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

We can compute explicitely the Green function.

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

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

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

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

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

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

We can compute the Fourier transform of the Matzubara function:

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

Remember as  $\omega_n$  is defined for fermionic fucntions

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

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

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

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

#### <span id="page-11-0"></span>1.4 Response functions

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

$$
S(t) = \langle A(t)A(0) \rangle \qquad S(\omega) \tag{1.62}
$$

$$
\chi(t) = i\theta(t) \langle [A(t), A(0)] \rangle \qquad \chi(\omega) \tag{1.63}
$$

$$
\chi(\tau) = \langle A(\tau)a(0) \rangle \qquad \chi(i\omega_n) \tag{1.64}
$$

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

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

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

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

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

$$
\chi(\omega) = \chi(i\omega_n \to \omega + 0^+) \tag{1.67}
$$

We will write explicity 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:

$$
H = H_s + H_{sp} \tag{1.68}
$$

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

$$
H_{sp} = gA_s A_p \tag{1.69}
$$

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:

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

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

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

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

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  $t = -\infty$ .

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

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

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

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

$$
\int dt e^{i\omega t} \sum_{f} \langle s_i | e^{iH_s t} A_s e^{-iH_s t} | s_f \rangle \langle s_f | A_s | s_i \rangle \tag{1.75}
$$

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

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

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

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

We can now compute the  $\chi$  function explicitely

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

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

<span id="page-12-0"></span>
$$
\chi(t) = i\theta(t) \sum_{mn} |\langle m|A|n\rangle|^2 e^{\beta F} \left(e^{-\beta E_m} e^{-\beta E_n}\right) e^{i(E_m - E_n)t}
$$
(1.80)

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

$$
\chi(\omega) = \int_{-\infty}^{\infty} \chi(t) r^{i\omega t} \sim \int_{0}^{\infty} dt e^{i\omega t} e^{i\alpha t} \qquad \alpha = E_m - E_n \tag{1.81}
$$

To regularize the integral we must write:

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

$$
\chi(\omega) \sim \left. \frac{e^{i\omega\alpha + i0^+}}{i(\omega + \alpha + i0^+)} \right|_0^\infty = \frac{i}{\omega + \alpha + i\delta} \tag{1.83}
$$

If we apply this to the Eq. [\(1.80\)](#page-12-0) we get:

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

If we take the imaginary part:

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

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

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

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

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

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

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

We get immediatly that:

$$
S(\omega) = 2\left[1 + n_B(\omega)\right] \chi''(\omega) \tag{1.91}
$$

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

$$
\chi(\tau) = \langle T_{\tau} A(\tau) A(0) \rangle_{\tau > 0} = \langle A(\tau) A(0) \rangle = \sum_{nm} e^{-\beta (E_m - F)} \langle m | e^{\tau H} A e^{-\tau H} | n \rangle \langle n | A | m \rangle
$$
\n(1.92)\n
$$
\chi(\tau) = \sum_{n} e^{-\beta (E_m - F)} \sigma(E_m - E_n) |\langle m | A | n \rangle|^2
$$
\n(1.93)

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

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

$$
\int_0^\beta d\tau e^{i\Omega_m \tau} e^{\tau \alpha} = \left. \frac{e^{i\Omega_m \tau} e^{\tau \alpha}}{i\Omega_m + \alpha} \right|_0^\beta = \frac{e^{\beta \alpha} - 1}{i\Omega_m + \alpha} \tag{1.94}
$$

This means that:

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

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

It is now preaty clear that:

$$
\chi(\omega) = \chi(i\omega_n \to \omega + 0^+) \tag{1.97}
$$

#### <span id="page-14-0"></span>1.4.1 Linear responce

We can define a new hamiltonaian

$$
H_t = H - h(t)A \tag{1.98}
$$

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

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

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

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

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

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

$$
\langle \psi_n(t) | B | \psi_n(t) \rangle \qquad i \frac{d \left| \psi_n(t) \right\rangle}{dt} = H_t | \psi_n(t) \rangle \tag{1.102}
$$

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

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

$$
\rho(t) = \sum_{n} c_n \left| \psi_n(t) \right\rangle \left\langle \psi_n(t) \right| \tag{1.104}
$$

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

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

We can use linear responce theory:

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

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

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

We can compute the commutator:

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

It is possible to solve this equation:

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

We can get the responce function:

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

This is is just:

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

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

As we have that:

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

The responce 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 responce. This can be used to derive the drude formula, which is preatty nice.

