



*“Our immersion in the present state of physics makes it hard for us to understand the difficulties of physicists even a few years ago, or to profit from their experience. At the same time, a knowledge of our history is a mixed blessing - it can stand in the way of the logical reconstruction of physical theory that seems to be continually necessary.”*

Steven Weinberg

*“An equation for me has no meaning unless it expresses a  
thought of God.”*

Srinivasa Ramanujan



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# The Luttinger-Ward Theorem

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# Thanksgiving

To my girlfriend Francesca, for being always willing to be the closest to me and for being the most loving and careful person I've ever met, I devote this thesis.

As well, for all the time they have spent since I was a child to make me grow and to nourish and support me in everything good that I've done and that I strive to do during mine, not to mention their efforts to be first of all examples to follow rather than supervisors to listen to, I want to express my deepest gratitude both to my mother Emanuela and to my father Giovanni.

Necessarily, I also have to thank many, many people, past and present, that I have been privileged enough to encounter in my life, for everything they have been able to teach me, always with the care not to school me unless it wasn't of the utmost necessity. To them I refer without mention, since it would digress from the main matter of this thesis, but still they are involved in my path, way before the beginning of my studies and up to the present days during the development of this important step.

Lastly, I have to express a huge amount of respect, gratitude and love both to my supervisor Luca Guido Molinari and to my advisor Mauro Pastore.

I've had the chance to know Mauro due to a random conversation we had for a little time when I was talking to his colleague in their office, and I immediately felt a deep empathy and respect towards him, having a strong feeling of his competence and skills as a physicist. When I was told about the need for an advisor for this thesis work, it became immediately clear that I would have preferred him to address such task more than anyone else, and I hope this little time spent together has been something positive not only for me as a physicist and a person, but, if possible, for him as well.

Luca Guido has fuelled me with incredible motivation, beginning with my confrontation and fascination with his intelligence - something that he surely won't be happy to read about - and with the way I've always seen him approach the computations on the blackboard during his lectures, way before having the honour to know him personally. I've learned all the most important things I know about how to face computations from the way I've always seen him attacking them. This was what made me go to him in order to ask for the chance of working on this project under his supervision. Nevertheless this is not the main thing I learned from him since in this piece of the road we have walked together I've found myself, without any exaggeration, embarrassed about what I think to be his greatest feature, and that is humbleness. He really is one of the most humble person I've ever met and this makes me consider him a master example to follow beyond the domain of being a physicist, since in my opinion humbleness is probably the greatest virtue amongst all.

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# Introduction

This thesis concerns Luttinger-Ward theorem, one of the foremost results of the whole many-body theory. The interest rises from the strong feeling of not grasping it after 70 years of involved literature, notwithstanding its apparent simplicity.

The content of the theorem can be stated in a simple form: the number of single-particle momentum states where the frequency-dependent Green function evaluated at the chemical potential is positive equals the number of particles of the system. We can rephrase it in an even simpler fashion: the inner volume of the Fermi Surface is an adiabatic invariant; i.e. it does not change when we switch-on the interactions.

It is an exact result whose presentation and discussion raised the interest of theoretical physicists like Joaquin Luttinger and John Ward or Igor Dzyaloshinskii to name some. Regardless its lingering history, we don't know how to cast this statement in a physical fashion. This fact by its own, even ignoring its huge range of applicability is, in my opinion, sufficient to devote to it the whole thesis. A surprising fact that anyone facing this theorem encounters is that, regardless its apparent simplicity, all the existing proofs are deeply technical.

The reader will find out that 60 years ago the vision on the state of affairs was slightly different from today's one. I will then present the line connecting them up in the most transparent and simple way I'll be able to. As well as J. Luttinger I won't deal with particles living in dimension different from three, since the arguments and definitions generalize trivially, with the only exception being given by one-dimensional systems. The latter demand a separate treatment, as could be felt thinking that it doesn't make sense to talk about cross-sections in one dimension.

The thesis is structured as follows: the first chapter begins with a presentation of the original proof of the Luttinger-Ward theorem. The chapter is divided in two parts: the first one concerns what nowadays we understand to be a collateral fact, namely the possibility for the momentum distribution function of an interacting fermionic system to develop a discontinuity in the zero temperature limit, just like it does in the non interacting case giving rise to the standard Fermi Surface. The second part dwells with the actual content of the theorem as we think it today, that is the conservation of the volume enclosed by the Fermi Surface when interactions are switched-on (making no reference to any discontinuity at all).

The proof given by Luttinger and Ward and almost any other proof of the same theorem in essence make use of the existence of a special functional that has to do with a diagrammatic dressed expansion for the Grand Potential of the theory. The second chapter is then devoted to the derivation and analysis of such expansion and to clarify how such functional could be constructed.

The content of the third chapter is the theory of quasi-particles. The Luttinger-Ward theorem has to do with them and the possibility that an elementary excitation of the interacting system behaves approximately like one of the non-interacting one, since an adiabatic switching-on of the interactions is reasonably involved in the validity of the Luttinger-Ward theorem and the conservation of the Fermi Sphere inner volume.

Quite the same reason makes out chapter number four dwell with the theory of the Fermi liquids. This paradigm involves ideas first devised by Landau in the early '60s, who was the first to put the understanding of the metallic behaviour of a system on a firm theoretical basis and to relate the macroscopic to the microscopic physics.

Chapter five brings closer to the present day since it deals with some recent proofs of the Luttinger-Ward theorem. In particular it is reported Dzyaloshinskii's derivation of it and extension of the very same theorem to non-Fermi liquids and Mott insulators, thus opening the doors to new questions to be addressed in order to understand properly what the full range of validity of the Luttinger-Ward theorem. Secondly it is given one more proof, by Giuliani and Vignale where they use a novel way to approach the result, still keeping an eye on the already existent ones.

The last chapter contains some considerations of mine that aim at offering some firm points in comprehension of the theorem. Starting with a formulation on a finite lattice, I use the Khällen-Lehmann representation of the propagator and with few hypothesis I obtain bounds and relations that clarify some of the main steps of the proof.

# 1 Luttinger-Ward Proof

There is a side fact about the theorem: under appropriate hypothesis the momentum distribution function develops a discontinuity and the points where it is discontinuous define a surface. We will discuss it before the proof of the theorem. The reason for doing so is that such fact seems somewhat separated from the theorem and somewhat involved all the same, so it seems logical to me to make it come first. We will then clarify whether or not it is a necessary consequence of our theorem and their precise relation.

## 1.1 The discontinuity in $n(k)$

Here follows Luttinger's investigation [2] of the possibility, pointed out first by Migdal [3], that in the interacting ground state of a fermionic system the mean occupation number of single-particle momentum states still possess a discontinuity, just like it does in the purely kinetic theory. If it is the case such singularity defines a surface, that should reasonably still be called the Fermi Surface (F.S.).

It was already clear to Luttinger that the existence of a F.S. should depend on the nature of the interactions. Indeed, for example, in a system of localized electrons there is no trace of such surface and we have experiments showing off that many systems exhibit those states, the most famous one being the Wigner solid [4] [5]. Moreover Luttinger's derivation is done under the explicit assumption that the perturbative theory is valid but whether or not it is so for practical cases was and still is an open question. With this in mind we can begin.

The partition function of the grand-canonical ensemble is

$$Z(\beta, V, \mu) = \text{Tr}\{\exp[-\beta(H - \mu N)]\} = \exp(-\beta\Omega)$$

and the mean occupation number for a state  $\mathbf{k}$  is defined by

$$n_k = \text{Tr}\{a_k^\dagger a_k \exp[\beta(\Omega - H + \mu N)]\} \quad (1)$$

It may be expressed in terms of the two-point Green function as

$$n_k = \lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_l \exp(\eta \zeta_l) \frac{1}{\zeta_l - \epsilon_k - \Sigma_k(\zeta_l)} \quad (2)$$

where the sum runs over the complex fermionic Matsubara frequencies

$$\zeta_l = \mu + i \frac{(2l+1)\pi}{\beta} \quad (3)$$

$\epsilon_k$  is the free-particle kinetic energy and  $\Sigma_k(\zeta)$  is the so-called “self-energy”, a precise definition of which is found later on in this paper. In the zero-temperature or equivalently  $\beta \rightarrow +\infty$  limit the series is said to become an integral. Reasonably this is legitimate in many cases, so we have

$$n_k = \lim_{\eta \rightarrow 0^+} \frac{1}{2\pi i} \int_{\mu-i\infty}^{\mu+i\infty} d\zeta \exp(\eta \zeta) \frac{1}{\zeta - \epsilon_k - \Sigma_k(\zeta)} \quad (4)$$

The contour is then closed to the left to encircle the portion of the real axis starting at  $\mu$  and extending to  $-\infty$ , turning the expression into

$$n_k = \frac{1}{2\pi i} \int_{-\infty}^{\mu} dx \left[ \frac{1}{x - \epsilon_k - K_k(x) - iJ_k(x)} - c.c. \right] \quad (5)$$

with  $K_k(x)$  and  $J_k(x)$  the real and imaginary part of the self-energy respectively. It’s noteworthy to say this expression may be derived starting at zero-temperature instead of going to the zero-temperature limit from the finite temperature theory. Before we take the thermodynamic limit, that is

$$N \rightarrow \infty, V \rightarrow \infty, N/V = \text{const.} \quad (6)$$

$\mathbf{k}$  is a discrete variable (taking values on a lattice in  $\mathbb{R}^3$  indeed) so we can’t talk about analytic properties. Conversely under such limit we can, and Luttinger himself says there is no reason not to expect  $\Sigma_k(\zeta)$  to become a smooth function of  $\mathbf{k}$ . This is still clearly an hypothesis and as it’s explicitly stated in his paper the existence of the singularity we are concerned with is a direct consequence of such assumption, which anyway is not the only one necessary to prove  $n_k$  is discontinuous somewhere, nor it seems necessary to assume something as strong as smoothness to do it. Still if the analyticity is satisfied then any possible discontinuous behaviour in  $n_k$  must result from a singularity in the integrand.

Then he makes use of the fact that  $J_k(x)$  approaches zero only in a neighborhood of  $x = \mu$ . Up to my knowledge this is an hypothesis too, without any kind of rigorous proof existing. As we’ll see later some exact constraints may be given about the behaviour of the imaginary part of the self-energy, but they’re surely not strong enough to guarantee the validity of the statement. Some perturbative arguments may be used to show such behaviour, but I remark we don’t know when the perturbative approach is valid. Anyway such issues will be dealt with later on in the thesis, so at the moment we’ll content ourselves of exploring the consequences of it. Let’s consider then all points in  $\mathbf{k}$ -space making out

$$\mu - \epsilon_k - K_k(\mu) = 0 \quad (7)$$

they lie on a surface in such space, that as expected is called the Fermi Surface of the interacting system. Remind that a more general and say modern definition of it will be given, without referring to any discontinuity in  $n_k$  at all. From here the best we can do is follow closely Luttinger paper since his description of his own proof is probably already as clean and precise as possible, regardless looking a little cumbersome to me. The proof consists in a sequence of changes in the integration variable and approximations from power series expansions, using the aforementioned hypothesis, to make the presence of the singularity in  $n_k$  explicit. Let's then consider those values of  $\mathbf{k}$  close the F.S. just defined. The equation

$$x - \epsilon_k - K_k(x) = 0 \quad (8)$$

will presumably in general have a solution  $x = E_k$  with  $E_k$  approaching  $\mu$ . It is natural to call  $E_k$  the true single-particle excitation energy. If we pick up the closest point to it on the F.S. and call it  $\mathbf{k}_0$  we have  $\mathbf{k} = \mathbf{k}_0 + \mathbf{y}$ , with  $\mathbf{y}$  perpendicular to the F.S. at  $\mathbf{k}_0$ . Now we expand at fixed  $\mathbf{k}$

$$x - \epsilon_k - K_k(x) = Z_k^{-1}(x - E_k) + \dots \quad (9)$$

with the so-called “quasi-particle weight”

$$Z_k^{-1} = 1 - \partial_x K_k(x)|_{x=E_k} \quad (10)$$

The reason for this name, if it's not yet, will be clear when we will deal with quasi-particles. Combining (9) with the perturbative result that  $J_k(x) = C_k(x - \mu)^2 + ..$  in a neighborhood of  $x = \mu$  the denominator in (5), when  $\mathbf{k}$  is close to  $\mathbf{k}_0$ , becomes

$$x - \epsilon_k - K_k(x) - iJ_k(x) = Z_k^{-1}(x - E_k) - iC_k(x - \mu)^2 + \dots \quad (11)$$

Then we split the integral in (5) as

$$\int_{-\infty}^{\mu} = \int_{\mu-a}^{\mu} + \int_{-\infty}^{\mu-a} \quad (12)$$

with  $a$  a fixed finite positive and small energy. It is clear that any possible discontinuous behaviour of  $n_k$  should come from the first integral since in the second one the integrand is never singular. We then write

$$n_k = n'_k + n''_k \quad (13)$$

and focus on  $n'_k$ . In the integral defining it we can use the aforementioned expansion to get

$$n'_k = \frac{1}{2\pi i} \int_{\mu-a}^{\mu} dx \left\{ \frac{1}{Z_k^{-1}(x - E_k) - iC_k(x - \mu)^2} - c.c. \right\} \quad (14)$$

at the leading order. Now we set

$$E_k = \mu - \Delta_k \quad (15)$$

and use

$$E_k = E_{k_0+y} = E_{k_0} \pm |y| |\nabla_{k_0} E_{k_0}| = \mu \pm |y| |\nabla_{k_0} E_{k_0}| \quad (16)$$

where the  $\pm$  depends on whether  $\mathbf{y}$  is parallel or anti-parallel to the normal to the F.S. at  $\mathbf{k}_0$ . Moreover at the lowest order

$$\Delta_k = \mp |y| |\nabla_{k_0} E_{k_0}| \quad (17)$$

so if we define  $r = \mu - x$  in (14) we are left with

$$n'_k = \frac{1}{2\pi i} \int_0^a dr \left\{ \frac{1}{Z_k^{-1}(\Delta_k - r) - iC_k r^2} - c.c. \right\} \quad (18)$$

again to the leading order. There is only one more change of variable to do. Putting

$$t = |\Delta_k|/r \quad (19)$$

yields for (18)

$$n'_k = \int_{|\Delta_k|/a}^{+\infty} dt \frac{(\alpha_k/\pi)}{(Z_k^{-1})^2(t \mp 1)^2 t^2 + \alpha_k^2} \quad (20)$$

with

$$\alpha_k = C_k |\Delta_k| \quad (21)$$

and the  $\mp$  sign according to  $\Delta_k$  being greater or less than zero respectively. If we let  $\mathbf{y}$  go to zero we are going closer to the F.S. so also  $\alpha_k$  goes to zero. This makes the argument of the integral approach the Dirac delta-function starting from a sort of Lorentzian peak, so we can write:

$$n'_k = \int_0^{\infty} dt \delta[|Z_k^{-1}|(t \mp 1)] \quad (22)$$

The small values of  $t$  near zero give no contribution since  $\alpha_k^2$  is negligible with respect to the first term in the denominator of (20). The only way to get a non-zero contribution is then to have the minus sign in the expression

(22). We have thus obtained that, in crossing the F.S.  $n_k$ , changes by the finite amount  $|Z_{k_0}|$ . Since the occupation number can't be greater than one one can guarantee also

$$|Z_{k_0}| \leq 1 \tag{23}$$

Besides this the manipulation above shows that the F.S. is the only discontinuity found in  $n_k$  under Luttinger hypothesis. The state of affairs looks a little discouraging to me, the reason being the following: the game we play consists often in saying something about the analytic structure of functions (forgive my tiny tortuous sentence) that should be obtained as the limit of a sequence of functions defined over some set of discrete variables, like for example the self-energy as a function of  $\mathbf{k}$  before the thermodynamic limit is taken.