#### <span id="page-15-0"></span>1.4.2 Density buble

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

$$
\int V(x,t)\rho(x,t)dx\tag{1.114}
$$

We want to compute the Matzubara responce:

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

We have to establish what is the quantity we want to compute. This is solve by linear responce 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:

$$
\sigma(\beta, 0) = 1 \tag{1.116}
$$

$$
\chi^{0}_{\rho\rho} = \langle \psi^{\dagger}(r,\tau)\psi(r,\tau)\psi^{\dagger}(0,0)\psi(0,0)\rangle \tag{1.117}
$$

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

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

We have two possible contractions:



The only cointraction that matters is:

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

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

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

We Fourirer Transform the Green's functions:

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

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

$$
-q + k - k' = 0 \tag{1.122}
$$

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

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



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

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

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

$$
i\omega_n = (2n+1)\pi T \tag{1.125}
$$

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 Matzubara fermionic frequencies:

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

We can compute the residual of the fermi functions:

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

This means that the Matzubara sum can be pefromrmed as:

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

Where the path on the complex plane goes around



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

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

In pratice we have:

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

We have two poles:

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

The Fermi function is periodic in the bosonic matzubara frequencies:

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

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

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

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

$$
\chi'(q=0;\omega) = 0 \tag{1.134}
$$

$$
\lim_{q \to 0} \chi'(q, \omega = 0) = \frac{1}{\Omega} \sum_{k} \frac{\partial f}{\partial \xi_k} \to N_F \tag{1.135}
$$

#### <span id="page-18-0"></span>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:

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

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

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

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

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

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

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

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

If we can introduce a Delta function for the complex exponential

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

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

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

Therefore, the intensity is of the probe is:

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

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

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

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

Then the greens function that obtain this quantity is:

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

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.

### <span id="page-19-0"></span>1.5 Optical conductivity

#### DRUDE THEORY

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

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

The final conducibility is:

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

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

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

$$
\vec{p} \to \vec{p} - \frac{e}{c}\vec{A} \tag{1.149}
$$

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

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

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

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

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

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

We can integrate by part.

$$
\int c^{\dagger}(c)(\nabla A)c(x) = -\int \nabla c^{\dagger}Ac - \int c^{\dagger}A\nabla c \qquad (1.153)
$$

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

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

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

The last term is:

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

Therefore the current is:

 $\overline{1}$ 

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

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

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

$$
\vec{v}_k = \frac{\partial \varepsilon_k}{\partial \vec{k}} \tag{1.159}
$$

This means that the vertext of the Feynman theory are



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

$$
J_{\mu}(q) = eK_{\mu\nu}(q)A_{\nu}(q)
$$
\n(1.160)

Where

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

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

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

Now it is possible to define the optical conductivity.

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

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

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

In a compleately unrealistic case it is equvalent 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 square brakets is zero. However, it is usefull to write it in this way because we can write a sum rule:

$$
\int_{-\infty}^{\infty} d\omega \Re \sigma(\omega) = \frac{\pi e^2 n}{m} - \pi e^2 \Pi_{xx}(0) + e^2 \int d\omega \frac{\Im \Pi_{xx}(\omega)}{\omega}
$$
(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 Π matrix. We will do the same as before, considering the velocity in the vertex. The bare bouble approximation is:

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

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

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

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:

$$
A(k, z) = \frac{1}{\pi} \frac{\Gamma}{(z - \xi_k)^2 + \Gamma^2}
$$
 (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 rapresentation for the Greens Functions:

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

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

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

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

$$
i\Omega_m \to \omega + i\delta \tag{1.172}
$$

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

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:

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



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

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

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

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

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

What we get is:

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

This formula can just be rewritten in this way:

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

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 emprically some of the vertext corrections. Computing optical response remains very difficult. For Fermi liquids one can more or less resolve this kind of approximation.

## <span id="page-24-0"></span>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 compleatly not evident. For magnetic systems it is evident the braking symmetry (spin alignment). The Heisenberg hamitlonian 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 mutch 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.

#### <span id="page-25-0"></span>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:

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

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

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

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:

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

$$
\chi_{\rho\rho}(\omega=0, q \to 0) = N_f \tag{2.4}
$$

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

The real part of the conductivity is:

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

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

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

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

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

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

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

Then the total potential can be written as:

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

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



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

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

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

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

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

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

$$
H = H_0 - U \sum_k \rho^{\dagger}(q)\rho(q) \tag{2.15}
$$

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

### <span id="page-27-0"></span>2.2 BCS model

The BCS Hamiltonian is:

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

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

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

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

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

If we introduce a spinor:

$$
\psi_k = c_{k\uparrow} c_{-k\downarrow}^\dagger \tag{2.20}
$$

It is possible to rewrite the HF hamiltonian as:

$$
H = \sum_{k} \psi_{k}^{\dagger} \hat{H} \psi_{k} + \sum_{k} \xi_{k} + \frac{\Delta_{0}^{2} \Omega}{g}
$$
 (2.21)

$$
\hat{H} = \begin{pmatrix} \xi_k & \Delta_0 \\ \Delta_0 & -\xi_{-k} \end{pmatrix}
$$
 (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 consisten equation of the Hartree-Fock theory, that will result in the self consistent gap equation:

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

The eigenvalues are:

$$
\lambda = \pm \sqrt{\xi_k^2 + \Delta_0^2} = \pm E_k \tag{2.24}
$$

Now we can write the partition function as:

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

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

So we have for the partition function

$$
Z = \prod_{k} (1 + e^{-\beta E_k})(1 + e^{\beta E_k})
$$
\n(2.27)

We can obtain the free energy:

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

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

$$
\frac{\partial F}{\partial \Delta_0} = 0 \tag{2.29}
$$

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

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

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

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:

$$
\Delta_0 = \sum_k \langle c_{k\uparrow} c_{-k\downarrow} \rangle \tag{2.33}
$$

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:

$$
n = -\frac{1}{\Omega} \frac{\partial F}{\partial \mu} = \frac{1}{\Omega} \sum_{k} \left( 1 - \frac{\xi_k}{E_k} \tanh \frac{\beta E_k}{2} \right)
$$
 (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 pratice we have to solve two coupled equations, one for the Gap and one for the chemical potential.

#### <span id="page-29-0"></span>2.3 Self consistent Gap equation

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

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

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

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

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

$$
1 \approx gN_0 \ln \frac{2\omega_D}{\Delta_0} \tag{2.37}
$$

Therefore we solve the equation for the Gap:

$$
\Delta_0 = 2\omega_D e^{-\frac{1}{gN_0}}\tag{2.38}
$$

This is a quite remarkable equation. Regardeless 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 decresees we have smaller  $\Delta_0$ . If you increase the energy of the bosonic  $\omega$ . Peaple tried to work on q 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 behund where its definded. 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  $\Delta_0(T) \to 0$ :

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

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

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

Therefore we can extimate the  $T_c$ :

$$
T_c \sim \omega_D e^{-\frac{1}{\beta N_0}} \tag{2.41}
$$

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

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

$$
\Delta_0 = 1.76 \cdot T_c \tag{2.43}
$$

### <span id="page-30-0"></span>2.4 BCS ground state: the Cooper pairs

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

$$
\vec{v} = \begin{pmatrix} a \\ b \end{pmatrix} \tag{2.44}
$$

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

$$
b = -\frac{\xi - E_k}{\Delta_0} a \tag{2.46}
$$

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

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

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

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

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

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

$$
U_k = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \tag{2.51}
$$

Then we have

$$
\hat{H}U_k = U_k \Lambda \qquad \Lambda = \begin{pmatrix} E_k & 0\\ 0 & -E_k \end{pmatrix} \tag{2.52}
$$

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

$$
H = \sum_{k} \psi_{k}^{\dagger} \hat{H} \psi_{k} = \sum_{k} \psi_{k}^{\dagger} U_{k} \Lambda U_{k}^{\dagger} \psi_{k} = \sum_{k} \phi_{k}^{\dagger} \Lambda \phi_{k}
$$
(2.53)

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

$$
\phi_k = U_k^{\dagger} \psi_k \qquad \psi_k = \begin{pmatrix} c_k \uparrow \\ c_{k\downarrow}^{\dagger} \end{pmatrix} \tag{2.54}
$$

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

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

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

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

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.

$$
\gamma_{k\uparrow} \left| BCS \right\rangle = 0 \tag{2.58}
$$

$$
\gamma_{k\uparrow}^{\dagger} BCS = |E_k\rangle \tag{2.59}
$$

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:

$$
H = \sum_{k} E_{k} \left( \gamma_{k\uparrow}^{\dagger} \gamma_{k\uparrow} - \gamma_{-k\downarrow} \gamma_{-k\downarrow}^{\dagger} \right)
$$
 (2.60)

I can use a anticommutation operator to write it as:

$$
H = \sum_{k\sigma} E_k \gamma_{k\sigma}^{\dagger} \gamma_{k\sigma} - \sum_k E_k
$$
\n
$$
E_{gs}
$$
\n(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 Bogoliugov transformation. This introduces the fermionic creation and annihilation operators  $\gamma^{\dagger}_{k\sigma}$  and  $\gamma_{k\sigma}$ .

Then the Hamiltonian can be rewritten as:

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

Here  $E_k$  are all positive numbers:

$$
E_k = \sqrt{\xi_k^2 + \Delta_0^2} \tag{2.63}
$$

The occupatoin number of the new fermionic excitations:

$$
f(E_k) = \frac{1}{e^{\beta E_k} + 1} \stackrel{T=0}{\to} 0
$$
\n(2.64)

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

$$
\gamma_{k\sigma} \left| BCS \right\rangle = 0 \tag{2.65}
$$

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

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

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

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

We will use the property:

$$
[A, BC] = \{A, B\} C - B \{A, C\}
$$
\n<sup>(2.68)</sup>

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

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.