The problem is that before the limit there is no analytic structure at all, and a mathematical theory of the analytic properties of functions emerging in the way described is completely absent. So if one is unable to produce explicit and exact expressions of the objects he wishes to take the limit of then he's left with an unsolved problem. The best we can do to address this issue is to assume that the output of our limits will be made of piece-wise analytic functions.

In the next part of the paper Luttinger, simply referring back to a previous work he made with J.C.Ward [1], points out in few lines that the volume of the F.S. defined above is exactly the same of the free theory. The next logical step is then to follow their construction, that is what we're going to do.

## 1.2 Fermi Sphere inner volume

Here we will reconcile a little with the contemporary view. Indeed Luttinger idea was to use the discontinuity in  $n_k$  to define a surface and then to show the enclosed volume is conserved. We don't need this. What is going to be proved presenting the content of Luttinger and Ward paper [1] is essentially the statement of the theorem we use nowadays, as found in the introduction. So we'll end up with a conserved volume without any necessary reference to the aforementioned discontinuity.

There will be again subtleties concerning the analytic structures in trying to relate to the singularity in  $n_k$  we talked so far, as could be expected. Just think for example that the level set of a generic real function on  $\mathbb{R}^3$  satisfying nothing but being non-negative and with a well defined integral could be literally anything. So if one wishes to define a surface from the level set of a function it has to be a somehow regular function or the definition is

not possible. I pointed this out since we're going to prove that the volume where a function is positive is invariant with respect to some changes in the underlying theory. Of course this volume would be the inner volume of the Fermi Surface (as the reader is probably thinking) and the F.S. has to be defined to be the boundary of such volume.

Nevertheless without assumptions upon the analytic structure this boundary doesn't even need to be a two-dimensional set in  $\mathbb{R}^3$ . Having said so, we proceed with Luttinger-Ward's proof that there is a volume in momentum space that does not depend on interactions.

The proof makes use of what in the present day literature we call the "Luttinger-Ward functional". A modern expression for it is given by [6] where is found

$$\Omega_{LW}[G, v] = \Omega_0 \mp \frac{1}{\beta} \{ \Phi[G, v] - \text{Tr}[\Sigma[G, v]G + \log(1 - G_0\Sigma[G, v])] \} \quad (24)$$

In the equation above  $G_0$  and  $G$  are the free and interacting Green functions of the system under consideration,  $v$  is the two points interaction function and the lower sign is for fermions. The  $\Phi$ -functional that appears is the subject of next chapter so we won't describe it much now. Almost the same functional is constructed by Luttinger and Ward in the first part of the paper [1] and we report it here using a little more standard notation

$$Y = \lim_{\eta \rightarrow 0^+} -\frac{1}{\beta} \sum_{k,l} \exp(\eta\zeta_l) \{ \log[\epsilon_k + \Sigma(k, \zeta_l) - \zeta_l] + G(k, \zeta_l)\Sigma(k, \zeta_l) \} + Y' \quad (25)$$

For  $Y'$  is given a diagrammatic definition that makes it a functional of full propagator and proper self-energy, contrary to [6] that uses  $G$  and  $v$ .

$$Y' = \sum \text{Closed Linked Skeleton Diagram} \quad (26)$$

and is the equivalent of the  $\Phi$ -functional in the previous equation. The precise meaning of these words will be clear when we will study such functional in detail. Here we don't need to. The functional  $Y$  is stationary when  $\Sigma, G_0$  and  $G$  are related by the Dyson equation. The stationary property is mentioned since the proof makes use it. Such  $Y$  is constructed starting from the standard expansion of the Grand Potential in terms of bare propagator and interaction. What matters now is that  $Y$  equals the value of the Grand Potential at the stationary point. Thus we may use it to compute the total number of particles, that is

$$N = -\frac{d}{d\mu} Y \quad (27)$$



In such derivation two sources of terms are distinguished:

- the  $\mu$  dependence which arises from the complex Matsubara frequencies  $\zeta_l$  defined in equation (3). For it  $\partial_\mu$  can be replaced by  $\partial_{\zeta_l}$ .
- the intrinsic  $\mu$  dependence of  $\Sigma$  at the stationary point. This could be ignored anyway since there we would get something like

$$\frac{\partial \Sigma(k, \zeta_l)}{\partial \mu} \frac{\delta}{\delta \Sigma(k, \zeta_l)} Y \quad (28)$$

that vanishes thanks the stationary property.

So the expression for  $N$  turns into

$$N = \lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_{k,l} \exp(\eta \zeta_l) \partial_{\zeta_l} \{\dots\} - \frac{1}{\beta} \sum_{k,l} \Sigma(k, \zeta_l) \partial_{\zeta_l} G(k, \zeta_l) \quad (29)$$

where the second term comes from the derivative of  $Y'$  and cancels out with the same term but from the curly bracket, leaving us with

$$N = \lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_{k,l} \exp(\eta \zeta_l) \{ \partial_{\zeta_l} \log [\epsilon_k + \Sigma(k, \zeta_l) - \zeta_l] + G(k, \zeta_l) \partial_{\zeta_l} \Sigma(k, \zeta_l) \} \quad (30)$$

In the zero temperature limit the sum is switched to an integral over the continuous variable  $\zeta$ . The authors themselves put the reader in warning about the fact this substitution may hide subtleties and that corrections to such limit may occur. Nevertheless when valid this gives for the last term in (30)

$$\lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_k \sum_l \exp(\eta \zeta_l) \{ \partial_{\zeta_l} [G(k, \zeta_l) \Sigma(k, \zeta_l)] - \Sigma(k, \zeta_l) \partial_{\zeta_l} G(k, \zeta_l) \} = \quad (31)$$

$$= \lim_{\eta \rightarrow 0^+} \frac{1}{2\pi i} \int_{\mu-i\infty}^{\mu+i\infty} d\zeta \exp(\eta \zeta) [-\Sigma(k, \zeta) \partial_\zeta G(k, \zeta)] \quad (32)$$

since the boundary term coming from the total derivative vanishes when the sum is replaced by the integral. The argument proceeds the following: first one notes that, because of the diagrammatic definition, this term is equivalent to the differentiation of every skeleton diagram with respect to  $\zeta_l$  followed by the replacement of sums by integrals. Then one uses the fact he has integrals in which partials derivatives with respect to the integration

variables appear. A partial integration with respect to them yields a term proportional to

$$(\partial_{\zeta_1} + \partial_{\zeta_2} + \partial_{\zeta_3} + \partial_{\zeta_4})\delta(\zeta_1 + \zeta_2 - \zeta_3 - \zeta_4) \quad (33)$$

due to the fact the Hamiltonian is time-independent. This makes the contribution to  $N$  disappear when the sum over  $\mathbf{k}$  is performed. This exact cancellation is crucial to prove the theorem. We will then try to understand it in a modern formulation. Having said all of this we're left with a single term that of course can't cancel out

$$N = \lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_{k,l} \exp(\eta \zeta_l) \partial_{\zeta_l} \log [\epsilon_k + \Sigma(k, \zeta_l) - \zeta_l] \quad (34)$$

To do this last summation we employ the following trick, that is common when dealing with Matsubara frequencies. Consider the function

$$f(\zeta) = \frac{1}{1 + \exp(\beta(\zeta - \mu))} \quad (35)$$

Its poles lie exactly on the values of  $\zeta$  we want to sum on. So if we multiply it with the argument of (34) and choose a convenient contour  $\Gamma$  for the integration in  $\zeta$ , we get

$$\lim_{\eta \rightarrow 0^+} \frac{1}{\beta} \sum_l \dots = \lim_{\eta \rightarrow 0^+} \frac{1}{2\pi i} \int_{\Gamma} d\zeta \exp(\eta \zeta) f(\zeta) \partial_{\zeta} \log [\epsilon_k + \Sigma(k, \zeta) - \zeta] \quad (36)$$

The contour  $\Gamma$  may be deformed into  $\Gamma_0$  as shown in fig. 1. Now we can use partial integration to make  $\partial_{\zeta}$  act on  $f(\zeta)$ . This gives a delta function  $\delta(\zeta - \mu)$  when  $\beta \rightarrow \infty$  and  $\zeta$  approaches the real axis. So all is left is

$$N = \lim_{\eta \rightarrow 0^+} \sum_k \frac{1}{2\pi i} \{\log [\epsilon_k + \Sigma(k, \mu) - \mu + i\eta] - \log [c.c.]\} \quad (37)$$

Now the branch-cut discontinuity of the logarithm of a complex number makes out the result we wondered: the argument of the curly brackets in (37) is zero when we're upon the positive part of the real axis and equal to  $2\pi i$  on the negative one, so the expression for  $N$  turns into

$$N = \sum_k \theta(\mu - \epsilon_k - \Sigma(k, \mu)) \quad (38)$$

with  $\theta(\cdot)$  the Heaviside theta-function.

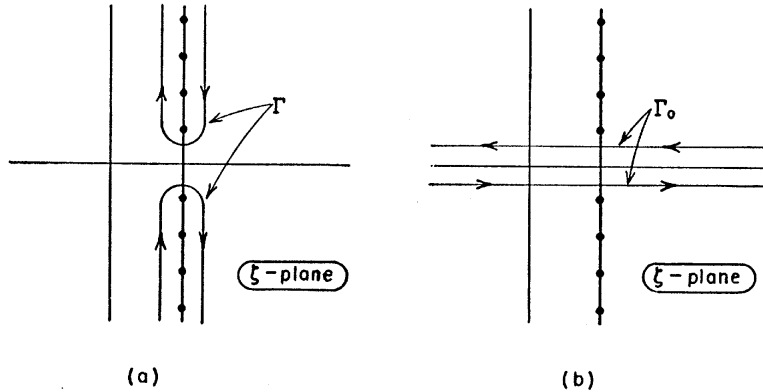


Figure 1: Paths involved in the contour integrals. Luttinger and Ward [1]

### 1.3 Some comments about the proof - why the thesis should go on?

The proof of the theorem we have just seen is somehow an unsatisfactory one, at least for the physicist. The good mathematician could feel that anything is OK and that the given proof extinguishes any doubt, leaving one with no possible question about it. However his is not mathematics so we cannot content ourselves saying that a bunch of “hoketi poketi” math tricks (as Richard Phillips would have called them) leaves us satisfied and prone to focus on other issues.

First of all we don’t have any physical interpretation of the Luttinger-Ward theorem and secondly it’s not even clear if it is just telling us about a somehow accidental mathematical fact with no real relation with the physical world or if it could be based on the experimental ground. Personally I think it would be really strange if the first one is the case.

My wish is to rule out as much as possible what is going on physically and that’s why in the following we will relate this theorem to the theory of fermionic condensed matter that we can test with the experiments and clarify the situation as much as we’ll be able to.

Of course I don’t presume to be able to address the issue to the necessary extent, many other much more skilled than me tried to do it before unsuccessfully. Nevertheless every drop is involved in making out the ocean so I won’t just sit apart in silence but follow the hope that mine could be another meaningful (regardless microscopic) contribution.

## 2 Dressed Expansion of the Grand Potential

In this chapter we will be concerned with all the functionals and diagrammatic expansions mentioned insofar. It is necessary to do it because of the central role they play in the theorem and almost in every known proof.

### 2.1 Introducing the bubble-diagrams

Recall the fundamental equation

$$Z = \text{Tr}[\exp[-\beta(H - \mu N)]] = \exp(-\beta\Omega) \quad (39)$$

The operator we are taking the trace of is closely related to time-evolution in Quantum theories, meaning that

$$\exp[-\beta K] = U_K(-i\tau)|_{\tau=\beta} \quad (40)$$

where  $K = (H - \mu N)$  and  $U_K(t)$  the unitary operator giving time translations with  $K$  taken as a sort of Hamiltonian. If we have

$$K = K_0 + V \quad (41)$$

it is a standard result from Quantum Mechanics that we can write

$$U_K(t) = U_{K_0}(t)U_I(t) \quad (42)$$

with  $U_I(t)$  given by

$$U_I(t) = \mathcal{P} \exp \left[ -i \int_0^t dt' V_{K_0}(t') \right] \quad (43)$$

and  $\mathcal{P} \exp[.]$  denoting the path-ordered exponential. One should note that these are exact relations. Using (40) and (42) in (39) gives

$$Z = \text{Tr}[U_{K_0}(-i\tau)U_I(-i\tau)|_{\tau=\beta}] \quad (44)$$

That by definition corresponds to

$$Z = Z_0 \langle \mathcal{P} \exp \left[ - \int_0^\beta d\tau V_{K_0}(\tau) \right] \rangle_0 \quad (45)$$

with  $\langle \dots \rangle_0$  denoting the thermal average given by the free theory  $K_0$ . This is an exact relation too and opens the doors to the diagrammatic expansions.

As could have been presumed there are many different kinds of them, indeed the title of the chapter makes it explicit we will deal with a so-called “dressed” one. It is logical anyway to arrive there starting from the most natural one coming, that is the following: by definition the  $\exp[\dots]$  is given by a power series in the argument, so we can explicitly write it down and consider for example the first few terms

$$Z = Z_0 \langle 1 + (-) \int_0^\beta d\tau V_{K_0}(\tau) + \frac{(-)^2}{2!} \int_0^\beta d\tau d\tau' T[V_{K_0}(\tau)V_{K_0}(\tau')] + \dots \rangle_0 \quad (46)$$

The first non-trivial one contains

$$\langle \int_0^\beta d\tau V_{K_0}(\tau) \rangle \quad (47)$$

Since we don’t need to be completely general we will focus only on a subset of all the possible diagrammatic expansions, that is the one encountered when dealing only with two-point interactions in a Many-Body theory. So without loss of generality we can write down

$$V = \frac{1}{2} \sum \langle l, n | v | r, s \rangle a_l^\dagger a_n^\dagger a_s a_r \quad (48)$$

where as probably already clear  $\langle l, n | v | r, s \rangle$  is the two-particles interaction matrix element and the  $a$ ’s are second-quantized field operators. The “imaginary-time” evolution of an operator  $O$

$$O(\tau) = \exp(\tau K) O \exp(-\tau K) \quad (49)$$

could be invoked to setup a time-dependent perturbation theory but I prefer a slightly different and simpler diagrammatic technique since it fits our purposes and it can be related to the imaginary-time  $\tau$  one only as much as necessary. It is noteworthy to say this kind of approach is similar to the one used by T.D.Lee and C.N.Yang in [7] to express  $\Omega$  in terms of mean occupation numbers, as it’s pointed out in [1] also, where Luttinger and Ward say their functional is just the translation of Lee and Yang work into the “modern” propagator language. For the moment let’s then content ourselves to begin with the direct computation of (47). To do it one simply proceeds the following:

- Exploit the  $\mathbb{C}$ -number  $\tau$ -dependence of the free Hamiltonian field operators, explicitly

$$a_k(\tau) = \exp(-\tau w_k) a_k(0) \quad (50)$$

$$a_k^\dagger(\tau) = \exp(\tau w_k) a_k^\dagger(0) \quad (51)$$

to separate the contribution in two factors, one of which is time independent and given by

$$\frac{1}{Z_0} \text{Tr}[\exp(-\beta K_0) a_l^\dagger a_n^\dagger a_r a_s] \quad (52)$$

contracted with  $v$ 's matrix element and the second one

$$\int_0^\beta d\tau \exp[-(w_r + w_s - w_l - w_n)\tau] \quad (53)$$

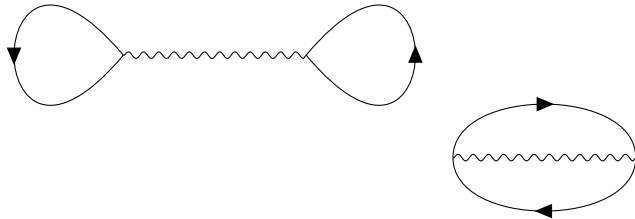
that can be easily solved exactly.

- Make use of the fact that for the free Hamiltonian the field operators map exact eigenstates into exact eigenstates. This allows to compute explicitly (52) and products of that form involving an arbitrary number of field operators.

It is now clear why we can focus on (52). Let me say this is nothing new in standard literature. The algorithm for the computation of such kind of product-forms is the content of G.Wick theorem [8] in its time-independent version. An excellent and complete discussion on it is given by L.G.Molinari in [9] so we won't give it more space here. We will focus on the diagrammatic representation of such product form instead because that is what we need for our theorem. It's a matter of fact that

$$\sum_{K_0} \frac{1}{Z_0} \exp(-\beta K_0) \langle K_0 | a_l^\dagger a_n^\dagger a_r a_s | K_0 \rangle \quad (54)$$

multiplied by the corresponding interaction matrix element according to (48) may be depicted graphically in the following way



$$(55)$$

$$\ln Z = \ln Z_0 + \frac{1}{2} \text{ (bubble)} + \frac{1}{2} \text{ (self-energy)} + \frac{1}{2} \text{ (self-energy with bubble)} + \frac{1}{4} \text{ (self-energy with two bubbles)} + \frac{1}{2} \text{ (self-energy with three bubbles)} + \frac{1}{4} \text{ (self-energy with four bubbles)} + \dots$$

Figure 2: Diagrammatic representation of  $\log(Z)$  in terms of the bare propagator and interaction. Stefanucci-van Leeuwen [6]

where the two diagrams correspond to different contributions that have to be summed over. The wiggly and straight lines should then be labelled by the momenta that flow into them, a numerical factor that accounts for the order of the diagram symmetry group has to be stick to it and then a sum over all these labels has to be performed to compute (47). Since this is again a standard procedure we don't give it space here.

The only thing of importance to us is that this procedure may be extended to arbitrary order giving us a diagrammatic representation of the partition function of the grand canonical ensemble. To obtain the Grand Potential one almost has to take the logarithm of it. This has the effect of leaving one with the sum of every possible topologically distinct and connected diagram taken just once. So we reached the conclusion that the the Grand Potential of our theory may be expressed as such sum of bubble diagrams. On the graphical level this is shown in fig. 2

## 2.2 Resummation of diagram classes - the proper self-energy

The diagrammatic interpretation we have come to opens the door to new computational possibilities. Indeed it is well-known that usually is possible to collect some specific classes of diagrams and sum all the elements of them to cast the whole expression one was to compute into a new - and usually simpler - one.

For example one may consider the class of diagrams specified by the fact that a single straight line goes in and a single straight line comes out. This of course gives what is commonly referred to as the improper self-energy. Then one may consider a subclass of all such diagrams, that is the one given by the same class just specified but with the additional restriction that none of them may be cut into two distinct pieces by removing one single straight

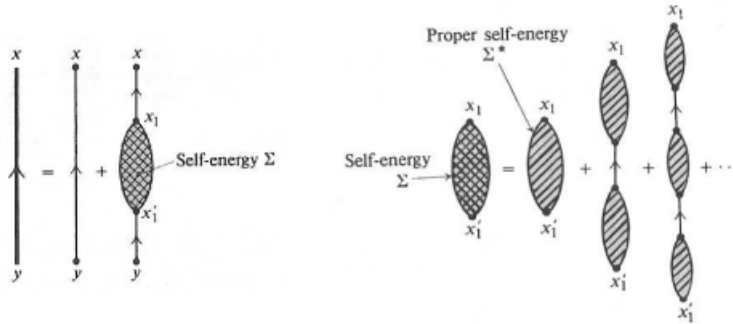


Figure 3: Graphical definition of the self-energy. Google Images

line. This is another standard procedure and the object obtained is known as the proper self-energy. The graphical representation of such procedure is summarized in fig. 3

### 2.3 G-skeleton bubble diagrams

Having seen some of the possibilities given by the diagrammatic interpretation of the quantities we usually wish to compute we can focus on the construction of the celebrated  $\Phi$ -functional involved in Luttinger-Ward theorem's proof. Such functional is defined at the algebraic level asking that its functional derivative with respect to the full (or interacting) Green function gives back the proper self-energy just defined.

This definition however doesn't help much if one wish to come to some explicit expression of such functional, nor it serves in order to rule out its very existence. Here the diagrammatic interpretations comes into play; indeed it doesn't take much to convince oneself that if we take the functional derivative of, for example,  $\log(Z)$  with respect to the bare propagator this has the effect of removing one single  $G_0$  line from every possible place where it appears in the diagrams involved.

It is straightforward to check that all such diagrams with a single  $G_0$  line removed constitute something that at least is related to the improper self-energy. Actually if one writes  $\log(Z) = \log(Z_0) - \Phi_r[G_0, v]$  it turns out that the second addend does exactly such thing: its functional derivative with respect to  $G_0$  coincides with the improper self-energy. This suggest we can



$$\begin{aligned}
\pm \Phi[G, v] = & \frac{1}{2} \text{ (two circles connected by a wavy line)} + \frac{1}{2} \text{ (circle with a wavy self-energy loop)} + \frac{1}{4} \text{ (two circles with two wavy lines between them)} \\
& + \frac{1}{4} \text{ (circle with two wavy self-energy loops)} + \frac{1}{2} \text{ (circle with three wavy self-energy loops)} + \frac{1}{6} \text{ (circle with four wavy self-energy loops)} + \dots
\end{aligned}$$

Figure 4: Graphical representation of the  $\Phi$ -functional. Stefanucci-van Leeuwen [6]

sharpen our diagrammatic construction in order to get a functional with the aforementioned property. Luckily it is the case. To have an intuition one may think that taking the diagrammatic expression for  $\log(Z)$  and re-absorbing all the contribution to a single diagram that “dress” a single  $G_0$  line could do the work. At the end of this resummation the structure of the original diagrams would be the same we had at the beginning but with the full propagator  $G$  appearing in place of  $G_0$ . Moreover it’s not difficult to convince oneself that in such expansion there will be no diagrams containing self-energy insertions, since all of them have been absorbed into the full propagator lines.

These are called the “G-skeleton” diagrams. The only issue left is about symmetry factors. These are often annoying to keep track of and usually doing it doesn’t help much to the extent of deepening the achieved comprehension of the state of affairs. So here we simply report that the correct factor to all the G-skeleton diagrams of order  $n$  is exactly  $1/2n$ . The final expression for the  $\Phi$ -functional we arrived to is then graphically given by (lower sign for fermions)

which in formulae corresponds to

$$\Phi[G, v] = \sum_n \frac{1}{2n} \frac{1}{(2\pi)^4} \int dw d^3k \Sigma_n(k, w) G(k, w)$$

where  $\Sigma_n(k, w)$  is the sum of all the topologically distinct G-skeleton self-energy diagrams of order  $n$  with  $G_0$  replaced by  $G$ .

## 2.4 Coming to the Grand Potential

We are left to relate the construction above to the expression for the Grand Potential, defined to be  $-(1/\beta)\log(Z)$ . One could have an intuition of how this would happen, indeed we have seen that  $\log(Z)$  has a natural diagrammatic expression in terms of the bare propagator and interaction and this expression may be manipulated in order to cast it in a form which makes it depending on the dressed propagator and bare interaction instead.

The actual state of affairs is a little bit more complicated than our simplification. Nevertheless it's just a matter of some algebra to relate the  $\Phi$ -functional we constructed to the dressed expansion of  $\log(Z)$ . Since it won't be illuminating and it's not what we really need for the investigation of Luttinger-Ward theorem, for which the  $\Phi$ -functional suffices, it seems meaningless to repeat here such algebraic steps.

What should be mentioned in my opinion is that to arrive to the exact expression of the Grand Potential  $\Omega$  in terms of  $\Phi$  and self-energy of G-skeleton diagrams one has to start from a re-scaled interaction of the form  $\lambda V$  in the Hamiltonian, compute the corresponding  $\lambda$ -dependent  $\Omega$  and then manipulate the expression obtained always at the algebraic level (so with no diagrammatic interpretation) to get rid of such  $\lambda$  keeping an eye on the desired result. This procedure is given in details in the book by Stefanucci and van Leeuwen [6] so we refer the reader to their work without falling into technicalities. The final expression is

$$\beta(\Omega - \Omega_0) = -\{\Phi[G, v] - \text{Tr}[\Sigma G + \log(1 - G_0 \Sigma)]\}$$

which was first derived in almost the same form by Luttinger and Ward themselves. It may be formally regarded as a functional of the independent variables  $G_0, \Sigma$  and  $G$ , which takes the value of the Grand Potential of the physical theory when the three variables are related by the Dyson equation ( $G = G_0 + G_0 \Sigma G$ ) that turns out to be a stationary point for such functional. In honor of its fathers in literature it is referred to as the Luttinger-Ward functional.

### 3 Quasi-particles

This chapter will be devoted to one of the most prominent concepts of condensed matter physics: the quasi-particle one. The reason for doing so is that it is closely related with the Luttinger-Ward theorem.

This relation is reasonably based on the fact that such theorem is telling us about a preferred set of single-particle states such that their number exactly equals the number of particles. It comes natural then to think that such states will have something to do with the particle-like behaviour of the elementary excitation of the physical system, thus involving the quasi-particle theory.

The chapter is organized as following: first of all the presence of quasi-particles will be related to the analytic structure of the two points Green function of the theory (note there is no ambiguity in the previous sentence since we implicitly assumed that any anomalous correlation function vanishes, so there is only one meaningful two points Green function). Then the spectral representation of the propagator and the so-called “spectral function” is introduced since from it we can deepen the analysis of the quasi-particle content of the aforementioned Green function.

It follows a section where we present the physics of the system and its properties starting from an ansatz on the form of such spectral function. Eventually the chapter is concluded with an eye on the experimental counterpart of the quasi-particle theory, in particular showing how incredibly for a huge variety of physical system the whole effect of the presence of the interactions is to modify a very small set of measurable parameters, the most relevant of which being given by the effective mass.

#### 3.1 The single particle propagator

The zero-temperature single particle propagator in the time domain is defined by

$$iG(xt, x't') = \langle T\psi(xt)\psi(x't')^\dagger \rangle \quad (56)$$

This function describes the amplitude for the propagation of the system when at a certain time one particle or one “hole” is added to the ground-state of the system (here denoted “ $\psi$ ”) somewhere in space and then it is destroyed somewhere else at a later time.

For a non-interacting system, as could be expected, the propagator is just that of a free particle which propagates freely, conserving energy and momentum. Time and space translations invariance make  $G(xt, x't')$  a function of  $x - x'$  and  $t - t'$  so its Fourier transform is  $G(k, w)$ .

### 3.2 The Spectral Function

As we will derive in section (4.1), regardless the interaction we have the so-called “spectral” or “Källén–Lehmann” representation for it, that is we can write

$$G(k, w) = \int_{-\infty}^{\infty} ds \frac{A(k, s)}{w - s + i\eta \operatorname{sgn}(s - \mu)} \quad (57)$$

where the limit  $\eta \rightarrow 0^+$  is implied if not otherwise stated. The function  $A(k, s)$  is reasonably called the “spectral function” of the theory, it is real and non-negative and satisfies the normalization condition

$$\int_{-\infty}^{\infty} ds A(k, s) = 1 \quad (58)$$

So we see that

*$G(k, w)$  is always given by some sort of weighted superposition of free particle propagators.*

$A(k, s)$  is in fact the weight of a free particle that propagates with frequency  $s$  and momentum  $k$ . This is important since the exact free particle behaviour of  $G(xt, x't')$  in a free theory is a strict consequence of

$$A(k, s) = \delta(s - \epsilon_k) \quad (59)$$

where  $\epsilon_k$  is the free particle excitation spectrum. With this under consideration it comes natural to ask oneself when it happens that our single particle propagator still behaves approximately like that of a free particle one, if interactions are turned on. Of course we can't expect an exact behaviour of such kind, otherwise the single particle momentum state involved won't be interacting with the remainder of the physical system.

Nevertheless it is reasonable that an elementary excitation of a somehow weakly coupled system could still exhibit single particle properties, like satisfying some kind of dispersion relation. The spectral function in a free theory is a delta function centered at the dispersion relation indeed. This is the same as saying that  $G(k, w)$  has only a single pole when  $w$  varies at fixed  $k$  and this pole is also real. We thus investigate the implications of single poles presence.

### 3.3 Quasi-Particle poles

Following L.G.Molinari [10] we *define* a quasi-particle to be a pole in the propagator of the interacting theory

$$w - \epsilon_k - \Sigma(k, w) = 0 \quad (60)$$

It seems necessary for it to be the only simple pole at fixed  $k$ , otherwise the single-particle picture becomes meaningless. If the pole is given by

$$w_{pole}(k) = w_1(k) + iw_2(k) \quad (61)$$

the propagator splits up into a quasi-particle propagator plus a regular part

$$G(k, w) = \frac{Z(k)}{w - w_1(k) - iw_2(k)} + G^{reg}(k, w) \quad (62)$$

The residue at the pole  $Z(k)$  is naturally called “quasi-particle weight” and it is a real number satisfying

$$0 \leq Z(k) \leq 1 \quad (63)$$

thanks the normalization condition (58). At the same time (57) tells us  $w_2(k)$  has the same sign of  $\mu - w_1(k)$ . So we can go back to time domain and write

$$iG(k, t) = Z(k) \exp[-iw_1(k)t - w_2(k)t] + iG^{reg}(k, t) \quad (64)$$

when  $t > 0$  and  $w_1(k) > \mu$ . It should be noted now that in the region of  $k$  – space where  $Z(k)$  approaches the value 1 the quasi-particle propagator effectively describes the whole physical system. Moreover if the imaginary part of  $w_{pole}(k)$  is small the resulting excitation’s lifetime becomes long, resembling the infinite lifetime of a free particle. Since  $w_2(k)$  is a dimensional quantity saying it’s small doesn’t mean nothing. The requirement is made precise when we ask for

$$\left| \frac{w_2(k)}{\mu - w_1(k)} \right| \ll 1 \quad (65)$$

This is peculiar, indeed it is well-known //cita autori// that for a wide class of interacting theories  $G(xt, x't')$  is constrained to vanish for large times, i.e.

$$\lim_{|t-t'| \rightarrow \infty} iG(xt, x't') \rightarrow 0 \quad (66)$$

as described in [6], so the particle-like behaviour of  $G(k, t)$  must be circumscribed in time and cannot last forever.