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

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

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

Therefore their sum gives zero. The application the destruction Bogoligov operator I get zero. The BCS state is a very creazy state. It is the superposition of a vacuum and double occupied state. We can also write the BCS ground state as:  $\overline{1}$  $\overline{ }$ 

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

$$
b^{\dagger} = \sum_{k} \alpha_{k} c^{\dagger}_{-k\downarrow} c^{\dagger}_{k\uparrow}
$$
 (2.74)

I can rewrite the bcs using an exponential notation:

$$
|BCS\rangle = \prod_{k} e^{\sum_{k} \alpha_{k} c_{-k\downarrow}^{\dagger} c_{k\uparrow}^{\dagger}} |0\rangle = e^{b_{k}^{\dagger}} |0\rangle \tag{2.75}
$$

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

$$
e^{b^{\dagger}} \left| 0 \right\rangle = \sum_{k} \frac{1}{n!} (b^{\dagger})^n \left| 0 \right\rangle = \sum_{k} \frac{1}{n!} \left| n \right\rangle \tag{2.76}
$$

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.

$$
N = 2\sum_{k} v_k^2 \tag{2.77}
$$

However, the average value has a finite variance:

$$
\langle N^2 \rangle - \langle N \rangle^2 = 2 \sum_k u_k v_k \tag{2.78}
$$

Therefore, since there is a indefined 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:

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

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

$$
\xi \sim \frac{1}{\delta k} \sim \frac{v_f}{\Delta_0} = \frac{m v_f^2}{\Delta_0 m v_f} = \frac{E_f \lambda_f}{\Delta_0} \tag{2.80}
$$

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 unconvensional superconductors, we have highter temperatures, with smaller fermi energy, so the mean-field theories do not hold any more.

#### <span id="page-33-0"></span>2.5 Green's function on BCS

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

$$
U = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \qquad HU = U\Lambda \tag{2.81}
$$

$$
\Lambda = \begin{pmatrix} E_k & 0\\ 0 & -E_k \end{pmatrix} \tag{2.82}
$$

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

$$
G^{-1} = i\omega I - H_{HF} \tag{2.83}
$$

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

We can invert the matrix easily:

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

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

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

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

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

Then we can rewrite the matrix as:

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

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

Then we can compute the spectral function:

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

$$
\Im G(k, i\omega_n \to 0^+) = A(k, i\omega_n) = u_k \delta(\omega - E) + v_k^2 \delta(\omega + E)
$$
 (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 groowing 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.

### <span id="page-34-0"></span>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:

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

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

$$
\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} \tag{2.94}
$$



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).

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

Thereforce we get:

<span id="page-35-0"></span>
$$
\frac{d}{dt}\left(\vec{A} + \frac{mc}{n_s e^2}\vec{J}\right) = 0\tag{2.96}
$$

The London hypothesis is that:

<span id="page-35-1"></span>
$$
\vec{A} + \frac{mc}{n_s e^2} \vec{J} = 0 \tag{2.97}
$$

This is not only the solution of Eq. [\(2.96\)](#page-35-0), but it is a much stronger assumption. This is a gauge fixed relation, so we must chose the Coulomb Gauge:

$$
\vec{\nabla} \cdot \vec{A} = 0 \tag{2.98}
$$

From this assumption we can derive the Meissner effect:

$$
\vec{J} = \frac{c}{4\pi} \vec{\nabla} \times \vec{h} \qquad \vec{h} = \vec{\nabla} \times \vec{A} \tag{2.99}
$$

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

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

$$
\vec{\nabla}^2 \vec{h} = \frac{1}{\lambda^2} \vec{h} \tag{2.102}
$$

The London assumption Eq. [\(2.97\)](#page-35-1) has the Meisnerr 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 maxweel equation we get:

$$
\vec{\nabla} \cdot \text{ vech} = 0 \qquad h_z = const \tag{2.103}
$$

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

$$
H = \frac{p^2}{2m} \qquad \vec{p} \to \vec{p} - \frac{q}{c}\vec{A} \tag{2.105}
$$

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

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

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

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:

$$
\psi_0 \nabla_0^{\psi} - (\nabla \psi_0^*) \psi_0 = 0 \tag{2.108}
$$

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 superconducor rigidity. The if  $\psi$  remains equal to  $\psi_0$ , than we have only the diamagnetic function:

$$
\vec{j} = -\frac{q^2}{mc}\vec{A}|\psi|^2 = -\frac{qn}{mc}\vec{A}
$$
\n(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:

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

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.