### 3.4 A Lorentzian approximation

Since we have seen that

- the spectral function of a free theory is a delta function

- the simple poles in  $G(k, w)$  give quasi-particle properties

we can expect that for weak interactions the delta function behaviour gets smoothed and broadened to some larger probability distribution maintaining a well defined central peak somewhere and decaying indefinitely as  $s$  runs away from it. A behaviour of this kind could be obtained if we set  $A(k, s)$  to be a Lorentzian function

$$A(k, s) = \frac{1}{\pi} \frac{\Gamma_k}{(s - \epsilon_k)^2 + \Gamma_k^2} \quad (67)$$

As well known by mathematicians this is the prototypical example of a pathological distribution, since almost none of its momenta are finite. Nonetheless it possesses finite limits and since  $\Im G(k, w) \approx A(k, w)$  we must have  $A(k, \mu) = 0$ . In this case the propagator becomes

$$G(k, w) = \frac{1}{w - \epsilon_k + i\Gamma_k \operatorname{sgn}(\epsilon_k - \mu)} \quad (68)$$

where it is evident the imaginary part has a finite discontinuity crossing  $\epsilon_k = \mu$ . Of course if we make  $\Gamma_k \rightarrow 0^+$  we reproduce the propagator of the free system. If we go back to time domain we have

$$G(k, t) = \exp(-iw_k t - \Gamma_k t) - \Gamma_k \int_{-\infty}^{\mu} dw \frac{1}{\pi} \frac{\exp(-iwt)}{(w - \epsilon_k)^2 + \Gamma_k^2} \quad (69)$$

and when  $w_k \gg \mu + \Gamma_k$  the second term is negligible compared to the first one, which in turn gives a quasi-particle propagating with energy  $w_k$  and lifetime  $\Gamma_k^{-1}$ . Keep in mind that since in Quantum theories the action is dimensionless  $\epsilon_k$  and  $w_k$  are nothing but the same thing so I use them interchangeably. Under our Lorentzian approximation it is straightforward to check the momentum occupation number becomes

$$n_k = \frac{1}{2} + \frac{1}{\pi} \arctan \frac{\mu - \epsilon_k}{\Gamma_k} \quad (70)$$

$n_k$  gives back the free distribution  $n_k^0$  when  $\Gamma_k$  goes to zero but is a smooth function whenever such limit is not taken. Contrary to this we have that the presence of a quasi-particle pole in the propagator (64) affects the analytic structure of  $n_k$ . Indeed

$$n_k = \int_{-\infty}^{+\infty} dw \frac{1}{2\pi i} \exp(iw\eta) G(k, w) \quad (71)$$

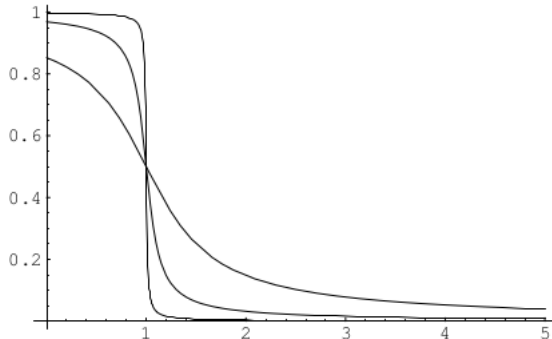


Figure 5: Momentum occupation number in the Lorentzian approximation;  $\mu$  is the energy unit,  $\Gamma/\mu = 0.01, 0.05, 0.1$  respectively, starting from the steepest curve. Molinari [10]

may be computed exactly and the residue theorem gives

$$n_k = n_k^{reg} + Z(k)\theta(\mu - \epsilon_k) \quad (72)$$

So we see that  $n_k$  has a discontinuous drop of magnitude  $Z(k)$  in crossing  $\epsilon_k = \mu$ . Such locus of points in  $k$ -space is a two-dimensional surface whenever  $\epsilon_k$  is a sufficiently regular function of  $k$ . This two dimensional surface should be called the Fermi Surface. So it is always true that if there are quasi-particles the system will exhibit a Fermi Surface and such surface will be the only singularity in the occupation numbers but we can't confidently state the converse anyway. Moreover at this level we can't state much about the FS volume. Still we can say something about such surface. Indeed for example Compton scattering experiments allow the step  $Z(k)$  to be measured [11]. Moreover we can relate it to the representation

$$G(k, w) = \frac{1}{w - \epsilon_k - \Sigma_k(w)} \quad (73)$$

since separating the real and imaginary part of (60) using (61) gives

$$w_1(k) - \epsilon_k - \Re\Sigma_k(w_1(k)) = 0 \quad (74)$$

$$w_2(k) = Z(k)\Im\Sigma_k(w_1(k)) \quad (75)$$

thus we have

$$Z(k) = (1 - \partial_w \Re\Sigma_k(w))^{-1}|_{w=w_1(k)} \quad (76)$$

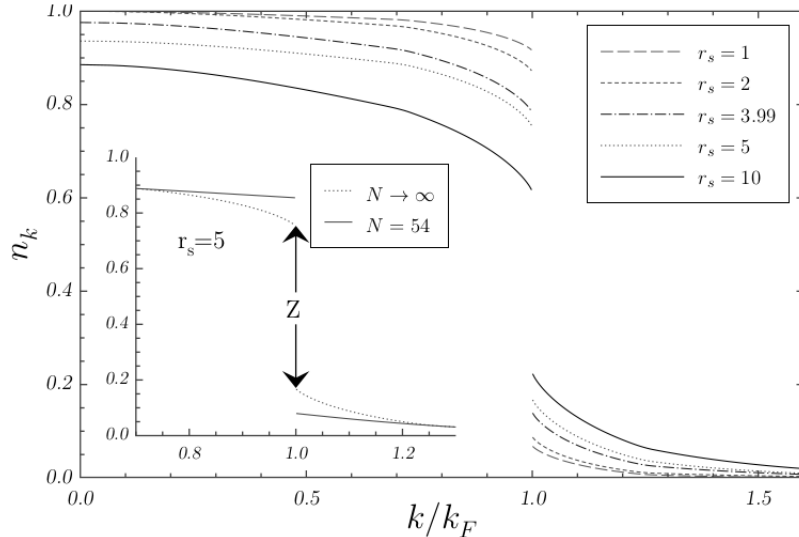


Figure 6:  $n_k$  for different values of  $r_s$  in the homogeneous electron gas. Ceperley et al. [25]

### 3.5 Mass renormalization in metals

Near the FS the imaginary part of the self-energy  $\Im\Sigma_k(w)$  approaches zero, making quasi-particles lifetime in that region considerably long. I find noteworthy to say experiments in metallic quantum wells done with thin Lead (Pb) films on Silicon (Si) show lifetimes ranging around hundred of femtoseconds (100fs) [12] and similar values are also found in graphene layers [13]. A detailed discussion of quasi-particles lifetime in the two and three dimensional electron liquid including temperature effects may be found in [14]. If  $Z(k)$  is close to one we can expand the dispersion relation near the FS. Assuming isotropy

$$w_1(k) = \mu + \frac{1}{2m^*}k_F(k - k_F) + \dots \quad (77)$$

with  $m^*$  the effective mass of the quasi-particle. So using (76) and the fact we're close the FS gives

$$\frac{m}{m^*} = Z(k_F)\left(1 + \frac{m}{k_F}\partial_k\Re\Sigma_k(\mu)|_{k=k_F}\right) \quad (78)$$



As could be expected the lifetime is related to  $\Im\Sigma_k(w)$ , so for our quasi-particle we have

$$\frac{1}{\tau_k} = -2Z(k)\Im\Sigma_k(w_1(k)) \quad (79)$$

The parameters  $m^*$ ,  $\tau_k$  and  $Z(k)$  for the homogeneous electron gas can be computed by means of different approximation techniques, as can be found in [15] and [16]. In the first case we have

$$\frac{m}{m^*} = 1 - 0.083 r_s(\log r_s + 0.203) + \dots \quad (80)$$

$$\frac{1}{\tau_k} = 0.252 (r_s)^{1/2} \frac{1}{2m} (k - k_F)^2 + \dots \quad (81)$$

where  $r_s$  is the so called Seitz radius of the system. It is defined to be the radius of the sphere that contains exactly one electron in units of the Bohr radius, that is the length scale given by the elementary charge and electron mass,  $a_{Bohr} = 1/me^2$ . In symbols

$$\frac{4}{3}\pi\left(\frac{r_s}{a_{Bohr}}\right)^3 = n^{-1} \quad (82)$$

It is interesting the mass renormalization in metals ranges wide since it could run from few points percent up to hundred times the bare value for strongly correlated materials [17]. Recently it has even been shown that the effective mass could show divergences in two-dimensional electrons systems [18].

## 4 The Fermi Liquid Theory

Since we have explored many particular aspects and peculiar facts concerning the many-body physics it is appropriate to devote this next chapter to a little contextualization of them. There is indeed a natural theoretical environment in which the matter discussed find their place: the Landau-Fermi liquid framework.

An excellent and complete treatment of it is given amongst many others by Giuliani and Vignale [17], that will be referred to also for the alternative proof of Luttinger-Ward statement they gave and that we will explore later. The starting point for the Fermi Liquid Theory (usually an electron liquid) is the experimental ground. Indeed we have evidences showing off that for many common metals the valence or conduction electrons behave just like if they were independent free particles, notwithstanding the actual mutual interaction strength.

Since the early 30's many aspects of their behaviour was predicted in terms of the degenerate Fermi gas picture. The justification of such fact made the physicists of that time struggle: for densities in the metallic range ( $r_s \approx 2-5$ ) the Coulomb interaction is even larger than the corresponding free gas Fermi energy, so in principle it should not be valid to regard it as a perturbation to the free system. For example in metallic Sodium (Na)

- $r_s \approx 3.9$
- $\epsilon_F \approx 3.2 \text{ eV}$
- $u_{int} \approx 4.3 \text{ eV}$

Around 1960 it was the genius of Lev Davidovich Landau that gave us the basis to understand what is nowadays called the “normal” or low-energy behaviour of an interacting Fermi system. As usual for him the good Lev never provided a rigorous solution of the problem: he just gave us a working one.

His work, nowadays referred to as the Landau-Fermi liquid theory, has been proved so successful in describing metals that deviations from its forecast are considered somehow exotic and are often prompt to rise the many-body community interest. Standard exceptions may be found in low and especially one-dimensional systems, where the physics itself literally becomes different as we already told in the introduction.

## 4.1 A continuity principle

The key idea grounding Landau's theory is that, for a wide class of fermionic systems where interactions are through repulsive potentials, it is possible to deform somehow continuously an elementary excitation of the free system into one of the interacting one.

From a technical point of view today we know this connection is obtained by means of the Gell-Mann and Low theorem. The classical derivation of it, regardless unwieldy, has been given by several authors and among these I prefer Fetter and Walecka's one [19].

Still besides those proofs fortunately we can cite a modern and radically different approach to such theorem, given by Molinari [21], where the Schrödinger equation for the propagator is taken as starting point for a much simpler proof. Anyway we don't need to fall into its proof technicalities, which often merely tend to obscure what should be clear from the very beginning. Indeed what happens essentially is that one introduces a fictitious and suitably slow switching-on of the interactions, i.e.

$$H(t) = H_0 + f_\eta(t) V \quad (83)$$

$$f_\eta(t) = \exp(-\eta|t|) \quad (84)$$

and uses the corresponding time evolution to evolve the eigenstates of the free theory, with the hope that when the switching-on is made infinitely slow one obtains something, so that the limit

$$\lim_{\eta \rightarrow 0^+} \lim_{t' \rightarrow +\infty} \frac{U_\eta(0, -t')|E_0\rangle}{\langle E_0|U_\eta(0, -t')|E_0\rangle} \quad (85)$$

exists. This procedure is called adiabatic switching-on of the interaction and the corresponding unitary evolution the adiabatic evolution. In this case the aforementioned theorem tells us this limit is an eigenstate of the interacting Hamiltonian.

If the limit does not exist it is still possible that for very small values of  $\eta$  the state obtained behaves approximately like an eigenstate, at least for time intervals

$$\Delta t \ll \eta^{-1} \quad (86)$$

Of course this behaviour is reminiscent of the quasi-particle properties seen in the previous chapter and the condition (86) relates to quasi-particle's lifetime. Another thing to mention is that it seems quite nothing can be said about the occurrence of level-crossing: we can start with a couple of eigenstates of the free theory  $|E_0\rangle, |E'_0\rangle$ , evolve them adiabatically and get

a couple of states  $|E\rangle, |E'\rangle$  with  $E_0 < E'_0$  but  $E > E'$  (assuming the limit exists). An example of such change of symmetry but in a few-body problem is given by [20]. We will explore in the next chapter some relevant facts happening if such level-crossing occurs on the ground state of the free theory.

## 4.2 Landau Effective Hamiltonian

Basing on the aforementioned continuity principle Landau postulated that, since the occupation numbers  $n_0(k)$  defined by

$$n_0(k) = \langle a_k^\dagger a_k \rangle \quad (87)$$

specify the eigenstates of the free theory, at least for the low-energy sector of the interacting theory

$$E_{exc} - E_{gs} \approx \mu + \Delta = \mu[1 + (\Delta/\mu)] \quad (88)$$

$$\Delta/\mu \ll 1 \quad (89)$$

it should be possible to describe the elementary excitation of the interacting theory using the same set of quantum numbers. Incidentally it is peculiar that the conditions (87),(88) together tell us we are not describing any collective excitation of the system, in case of which one would expect

$$E_{exc} - E_{gs} \approx N\mu \quad (90)$$

or at high temperatures something like

$$E_{exc} - E_{gs} \approx N\beta^{-1} \quad (91)$$

Of course these  $\mathcal{N}_k$  represent no more the occupations of single-particle's momentum states. They rather represent, as should be quite clear now, the occupation number of quasi-particle (or quasi-hole) states carrying the same momentum. Another way to remark this is to say

$$[a_k^\dagger a_k, V] \neq 0 \quad (92)$$

with  $V$  the interaction potential, so the  $n_0(k)$  will in general have a non-trivial time evolution even during the adiabatic switch-on and won't be constants of the motion anymore. Since the free ground state is a filled Fermi Sphere the line we're following suggests then that the interacting ground state would resemble a suitable "Fermi Surface" but filled with the quasi-particles instead.

This makes a variation of Luttinger-Ward statement immediate: the number of quasi-particles in the interacting ground state equals the number of bare particles of the non-interacting one. We are thus dealing with two number-distributions at the same time:

- $n(k) = \langle a_k^\dagger a_k \rangle$  = number of bare particles with momentum  $k$  in the interacting ground state (or any other state as well)
- $\mathcal{N}(k)$  = number of quasi-particles carrying momentum  $k$  in the ground state (or in weakly excited states either)

Landau's postulate then brings to ask oneself how the energy could depend on the  $\mathcal{N}(k)$ . Concerning this he wrote down the most natural possible thing: an effective Hamiltonian (or rather an energy functional) expanded around  $E_{gs}$  to the second order in the  $\delta\mathcal{N}(k)$ , that is the deviation of  $\mathcal{N}(k)$  from their equilibrium distribution, i.e. a filled Fermi Sphere. So we ended up with is

$$E[\{\mathcal{N}(k)\}] = E_{gs} + \sum_k \varepsilon_k \delta\mathcal{N}(k) + \frac{1}{2} \sum_{k,k'} f_{k,k'} \delta\mathcal{N}(k) \delta\mathcal{N}(k') \quad (93)$$

where  $\varepsilon_k$  and  $f_{k,k'}$  are the quasi-particle "kinetic" energy and the interaction function. The conditions (88),(89) make clear the  $\mathcal{N}(k)$  should not deviate much from zero whenever  $k$  isn't close to the Fermi Sphere for this functional description to make sense.

This quasi-particle picture together with (93) gives us another way to approach some of the concepts seen in the previous chapter. For example since  $\varepsilon_k$  represents somehow a kinetic term for the quasi-particle the analogy with bare particles suggest to define the effective mass as

$$\frac{1}{m^*} = \frac{1}{k_F} \partial_k \varepsilon_k |_{k=k_F} \quad (94)$$

or that we have to identify

$$\varepsilon_{k_F} = \mu \quad (95)$$

Moreover it is noteworthy that the full single quasi-particle energy could be computed as

$$\tilde{\varepsilon}_k = \frac{\delta E}{\delta \mathcal{N}(k)} = \varepsilon_k + \sum_{k'} f_{k,k'} \delta\mathcal{N}(k') \quad (96)$$

with the second term representing a contribution to the kinetic energy given by the interaction with the remainder of the system, where the coefficient  $f_{k,k'}$  given by

$$f_{k,k'} = \frac{\delta^2 E}{\delta \mathcal{N}(k) \delta \mathcal{N}(k')} \quad (97)$$

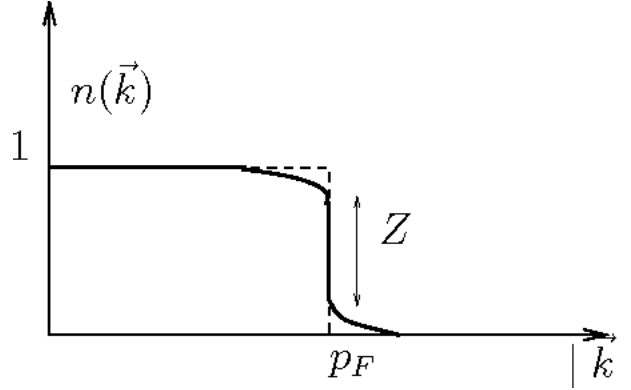


Figure 7: Particle vs quasiparticle momentum distribution function at zero temperature. Google Images

### 4.3 Entropy for the quasi-particle ensemble

Another remarkable fact concerning Landau-Fermi liquid theory is that we can formally regard the  $\mathcal{N}(k)$  as a set of occupation numbers specifying a grand-canonical ensemble. So it's straightforward that its statistics will be given by an entropy principle. The correct functional for it is (cf. [17])

$$S[\mathcal{N}(k)] = - \sum_k \mathcal{N}(k) \log \mathcal{N}(k) + (1 - \mathcal{N}(k)) \log (1 - \mathcal{N}(k)) \quad (98)$$

Armed with this expression we can write down the corresponding grand potential, that of course is

$$\Omega[\mathcal{N}(k)] = E[\mathcal{N}(k)] - \beta^{-1} S[\mathcal{N}(k)] - \mu \sum_k \mathcal{N}(k) \quad (99)$$

At this level  $\mu$  should be obtained minimizing  $\Omega[\mathcal{N}(k)]$ . Since expressions (93) and (98) are given explicitly such computation is easily possible and gives us the quasi-particle equilibrium distribution function at finite temperature

$$\mathcal{N}^{eq}(k) = \frac{1}{1 + \exp[\beta(\tilde{\varepsilon}_k - \mu)]} \quad (100)$$

The last comment here is the latter equation should be solved at the same time of (96) so a sort of self-consistency in this quasi-particle ensemble picture is evident.

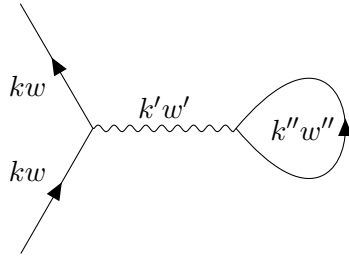
## 4.4 Freezing particles on the Fermi Surface

Having understood that continuity is the key to transform the non-interacting low-energy sector of the statistical ensemble into the interacting one, whether or not Landau-Fermi liquid theory could effectively describe the physical system in such sector relies on the actual ineffectiveness of the occurrence of the interactions to change the momentum occupation numbers when we are close to the Fermi Surface.

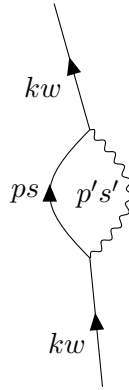
We will reach this conclusion in a twofold way, one of which is a simple application of standard perturbation theory while the other one is a more qualitative argument.

### 4.4.1 A diagrammatic interpretation

As promised the result may be obtained by means of a perturbative diagrammatic expansion where, from the second order one, terms give the self-energy a non-trivial  $w$ -dependence. It is quite a general fact that at the first order the self energy is just a constant with respect to  $w$ . This could be seen easily looking at the two diagrams below



(101)



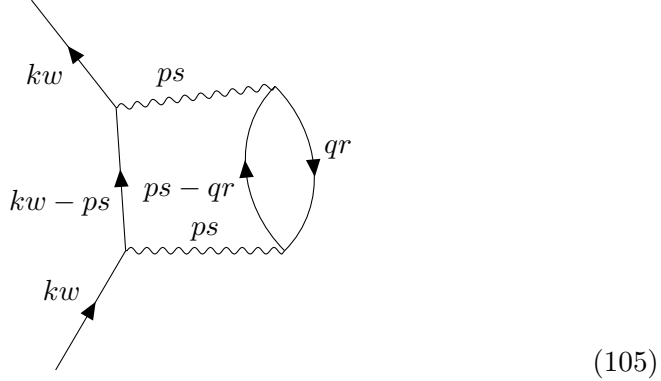
(102)

where the labels are couples of linear momentum and energy values respectively. For the theories we are interested in they are all the diagrams to be considered for the first order self-energy's computation and energy and momentum are exactly conserved quantities. So in the diagrams above we have to set  $k'w'$  equal to zero and  $ps = kw - p's'$ . Moreover the energy dependence of the bare interaction is trivial, thus summing over the internal labels we get a contribution independent of  $w$ . Of course the converse is not true for  $k$ . Explicitly

$$\Sigma^{(1)}(k, w) \approx u(0)(N/V) - (\beta V)^{-1} \sum_{ps} e^{is\eta} u(p) G_0(k-p, w-s) = \quad (103)$$

$$= u(0)n - \sum_p u(p)n_0(k-p) \quad (104)$$

which makes the independence of  $\Sigma^{(1)}$  on  $w$  evident. The conditions above do not hold if we consider higher order diagrams, where it's possible for the self-energy to acquire some  $w$ -dependence. Again an exemplification of this is given by



where the contribution to  $\Sigma^{(2)}$  turns out to be proportional to

$$\frac{1}{(\beta V)^2} \sum_{ps} \{G_0(k-p, w-s)[u(p)]^2 \sum_{qr} G_0(qr)G_0(p-q, s-r)\} \quad (106)$$

so even without pushing the computation further it's easy to convince oneself the non-trivial convolutions of (106) may give  $\Sigma$  the  $w$ -dependence we mentioned insofar. It should be remarked that without it Luttinger-Ward theorem becomes trivial and the Fermi Surface simply becomes

$$\mu - \epsilon(k) = 0 \rightarrow \mu - [\epsilon(k) + \Sigma^{(1)}(k, \mu)] = 0 \quad (107)$$



This is evident since a propagator of the form

$$G(k, w) = \frac{1}{\mu + iw - x(k, \mu)} \quad (108)$$

would give an occupation number

$$n(k, \mu; \beta) = \frac{1}{e^{\beta[x(k, \mu) - \mu]} + 1} \quad (109)$$

that reasonably should satisfy

$$\lim_{\beta \rightarrow \infty} n(k, \mu; \beta) \rightarrow \theta(\mu - x(k, \mu)) \quad (110)$$

This is interesting since the value of  $\mu$  has to be fixed to give back the correct value for the total number of particles, that is

$$N = \sum_k \theta(\mu - x(k, \mu)) \quad (111)$$

is an equation to be solved for  $\mu$  and the thesis' theorem statement becomes somehow the result of a self-consistent condition. This fact is a characteristic of the free theories also and it's probably more involved in Luttinger-Ward theorem than we understand nowadays.

Apart from this one can compute all the second order diagrams and get the full contribution to  $\Sigma^{(2)}$ . This has been done by several authors (see for example the renowned book of Fetter and Walecka [19]) so it's quite meaningless to repeat here their calculations. We just content ourselves to state that at second order the imaginary part turns out to be proportional to

$$\Im \Sigma^{(2)}(k, w) \approx c(k)(w - \mu)^2 \quad (112)$$

This makes any excitation lifetime approach infinity when its momentum approaches the Fermi Surface that's what we wish to check. We will elucidate this in showing up the relation between it and the Spectral Function of the previous chapter. Equation (112) is so relevant that sometimes it's taken as a defining feature of the Fermi liquid.

#### 4.4.2 The Phase Space argument

As anticipated this will be a qualitative reasoning. Remark then that we wish to rule out the possibility that particles scatter out the Fermi surface. To avoid useless technicalities we will focus on the isotropic situation. So

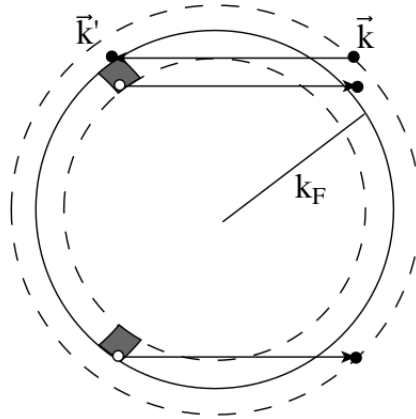


Figure 8: Schematic illustration of the quasiparticle decay process. Giuliani-Vignale [17]

the natural starting point here is to consider a wave-vector close to the FS but outside of it  $k : k > k_F$ . The admissible states for a decay process condense in a thin shell outside the FS, since all the states inside of it are already occupied. Since the probability of decay is proportional to the total number of possible “out” states we get a factor for it proportional to the shell thickness  $|k - k_F|$ .

Since we have to conserve energy and momentum during the process we have to excite a hole that lives in again in a shell of the same thickness but this time it has to be below the Fermi Surface, giving us another factor  $|k - k_F|$  for the probability of the decay. We then have that the scattering rate vanishes approximately like  $(k - k_F)^2$  as we approach the Fermi Surface. This is exactly the result we wanted. It should be remarked again that since the momentum occupation numbers are not exactly conserved quantities one would see them change if the system is observed for a long time.

#### 4.5 Making profit of the Golden Rule

When we deal with Fermi liquids the main process that can make a quasiparticle decay is the so-called “*electron-hole pair production*”. To avoid complications related to temperature we will assume it to be sufficiently low for our argument to be valid. So essentially what we do to estimate the quasi-particle lifetime is to apply directly the famous “*Fermi golden rule*” for the probability of the transition between the quasi-particle and electron-hole

couple states. Let's then consider a couple of electrons carrying momentum  $p$  and  $p'$  respectively. The scattering rate at exchanged momentum  $q$ , i.e.

$$\begin{aligned} p &\rightarrow p + q \\ p' &\rightarrow p' - q \end{aligned} \quad (113)$$

according to the golden rule is

$$R(q, p', p) = 2\pi |w(q)|^2 \delta[\varepsilon(p + q) + \varepsilon(p' - q) - \varepsilon(p') - \varepsilon(p)] \quad (114)$$

where  $w(q)$  is the matrix element of the interaction potential corresponding to the process and the  $\varepsilon(x)$  as usual are the free-particle energies at momentum  $x$ . I hope to be crystal clear for the reader that (114) is an approximate result. If we sum over all the possible decay processes where one of the two electrons has momentum  $p$  we get the total probability of decay for a particle with that momentum.

$$\tau_p^{-1} = \sum_{p', q} R(q, p', p) \{n(p') [1 - n(p' - q)] [1 - n(p + q)]\} \quad (115)$$

again with  $n(x)$  the free theory occupation number at momentum  $x$ . The three factors following  $R(q, p', p)$  have a simple physical interpretation, indeed of course the probability to scatter off against a state with momentum  $p'$  should be proportional to the actual number of particles carrying such momentum, thus giving the factor  $n(p')$  and quite the same reasoning applies for the remaining ones.

From equation (115) a certain number of approximations (the details of which are of no interest here and for which we refer back again to Giuliani and Vignale's book [17]) allow to do the calculation and cast the expression for  $\tau_p$  for a three-dimensional system in the somehow simpler form

$$\tau_p^{-1} = \frac{\pi}{8\mu} \frac{(\varepsilon(p) - \mu)^2 + \pi^2 \beta^{-2}}{e^{-\beta(\varepsilon(p) - \mu)} + 1} \xi(r_s) \quad (116)$$

where  $r_s$  is again the Seitz radius and the function  $\xi(r_s)$  is defined as

$$\xi(r_s) = \frac{1}{2[1 + g(r_s)]} + \frac{1}{2} \sqrt{g(r_s)} \tan^{-1}[1/\sqrt{g(r_s)}] \quad (117)$$

$$g(r_s) = (9/4\pi)^{1/3} (\pi/r_s) \quad (118)$$

An interesting fact is that when  $r_s \rightarrow 0$  we have  $\xi(r_s) \rightarrow \sqrt{r_s}$  so the decay rate turns out to be proportional to the elementary charge  $e$  instead of the  $e^4$

dependence one could have expected stemming from the standard scattering theory. It seems indicated to remark that the dependence on the elementary electric charge here is completely contained in the Seitz radius, explicitly:  $r_s = (me^2)[3/4\pi n]^{1/3}$ .

I conclude saying some reader may have imagined the naive result should not apply since it's a matter of a couple lines to show the Jellium hamiltonian may be cast in the form of an energy scale times a dimensionless operator whose sole parameter is the Seitz radius.

## 4.6 Summarizing the results

Last chapter we have explored many different aspects of the electron liquid theory and one may feel confused about the huge amount of information to be managed at once.

Nevertheless what is important in physics is always to try to keep evident what is relevant and to wash away any remainder. So basically in this chapter we have seen that a Fermi liquid is any physical system that can be obtained by a suitably slow and continuous switching-on of the interactions starting from a homogeneous electron gas. In this system we then found a remnant of the Fermi surface and the existence of many long lived particle-like excitation that we naturally called quasi-particles.

We investigated the possibility to describe the system as if these quasi-particles were the true elementary degrees of freedom, thus defining an effective Hamiltonian for them and a quasi-particle ensemble and we have shown it could be used in order to compute some properties of the system. In the end we have examined in details the mechanism giving an excitation close to the Fermi Surface an infinitely long lifetime, both from the qualitative and quantitative point of view, relating the microscopic physics to the intuitive results always working in the domain of perturbative approaches. A last comment is mandatory: the historical Landau-Fermi liquid theory has been recently revised in a novel fashion in the modern times, where the Renormalization Group approach to the theory has been devised by many authors [29] [30].

## 5 More proofs of the theorem

As anticipated in the introduction the scientific literature in about 70 years has literally clouded in folklore what the Luttinger-Ward theorem is and whether or not the Fermi (or Landau-Fermi) liquid picture gives a valid description of a physical system.

I think probably anyone having spent enough time scratching his head in this field of physics feels (or felt - we have to pay homage to the giants of the past whose shoulders we're trying to climb on) a concrete and strong sensation that these apparently disconnected issues hide a connection instead, way deeper than we can show and understand within the mathematics of the present days.

It comes by itself that our purpose, as well as it was for those who tried to do this before, is still try to address the question as much as possible. To this end it is natural to slow down a little and spend a couple of words trying to figure out what's going on from the physical point of view.

On one side we are considering a system of interacting electrons and we wish to tell when it behaves like if they were free particles. On the other side we have a theorem that tells us something we know how to state mathematically:

*The number of states such that  $G(k, \mu) > 0$  equals the number of particles.*

How could we say this physically?

As we pointed out earlier the propagator in the time domain has a simple interpretation. It gives the probability amplitude between the initial and final states after a certain time lapse, where both states are obtained adding a particle or a hole to the many-body ground state. It is of course a function of the time lapse only in our physical theories since there is no preferred point in time. When the time lapse is positive we are describing the propagation of a particle and when it's negative we propagate holes.

It is good practice to picture this making use of the experiments. We can inject holes by photo-emission on our bulk metal, shooting photons in it with some powerful laser beam to kick-out electrons and all the same we can inject an electron beam with a simple electron gun pulling electrons out some hot filament. Since we can control quite easily the momentum of the incident beam a measure of if for the outgoing one would give the value of the injected momentum, so we are really implementing the field operators  $a_k, a_k^\dagger$ .

What is the interpretation when we switch to frequency domain? Basically

we are taking the spectral components of  $G(k, t)$ ; that is we are looking at each portion of the propagation process happening with a well-definite energy separately. What is then so special in the energy value  $w = \mu$ ? We again have a simple answer: it is the energy value connecting the ground state of the  $N$  and  $N + 1$  particle systems. We can rephrase this saying that  $G(k, \mu)$  gives the amplitude to fall into the  $N + 1$  particles ground state when we inject an electron carrying momentum  $k$ . Since in the thermodynamic limit we expect

$$\mu_N - \mu_{N-1} \rightarrow 0 \tag{119}$$

we may assume  $G(k, \mu)$  simply also gets the contribution given by the amplitude that the system falls into the  $N - 1$  particle ground state when we remove an electron with the same momentum instead.

I feel necessary to comment that this hypothesis could hide subtleties from the mathematical point of view. To have an intuition that they are present one could simply think that, exactly in the same limit, (119) does not imply

$$G(k, \mu_N) - G(k, \mu_{N-1}) \rightarrow 0 \tag{120}$$

or any similar equation. This kind of result is evidently related to the continuity of  $G(k, w)$ . Again we see that the somehow emergent analytic structure, when we take an infinite system, plays a pivotal role even at the fundamental level of simply addressing the question: “What does the thing I compute this way represents on the experimental ground?”. Moreover even if we assume  $G(k, w)$  to be a continuous function it isn’t to any extent clear what should be the physical interpretation.

The best I’m able to reason out to this end is the following. The sole fact that  $\Im G(k, \mu)$  vanishes regardless of  $k$  tells us that the processes involved at the chemical potential energy are forced to interfere with a perfect phase or anti-phase match, that is to say the interference can only be completely constructive or destructive either.

From this perspective it seems the theorem, when cast in a physical fashion, is telling us that the whole set of processes whose interference is constructive must account for the total number of bare particles present in the system. The reason why it should be so to the present day is still a fascinating mystery to me which I hope someone to shed light on one day. In order to try to get closer to its solution it seems a good thing to explore other proofs that have been given during past year, probably with the very same purpose.

Apart of the preamble being given by my little apology here is the content of

the following chapter. First of all we will dwell with the proof of Luttinger-Ward theorem given by Dzyaloshinskii. There are two reasons for doing so. The first one is objective: such proof extends the validity of the theorem to the Mott Insulators and to non-Fermi liquids. For the thesis to be self-contained and for clarity I found appropriate to spend some words describing what they are, so there will be a couple of subsections reserved to them. The second one isn't objective and is that such proofs seems to me and to my supervisor one of the most beautiful appearing in the literature we examined.

Then it follows a little part in which we show, always according to the same author, how the extension of the theorem to electrons living in the crystalline states of matter is almost a mere technicality. After such part another original proof of the theorem, namely the one given by Giuliani and Vignale, is presented since it differs from the most standard ones in many ways.

The chapter is concluded with an argument given by Guraire which allows to infer the existence of the  $\Phi$ -functional involved in the proof we mentioned and discussed insofar. To conclude I wish to mention a recent publication by Pieri and Strinati [31] where they dwell with unbalanced Fermi system (thus taking spin into account) since in this thesis we never give space to such issue.

## 5.1 Dzyaloshinskii Proof

In a seminal paper dating back to the early 2000s [22] Igor Dzyaloshinskii showed that a careful analysis of Luttinger theorem brings to conclude there is a close analogue of the Fermi surface far beyond the metals domain. The branches of Luttinger's tree extend themselves pervading even the Mott insulator and Non-Fermi liquids theories indeed.

As already told, it seems indicated to me to spend few words describing them in order to appreciate the almost mystical wideness of the environment in which Luttinger-Ward theorem holds.

### 5.1.1 Mott Insulators

In the Mott insulators standard band theory does not work: it predicts we should have an ohmic behaviour but it turns out we really have insulators. Thus they are a genuine example of a system where the interactions break the free-particle picture.

Moreover they are really peculiar since in this kind of materials the metal-insulator transition takes place, as predicted by N.Mott himself [23] decades ago and the transition has been subsequently observed for example [24] in doped Silicon via electronic Raman spectroscopy.

### 5.1.2 Non-Fermi liquids

According to what we have understood about his counterpart, we can reasonably define a non-Fermi liquid to be any physical system of (necessarily) interacting fermions where the individuality of any low-energy excitation fades into collective phenomena. That is to say we don't find the particle-like behaviour anymore.

Even if we avoid most of the complications we should be concerned with when we describe a real system of interacting electrons (spin-glass states, superfluid states, magnetic ordering, topological phases etc.), the sole intake of the Coulomb interaction forces us to sketch a phase diagram with some crystalline (or localized electrons) phases in it. A more realistic numeric simulation makes out something looking like that in fig. 9. Naively one could think it is the case because in such system the average kinetic energy per electron should go like

$$\epsilon_{Kin} \approx n^{2/3} \quad (121)$$

while for the interaction one, assuming some sort of screening to assure the energy is extensive

$$u_{int} \approx n^{\frac{1}{3}} \quad (122)$$

where the formulas refer to three dimensions. Still this prediction is not the best one we can formulate, at least in my opinion, since whenever the Hamiltonian is a sum of homogeneous functions (depending only on the momentum or position of the particles) we can invoke the Virial theorem. Contrary to the equations above it gives us exact an relation between the averages of the total kinetic and potential energy on any true eigenstate of the full Hamiltonian. If we can apply such theorem the relation should run

$$2\langle T \rangle + \langle V \rangle = 0 \quad (123)$$

so it would be no more obvious that we could have crystals. Nevertheless for the systems we are dealing with (123) is wrong for more than one reason, indeed we lied to the reader in the lines above; it's not true that we can use the Virial theorem here since we're not dealing with any bound state of particles living in the euclidean space. Anyway what matter to us is that,



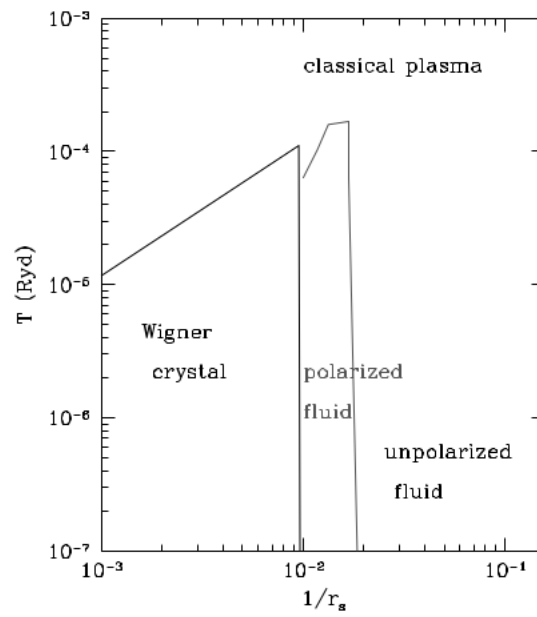


Figure 9: Phase diagram of the three dimensional HEG. Giuliani-Vignale [17]

as mentioned previously, we expect the emergence of crystalline states for sufficiently low temperature and density.

In these states it's not difficult to convince oneself that the most probable low-energy physics is that of a vibrating crystal or equivalently an ensemble of almost uncoupled harmonic oscillators, so only the collective excitations appear and the Fermi liquid behaviour is completely lost. We have thus an example of a real physical system of interacting electrons breaking the Fermi liquid theory. To the same end of giving examples of such systems in the real world it is noteworthy to mention one-dimensional systems also: they display a non-Fermi liquid behaviour indeed we know there will be a different physics, usually demanding a separate treatment.

### 5.1.3 The Luttinger Momentum

Having understood qualitatively what a Mott Insulator and a non-Fermi liquid is, we can focus back on Dzyaloshinskii paper. In it the author applied the Luttinger theorem in its modern (and “most general”, according to his own words) form, that is

$$\frac{N}{V} = \int \frac{d^3p}{(2\pi)^3} \theta[G(0, p)] \quad (124)$$

both to Mott Insulators and non-Fermi liquids. In the equation above  $\theta[.]$  is the Heaviside step-function and in the original paper an additional factor 2 accounts for spin multiplicity. Here we will ignore spin since it's not essential to the argument.

The careful reader may find himself confused at this point but there is no need to worry: we can use  $G(0, k)$  or  $G(\mu, k)$  in the relation above because they are different (and probably a little misleading) notations for the same object. Indeed we can think the frequency to be a purely imaginary number and use the first notation or we can include in the frequency a real part given by the chemical potential and use the second one.

The Luttinger momentum  $P_L$  is defined to be the locus where  $G(0, p)$  changes sign, regardless being continuous or finite at  $p = P_L$ . For his proof the author makes use of three kinds of propagators at finite temperature: the retarded (analytic in the upper half of the complex plane), the advanced (analytic in the bottom half) and the Matsubara one. The fact that Luttinger theorem is essentially a consequence of the analytic properties of the propagators is explicitly stated at the very beginning. The three propagators share an

Hilbert representation for  $\Im\epsilon \neq 0$

$$G_{r,a}(\epsilon) = \frac{1}{\pi} \int_{-\infty}^{+\infty} dx \frac{\rho(x)}{x - \epsilon} \quad (125)$$

where the equation holds whenever  $\Im\epsilon \neq 0$ . The Matsubara propagator is given by

$$M(\zeta_n) = G_{r,a}(i\zeta_n) \quad (126)$$

according to whether  $\zeta_n$  is positive or negative respectively. For the reader's convenience allow me to remark that here  $i\zeta_n$  is the purely imaginary Matsubara frequency  $i\pi(2n+1)/\beta$ . Sadly I also have to say that, because of a different sign convention, the spectral weight function  $\rho(x)$  here is said to be negative for all the values of  $x$ , contrary to the spectral function we defined earlier. In my opinion the best one could prove is that  $\rho(x)$  is never positive (or never negative according to the convention one chooses). Moreover we it is well-known that the spectral function is related to the imaginary part of the propagator that must vanish at least for  $w = \mu$ .

Nevertheless the proof goes on the following: starting from the expression for the density in terms of the Matsubara propagator

$$n(\mu, \beta) = \frac{1}{\beta} \sum_l e^{i\zeta_l \eta} \int \frac{d^3 p}{(2\pi)^3} M(\zeta_l, p, \beta) \quad (127)$$

(with the usual limit  $\eta \rightarrow 0^+$  taken at the end of the calculation) under the hypothesis of no phase transition at zero temperature the sum is switched to an integral over the continuous variable  $\zeta$ . In practice on the complex plane we integrate on a path moving upward on the imaginary axis. In formulae

$$\lim_{\beta \rightarrow \infty} n(\mu, \beta) = \int \frac{d\zeta d^3 p}{(2\pi)^4} e^{i\zeta \eta} M(\zeta, p, +\infty) \quad (128)$$

and from now on  $M(\zeta, p, +\infty)$  will be denoted simply by  $M(\zeta, p)$ . Then follows a transposition of some steps that appear in the original Luttinger-Ward proof we started with. I just mention them since there is really no need to write them down twice. So the integrand is rewritten as

$$-iM(\zeta, p)[\partial_\zeta M^{-1}(\zeta, p) + \partial_\zeta \Sigma(\zeta, p)] \quad (129)$$

where  $\Sigma$  is the self-energy and the second term is immediately dropped, referring back to the construction and effective argument given by Luttinger. My personal comment here is that again we see that this exact cancellation is cardinal for the validity of Luttinger-Ward theorem. We can literally rephrase the theorem (using modern notations) like

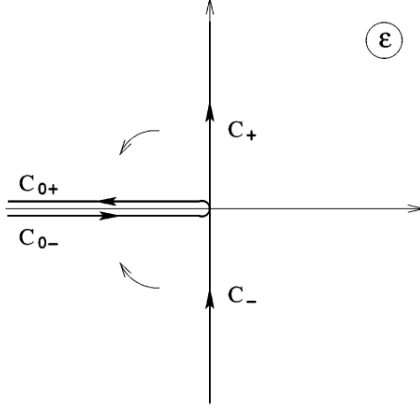


Figure 10: Contour deformation in the complex energy plane. Dzyaloshinskii [22]

*The integral  $\int d\zeta d^3p \Sigma(p, \zeta) \partial_\zeta G(p, \zeta)$  vanishes identically*

and i remark this result is linked with the dressed expansion of the grand potential as we have seen. The author is then left with the following expression for the density in the limit of zero temperature

$$n = \frac{i}{(2\pi)^4} \int d\zeta d^3p e^{i\zeta\eta} \partial_\zeta \log M(\zeta, p) \quad (130)$$

We encountered this expression already but from here the proof separates from that already seen. Indeed the author makes use of (126) to rewrite (130) as

$$n = \frac{i}{(2\pi)^4} \int d^3p \left\{ \int_{C^+} \dots + \int_{C^-} \dots \right\} \quad (131)$$

where  $C^+$  and  $C^-$  are the top and bottom halves of the imaginary axis and the dots stand for

$$d\epsilon e^{\epsilon\eta} \partial_\epsilon \log G_{r,a}(\epsilon, p) \quad (132)$$

respectively. The path of integration is then closed to the left, encircling the negative part of the real axis as shown in fig. 10. This can be done thanks the exponential factor and the hypothesis that both  $G$ 's never vanish on each logarithm is analytic. Then the expression turns into

$$n = \frac{i}{(2\pi)^4} \int d^3p \int_{-\infty}^0 d\epsilon \partial_\epsilon \log [G_r(\epsilon) / G_r^*(\epsilon)] \quad (133)$$

with  $*$  denoting the complex conjugate. (133) is then rewritten as

$$n = -\frac{1}{\pi(2\pi)^3} \int d^3p \int_{-\infty}^0 d\epsilon \partial_\epsilon \phi_r(\epsilon) \quad (134)$$

where  $\phi_r(\epsilon)$  is the phase of the retarded propagator, so we reached the conclusion that

$$n = \frac{1}{(2\pi)^3} \int d^3p \frac{1}{\pi} [\phi_r(-\infty) - \phi_r(0)] \quad (135)$$

Since  $G_r(-\infty)$  is real and negative  $\phi_r(-\infty) = \pi$ , Thus the only values of  $p$  that contribute to the integral are those for which  $G(0, p)$  is positive. For them the integrand has the constant value 1 so we ended up with the Luttinger-Ward theorem. The proof is valid regardless the system being a Fermi liquid, a non-Fermi liquid or a Mott Insulator either and the only way left to question the proof is then to assume the zero-temperature limit is discontinuous, thus involving a zero-temperature phase transition.

#### 5.1.4 Extension to crystalline states

In the same paper, after the completion of the proof we have just seen, Dzyaloshinskii points out a fact that the some reader could have expected already and that will be further generalized in last chapter: Luttinger-Ward theorem holds also when a static crystal lattice of nuclei is present in the background, giving an external potential for the electrons. This is important because it tells us the theorem applies in describing many of the common materials we deal with everyday.

The question whether or not the theorem holds if we allow crystal vibrations is not addressed instead. It's quite clear, at least on the experimental ground, that the attractive interaction given by phonon exchange does not break the validity of the theorem for many possible states of most physical system. Nevertheless when it causes the system to fall into superfluid states the theorem certainly cannot hold. A mathematical analysis of this issue goes beyond the scope of the present thesis and we left it an for a possible intriguing future work.

When a crystal background is present the good quantum numbers are the band index  $n$  (not to be confused with the density) and the crystal momentum  $k$ , taking values in the Brillouin zone  $B$ . So these are the entries on which the propagators depend, since we can add and destroy particles carrying such quantum numbers. Of course to get an expression for the full

density we must sum over all these states. We thus write

$$n = i \sum_n \int_B \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{+\infty} d\zeta e^{i\zeta\eta} M_{n,n}(\zeta, k) \quad (136)$$

where again  $M$  is the Matsubara propagator. Repeating the step we did before brings to

$$n = \frac{i}{(2\pi)^4} \int_{-\infty}^0 d\epsilon \int_B d^3k \partial_\epsilon \log[\det M(\epsilon, k)] \quad (137)$$

Again we can substitute  $G_{r,a}$  in place of  $M$ , so the expression above turns into

$$n = \frac{i}{(2\pi)^4} \int_{-\infty}^0 d\epsilon \int_B d^3k \partial_\epsilon \log\left[\frac{\det G_r}{\det G_a}\right] \quad (138)$$

The matrices  $G_{r,a}$  may be put in diagonal form and their spectra  $G_l(0, k)$  are real at zero energy since there they are Hermitian. So we end up with the natural generalization of the Luttinger-Ward formula for the electrons in a crystalline solid

$$n = \frac{1}{(2\pi)^3} \sum_l \int_B d^3k \theta[G_l(0, k)] \quad (139)$$

## 5.2 A different argument from Giuliani and Vignale

A quite different approach to some step in the theorem's proof has been given by Vignale and Giuliani in their book [17]. It is noteworthy to report their way to reach Luttinger-Ward statement since it may help having some more insight and because this is one of the few (if not the only) proof existing that does not start at finite temperature. Nonetheless we have seen a couple of proofs already and we have explored in detail many properties of electronic systems so it would be meaningless to start again from Adam and Eve. The in-medias-res beginning is surely the most appropriate so we start with the expression we already encountered before

$$n = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\mu} ds A(k, s) \quad (140)$$

with  $A(k, s)$  the spectral function introduced in the quasiparticle chapter, the very same definition of which implies

$$A(k, s) = -\frac{1}{2\pi i} [G(k, s + i\eta) - G(k, s - i\eta)] \quad (141)$$

Using the fact the propagator at the chemical potential is real allows to cast the expression for the total density as

$$n = \int \frac{d^3k}{(2\pi)^3} \int_C \frac{dz}{2\pi i} G(k, z) \quad (142)$$

where  $C$  is a path encircling counterclockwise the portion of the real axis extending from  $-\infty$  to  $\mu$  on the complex plane. Here comes the main difference: the authors suggest to perform the following  $k$ -dependent change of integration variable

$$z \rightarrow G(k, z) \quad (143)$$

where for the reader's convenience I remark

$$G(k, z) = \frac{1}{z - \epsilon(k) - \Sigma(k, z)} \quad (144)$$

so we have

$$dz = -\frac{dG}{G^2} + d\Sigma \quad (145)$$

Now we have to note that as  $z$  runs along the path  $C$  the variable  $G$  performs a closed path in the complex plane based at  $G = 0^-$ . It is evident that for arbitrary interactions this path will be arbitrarily complicated. Nevertheless the property we need to exploit can be deduced almost without calculations. The line of argument proceeds the following: since  $\Im G(k, z)$  vanishes only if  $z \rightarrow -\infty$  or  $z = \mu$  there are only two points in which our path intersects the real axis. So it encloses the origin, for fixed  $k$ , according to whether  $G(k, \mu)$  is positive or negative. Moreover looking at the relation between  $G$  and  $z$  it's not difficult to convince oneself that the path described by  $G$  is winding counterclockwise when it encloses the origin and vice versa. In both cases we call the path  $\Gamma$ . Plugging (145) into (142) yields

$$n = -\frac{1}{2\pi i} \int \frac{d^3k}{(2\pi)^3} \int_{\Gamma} \left\{ \frac{dG}{G} - G d\Sigma \right\} \quad (146)$$

As we argued many times the second term is dropped and the argument bringing to this conclusion is again the original one by Luttinger and Ward themselves; namely that we need a functional, say  $\Phi[G]$ , with the property

$$\frac{\delta\Phi}{\delta G(k, w)} = \Sigma(k, w) \quad (147)$$

So the final expression for the total density is left in the first term in (146)

$$n = -\frac{1}{2\pi i} \int \frac{d^3k}{(2\pi)^3} \int_{\Gamma} \frac{dG}{G} \quad (148)$$

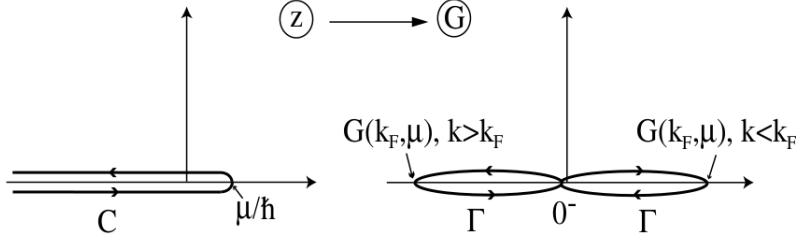


Figure 11: Schematic representation of the different contours in the  $z$  and  $G$  planes. Giuliani-Vignale [17]

The contour integral

$$-\frac{1}{2\pi i} \int_{\Gamma} \frac{dG}{G} \quad (149)$$

gives back the values 0 or 1 according to the two possibilities devised before, that is the sign of  $G$  evaluated at the chemical potential. So we end up again with the utter expression

$$n = \int \frac{d^3k}{(2\pi)^3} \theta[G(k, \mu)] \quad (150)$$

that is exactly the content of the Luttinger-Ward theorem.

### 5.3 What about the existence of the $\Phi$ -functional?

As we've seen in many ways, the theorem revolves around a special functional  $\Phi$  with the property that its functional derivative with respect to the interacting (or dressed) Green function gives back the proper self-energy of the electron or fermion we inject in the bulk and watch propagate.

Since there is a proof of the existence of such functional which differs from the original constructive one given by the authors whose theorem this thesis is named after I think appropriate to report it. In a recent work [26] Guraire infers that we can find a  $\Phi[G]$  such that the equality

$$\frac{\delta\Phi}{\delta G(k, w)} = \Sigma(k, w) \quad (151)$$

holds if we can prove that

$$\frac{\delta\Sigma(k, w)}{\delta G(k', w')} = \frac{\delta\Sigma(k', w')}{\delta G(k, w)} \quad (152)$$



Why it should be so? Actually the condition above can be interpreted thinking the self-energy as some kind of infinite-dimensional vector field: if the equation holds such vector field is irrotational. Alternatively one could think that we're asking for the (again infinite-dimensional) differential form

$$\int \frac{d^3k dw}{(2\pi)^4} \Sigma(k, w)[G]dG(k, w) \quad (153)$$

to be exact; i.e.

$$d \left\{ \int \frac{d^3k dw}{(2\pi)^4} \Sigma(k, w)[G]dG(k, w) \right\} = 0 \quad (154)$$

where the exterior derivative actually is a functional exterior derivative acting on the  $G$  dependence only so maybe it should be denoted by  $\delta$  instead of  $d$ . I ought to say I feel a little uncomfortable about this reasoning because there isn't almost any well-developed mathematical theory of PDEs at the functional level. Nevertheless the author concludes that the relation (152) holds by means of the following argument.

First one notes that by definition  $\Sigma(k, w)$  is given by all the possible OPI diagrams. Taking a functional derivative with respect to  $G(k', w')$  has the graphical interpretation of removing one dressed  $G$ -line from every one of those diagram in every possible way. All such diagrams taken together give rise to a vertex function for a process involving particles with energies and momenta given by  $k, w$  and  $k', w'$ .

Since the process should be symmetric under particle exchange we can switch the labels and reach the deserved conclusion that our functional differential form is in fact exact as we wanted to prove.

## 6 My two cents

For the sake of concreteness I will work under few assumptions that may not be the minimal ones. They are the following:

- particles live on some finite lattice covering a compact manifold with no boundary
- the Hamiltonian does not depend on time
- the number of particles is conserved

Moreover the thermodynamic limit is always taken at the very end of calculations. (The latter being rather a principle than some hypothesis)

First of all I wish to discuss the celebrated Källén–Lehmann representation for the propagator. This exact representation seems crucial. From it the proof of the theorem for the free fermions is promptly given. Such proof will then be useful finding out when and why the theorem holds if fermions interact.

### 6.1 The Källén–Lehmann representation

In a time-independent fermionic system the propagator is defined as:

$$iG_{\alpha\beta}(t) = \theta(t)\langle a_\alpha(t)a_\beta(0)^\dagger \rangle - \theta(-t)\langle a_\beta(0)^\dagger a_\alpha(t) \rangle \quad (155)$$

where  $\langle \dots \rangle$  is short for the expectation value on the N-particle ground state  $|E^0_N\rangle$ . Simply plugging in between the field-operators of  $G(t)$  a resolution of the identity in terms of simultaneous eigenstates of the Hamiltonian and Number of particles operator gives:

$$\begin{aligned} iG_{\alpha\beta}(t) = & \sum_s \theta(t) e^{-it(E_{N+1}(s) - E^0_N)} \langle E^0_N | a_\alpha | E_{N+1}(s) \rangle \langle E_{N+1}(s) | a_\beta^\dagger | E^0_N \rangle + \\ & - \sum_r \theta(-t) e^{it(E_{N-1}(r) - E^0_N)} \langle E^0_N | a_\beta^\dagger | E_{N-1}(r) \rangle \langle E_{N-1}(r) | a_\alpha | E^0_N \rangle \end{aligned} \quad (156)$$

and Fourier-transforming with respect to time yields

$$\begin{aligned} G_{\alpha\beta}(w) = & \sum_s \frac{\langle E^0_N | a_\alpha | E_{N+1}(s) \rangle \langle E_{N+1}(s) | a_\beta^\dagger | E^0_N \rangle}{w - (E_{N+1}(s) - E^{gs}_N) + i\eta} + \\ & + \sum_r \frac{\langle E^0_N | a_\beta^\dagger | E_{N-1}(r) \rangle \langle E_{N-1}(r) | a_\alpha | E^0_N \rangle}{w + (E_{N-1}(r) - E^{gs}_N) - i\eta} \end{aligned} \quad (157)$$

It is convenient to define the coefficients

$$C_{\alpha\beta}^+(s) = \langle E_N^0 | a_\alpha | E_{N+1}(s) \rangle \langle E_{N+1}(s) | a_\beta^\dagger | E_N^0 \rangle \quad (158)$$

$$C_{\alpha\beta}^-(r) = \langle E_N^0 | a_\beta^\dagger | E_{N-1}(r) \rangle \langle E_{N-1}(r) | a_\alpha | E_N^0 \rangle \quad (159)$$

leaving the  $N$ -dependence implicit and to manipulate the denominators as following:

$$E_{N+1}(s) - E_N^{gs} = (E_{N+1}(s) - E_{N+1}^{gs}) + (E_{N+1}^{gs} - E_N^{gs}) = \mu_N + \epsilon_{N+1}(s) \quad (160)$$

and similarly

$$-E_{N-1}(r) + E_N^{gs} = \dots = \mu_{N-1} - \epsilon_{N-1}(r) \quad (161)$$

to get

$$G_{\alpha\beta}(w) = \sum_s \frac{C_{\alpha\beta}^+(s)}{w - [\mu_N + \epsilon_{N+1}(s)] + i\eta} + \sum_r \frac{C_{\alpha\beta}^-(r)}{w - [\mu_{N-1} - \epsilon_{N-1}(r)] - i\eta} \quad (162)$$

that is, the Källén–Lehmann representation. It is important to note that reasonably all the  $\epsilon_{N\pm 1}(s/r)$  are non-negative. From this representation the exact analytic structure of  $G(w)$  for every  $w \in \mathbb{C}$  becomes evident. The transformation properties of  $G(w)$  make sure it is diagonalized by some possibly  $w$ -dependent operator  $U(w)$  but this is not sufficient to say there exists an orthonormal single-particle basis such that  $C_{\alpha\beta}^+(s) = \delta_{\alpha\beta} C^+(s; \alpha)$  and similarly for  $C_{\alpha\beta}^-(r)$ . This possibility comes from the very fact that symmetries in the Hamiltonian bring to conserved charges. (This is actually what happens when particles live in the usual square box with periodic boundary condition and still hold anytime we have enough symmetry, so we focus on these cases). Using some convenient set of field operators it's then true that

$$G_{\alpha\beta}(w) = \delta_{\alpha\beta} G(\alpha, w) \quad (163)$$

$$G(\alpha, w) = \left\{ \sum_s \frac{C^+(s; \alpha)}{w - [\mu_N + \epsilon_{N+1}(s)] + i\eta} + \sum_r \frac{C^-(r; \alpha)}{w - [\mu_{N-1} - \epsilon_{N-1}(r)] - i\eta} \right\} \quad (164)$$

the numerators being real non-negative coefficients that since  $\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}$  satisfy

$$\sum_r C^-(r; \alpha) + \sum_s C^+(s; \alpha) = 1 \quad (165)$$

Here setting

$$G(w) = G^+(w) + G^-(w) \quad (166)$$

seems quite natural and there is apparently no mean to be concerned with the viable presence of zeros of  $G(w)$  at the moment. Looking at the expression obtained may be used to conclude the following with  $w$  on the real axis:

$$\Im[G^-(w)] \geq 0 \quad (167)$$

$$\Im[G^+(w)] \leq 0 \quad (168)$$

Since all the  $\epsilon_{N\pm 1}(s/r)$  are non-negative  $G^+(w)$  is real and negative for  $w < \mu_N$  and  $G^-(w)$  is real and positive for  $w > \mu_{N-1}$ . So the whole contribution to the imaginary part of  $G(w)$  is separately given by  $G^+(w)$  and  $G^-(w)$  for real  $w$ . Of course all the properties stated refer to the spectral values of the propagator and hence still hold for every possible state's expectation value.

## 6.2 Free fermions

For the Hamiltonian we consider it may be reasonable to assume  $\mu_N > \mu_{N-1}$ . I will give a comment about this at the end of the section. The strong inequality seems necessary for the validity of the theorem and it ought to be noted it is equivalent to  $E^{gs}_N$  being a strictly convex function of  $N$ . Under such hypothesis in the vertical stripe  $\mu_N > \Re(w) > \mu_{N-1}$  the eigenvalues of  $G(w)$  are never singular so it is possible to set  $\eta = 0$ . This makes simultaneously  $G(w)$  real,  $G^+(w) \leq 0$  and  $G^-(w) \geq 0$  in such stripe for  $w \in \mathbb{R}$ . Having said that we can focus on the expression for the number of particles:

$$N = \sum_{\alpha} \lim_{\eta \rightarrow 0^+} -iG_{\alpha\alpha}(-\eta) = \sum_{\alpha} \lim_{\eta \rightarrow 0^+} -i \int \frac{dw}{2\pi} e^{i w \eta} G_{\alpha\alpha}(w) = \quad (169)$$

$$= \text{Tr} \left[ \lim_{\eta \rightarrow 0^+} -i \int \frac{dw}{2\pi} e^{i w \eta} G(w) \right] \quad (170)$$

A subscript  $N$  should appear in  $G(t)$  before taking limits, indeed  $\langle \dots \rangle$  denotes the  $N$ -particle ground-state expectation value. Also note the trace is not any abuse of notation,  $G(w)$  being a linear operator on the single-particle Hilbert space. A simple comparison with the previous section shows:

$$N = \sum_{\alpha} N_{\alpha} = \sum_{\alpha} \left\{ \sum_r C^-(r; \alpha) \right\} \quad (171)$$

It turns out  $N_\alpha = 1$  if and only if the corresponding single-particle state enters as a pure factor in the many-particles one. So for factorized states either  $C^+(s, \alpha)$  is zero for every  $s$  or  $C^-(r, \alpha)$  is for every  $r$ . This fact combined with the properties of  $G(w)$  just stated shows that for  $w \in \mathbb{R}$  the spectrum of  $G(w)$  in the region  $\mu_{N-1} < w < \mu_N$  is strictly positive for all those  $\alpha$  that are occupied and viceversa for all those that are not. This is exactly the Luttinger-Ward theorem for free fermions, the construction achieved looking solid to me.

About the assumption on the chemical potential we can say the following, that does not depend on the finite lattice hypothesis to any extent: since here particles live on a compact manifold with a certain extent of symmetry the kinetic Hamiltonian is almost always quite degenerate, so the strong inequality in practice never holds.

Nevertheless the weak one is always satisfied. This is good since we expect  $\mu(N, V)$  to become a function of the intensive variable  $N/V$ , that is the number density  $n$ , in the thermodynamic limit. Actually this is more than a hypothesis since there are exact results about this fact - see for example [27]. This function  $\mu(n)$  has to mimic the behaviour of  $\mu(N, V)$  but since we don't expect an infinite sequence of first order phase transitions rising  $n$  it has to be quite smooth almost everywhere. So the only possibilities are either  $\mu(n) = \text{constant}$  or  $\partial_n \mu(n) > 0$  with at most some isolated zeros. Obviously only the latter is physical. This completes the theorem's proof for the free theory in the thermodynamic limit.

### 6.3 Interacting fermions

A separation of  $G(w)$  into free and interacting contribution will serve the argument. I discuss here briefly such separation on a general footing.

#### 6.3.1 Another approach to the self-energy

Consider the many-body Hamiltonian describing the system. It can always be written as quadratic (say kinetic) plus non-quadratic terms in the field operators. The kinetic term alone yields the "free" theory, the remainder being external sources and interactions. We have suppressed sources anyway asking  $[N, H] = 0$ . The propagator for the free theory is denoted  $G_0(w)$ . The self-energy  $\Sigma(w)$  here is *defined* by:

$$\Sigma(w) = -[G^{-1}(w) - G_0^{-1}(w)] \quad (172)$$

where those above are matrix inverses.

$G_0(w)$  has always a virtually very simple form:

$$G_{0\alpha\beta}(w) = \frac{\delta_{\alpha\beta}}{w - \epsilon_\alpha + i\eta \operatorname{sgn}(\epsilon_\alpha - e_F)} \quad (173)$$

with the convention  $\operatorname{sgn}(0) = -1$ .

Here I must point out a subtlety: the above expression for  $G_0(w)$  is exact only if the single-particle Hamiltonian is non-degenerate. Otherwise the Fermi energy-level could be partially filled and for those empty states at the Fermi-level the signum times  $i\eta$  is simply wrong. Indeed it has to be  $-i\eta$  for all the states that are occupied and the opposite for the states that are not so.

If one thinks for example about the usual free electrons in the cubic box this issue becomes evident: the energy levels are in practice given by the sum of three integers squared and of course there are many ways to choose three different squares to sum up to the same value.

Anyway a frequency-independent function  $f(\alpha)$  with values in  $\{-1, 1\}$  multiplying  $i\eta \operatorname{sgn}(\epsilon_\alpha - e_F)$  could fix this issue. Moreover it's not necessary to work at the algebraic level: since the Hamiltonian considered does not break the symmetries of the manifold or lattice particles live onto,  $G(w)$  and  $G_0(w)$  are simultaneously diagonal and we can focus on their spectral values, denoted like  $G_\alpha(w)$  from now on. This allows the use of a simple criterion to state whether the perturbative expansion is valid: rewriting (172) as

$$G_\alpha(w) = G_{0\alpha}(w) \left\{ \frac{1}{1 - G_{0\alpha}(w)\Sigma_\alpha(w)} \right\} \quad (174)$$

makes evident that the aforementioned expansion is convergent if and only if

$$|G_{0\alpha}(w)\Sigma_\alpha(w)| < 1 \quad (175)$$

### 6.3.2 Retracing the proof footsteps

With the definition and notations presented above the propagator may be rewritten as:

$$G_\alpha(w) = -\partial_w \log G_\alpha(w) + G_\alpha(w)\partial_w \Sigma_\alpha(w) \quad (176)$$

and using them in the integral for the number of particles (here we switch back to matrices to suppress the index  $\alpha$  and lighten notation) gives:

$$N = -i \operatorname{Tr} \left\{ \lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} \int \frac{dw}{2\pi} e^{iw\gamma} [-\partial_w \log G(w) + G(w)\partial_w \Sigma(w)] \right\} = \quad (177)$$

$$= \text{Tr} \left\{ \lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} + i \int \frac{dw}{2\pi} e^{iw\gamma} [\partial_w \log G(w) + \Sigma(w) \partial_w G(w)] \right\} \quad (178)$$

Some comments about vanishing contributions are necessary.

The boundary term is dropped thanks the asymptotic behaviour of  $G(w)$  making out

$$\lim_{w \rightarrow \infty} \Sigma(w)/w \rightarrow 0 \quad (179)$$

and to convince myself that

$$\lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} \gamma \int \frac{dw}{2\pi} e^{iw\gamma} G(w) \Sigma(w) \quad (180)$$

vanishes I used the following argument, which turns out a little longer and makes use of the finite lattice hypothesis: if particles live on a finite lattice both free and interacting Green functions are meromorphic in  $w$ . This ensures  $\Sigma(w)$  also is. Thus it has a Laurent expansion out some sufficiently large disk centered at the origin, that is the only region to be considered to prove the convergence of the integral (remember that the limit  $\eta \rightarrow 0^+$  comes after the integration).

Combining this with  $\Sigma(w)/w \rightarrow 0$  in the same region makes the regular part of  $\Sigma(w)$  being at most a constant. The residue theorem can then be used showing the integral is finite and the limit itself zero. I find interesting that we need to make heavily use of the analytic properties in order to prove this, properties that may be broken by the intake of the thermodynamic limit.

Anyway the desired result is close. What comes into play now is the  $\Phi[G]$ -functional of chapter 2. Nevertheless to our purpose it may be thought to be defined by the following equation:

$$\Sigma(w) = \frac{\delta}{\delta G(w)} \Phi[G] \quad (181)$$

still its existence being proved only by means of a diagrammatic technique. As we have seen  $\Phi[G]$  is related to the so-called dressed expansion of the partition function, which in turn has to do with the normalization of the adiabatic state at zero temperature given by Gell-Mann & Low theorem. Using this functional to compute  $N$  we get

$$\text{Tr} \left\{ \lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} i \int \frac{dw}{2\pi} e^{iw\gamma} (\partial_w G(w)) \frac{\delta}{\delta G(w)} \Phi[G] \right\} \quad (182)$$

from the latter addend. The annoying  $e^{iw\gamma}$  still there. If the limit can jump inside the integral such factor disappears and the remainder becomes

the overall variation of  $\Phi[G]$  when  $G(w)$  is subject to a frequency shift. Many authors chorally say this variation is then zero since, thanks to Galilei invariance, a global shift in the energy leaves the whole theory unchanged. All the contribution to the total number of particles is then left in the logarithmic term, that is we can write:

$$N = \text{Tr} \left\{ \lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} i \int \frac{dw}{2\pi} e^{iw\gamma} [\partial_w \log G(w)] \right\} \quad (183)$$

From this equation we have already seen that there some possibilities to go on. One is to go back to finite temperature and repeat the steps of Luttinger and Ward (starting from eq. (34)). Another one is to follow the approach of Dzyaloshinskii (seen in chapter 5) and the last one we have seen is that of Giuliani and Vignale (presented also in chapter 5, section 5.2). I asked myself if it is possible to proceed differently.

The only way I found to do it but not without the help of a very dear friend of mine, that allowed me to get out some troubles I incurred in and that I must really thank for his everlasting supportive attitude, is the following.

First of all note that the exponential factor is tricky: it is often thought to be there just to tell us where we must close the contour when one wish to invoke contour integration techniques. But we are aware that the half-circle has to give no contribution at all, otherwise we don't end up with the value of the integral we started with. Further inspection reveals that - since the  $\gamma \rightarrow 0^+$  limit has to be performed - such factor can only affect what happens in the asymptotic region of the integral. No definite integral can be changed by it.

As a matter of fact at the end of the day it turns out that such exponential factor is responsible for the non-exact cancellation of the asymptotic contributions to the integral only. This will become clear in the following computation whenever it's not yet so.

The expression inside the curly brackets is broken into three pieces thanks the introduction of the fictitious parameter  $a$ , taken to be large enough to be way greater than any eigenvalue of the interacting Hamiltonian and made run to infinity eventually. In formulae

$$\lim_{\gamma \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} \lim_{a \rightarrow +\infty} \frac{i}{2\pi} \left( \int_{-\infty}^{-a} + \int_{-a}^a + \int_a^{+\infty} \right) dw e^{iw\gamma} [\partial_w \log G(w)] \quad (184)$$

We start focusing on the middle term. Since it is a definite integral the exponential factor can't affect the result, as we pointed out earlier, so it can be simply suppressed. The result is then determined by the difference



between  $\log G(w)$  at the extremes of integration.

$$\frac{i}{2\pi} \lim_{\eta \rightarrow 0} \lim_{a \rightarrow +\infty} \log[G(a)G^{-1}(-a)] \quad (185)$$

Here it's convenient to reintroduce the index  $\alpha$ . We can make use of the analytic properties of  $G_\alpha(w)$  (something we are granted of only because we set up the problem on a finite lattice) to extract its asymptotic behaviour in the following way: since it is a meromorphic function and all its poles are finite it has a Laurent expansion out some sufficiently large disk - here of radius  $a$  - centered at the origin. Moreover we know that the coefficient  $c_0$  vanishes thanks the asymptotic behaviour of  $G(w)$ , so we can write

$$G_\alpha(w) = \sum_{j=1}^{+\infty} c_j(\alpha) \frac{1}{w^j} \quad (186)$$

Of course for the same reason we know  $c_1 = 1$  for every  $\alpha$ . We need to work out the expression for  $c_2(\alpha)$ . In order to do it recall that we defined  $G(w) = G^+(w) + G^-(w)$ . Looking for example at the expression for  $G^+(w)$ , namely

$$G^+_\alpha(w) = \sum_s \frac{C^+(s; \alpha)}{w - [\mu_N + \epsilon_{N+1}(s)] + i\eta} \quad (187)$$

suggest we can do the following manipulations for  $w \rightarrow \infty$

$$\frac{C^+(s; \alpha)}{w - [\mu_N + \epsilon_{N+1}(s)] + i\eta} = \frac{1}{w} \left\{ \frac{C^+(s; \alpha)}{1 - [(\mu_N + \epsilon_{N+1}(s) - i\eta)/w]} \right\} = \quad (188)$$

$$= \frac{1}{w} \left\{ C^+(s; \alpha) \left[ 1 + \frac{(\mu_N + \epsilon_{N+1}(s) - i\eta)}{w} + \dots \right] \right\} = \quad (189)$$

$$C^+(s; \alpha) \left\{ \frac{1}{w} + \frac{(\mu_N + \epsilon_{N+1}(s) - i\eta)}{w^2} + \dots \right\} \quad (190)$$

where the dots represent highest order terms in  $1/w$ . So repeating the same steps for  $G^-_\alpha(w)$  gives in the same large  $w$  limit, using the "normalization condition" (165)

$$\begin{aligned} G_\alpha(w) &= \frac{1}{w} + \frac{1}{w^2} \left\{ \sum_s C^+(s; \alpha) [\mu_N + \epsilon_{N+1}(s) - i\eta] + \right. \\ &\quad \left. + \sum_r C^-(r; \alpha) [\mu_{N-1} - \epsilon_{N-1}(r) + i\eta] \right\} + \dots \end{aligned} \quad (191)$$

giving us for the coefficient  $c_2(\alpha)$  the expression

$$c_2(\alpha) = (\mu_N - i\eta)(1 - N_\alpha) + N_\alpha(\mu_{N-1} + i\eta) + \sum_s C^+(s; \alpha)\epsilon_{N+1}(s) - \sum_r C^-(r; \alpha)\epsilon_{N-1}(r) \quad (192)$$

where we have made use of (165) and (171) to perform the summations to get  $N_\alpha$  in the formula. Please note that accordingly we have for the imaginary part of  $G_\alpha(w)$  for large and real  $w$

$$\Im G_\alpha(w) \approx 2\eta(N_\alpha - \frac{1}{2})/w^2 \quad (193)$$

This equation by its own show a problem: we know that the sign of  $\Im G_\alpha(w)$  should be the same of  $w - \mu$  and this fact can't be taken into account simply going to higher orders in the power expansion. Nevertheless this is a very delicate issue and it's better to keep concentrated on our argument, that is certainly a working one since there are no mistakes until now. If one goes on the following is what happens. It is a matter of really just two lines to convince oneself that any meromorphic function of the form (186) satisfies

$$\lim_{w \rightarrow \infty} \frac{1}{G_\alpha(w)} \rightarrow w \left\{ 1 - \frac{c_2(\alpha)}{w} + \dots \right\} \quad (194)$$

where again we used  $c_1 = 1$ . So in the attempt to evaluate the expression (185), plugging our results back in the logarithm yields

$$\lim_{a \rightarrow \infty} \log \left\{ (-a) \left[ 1 - \frac{c_2(\alpha)}{(-a)} + \dots \right] \frac{1}{a} \left[ 1 + \frac{c_2(\alpha)}{a} + \dots \right] \right\} = \quad (195)$$

$$= \log \left[ -1 - 2 \frac{c_2(\alpha)}{a} + \dots \right] \quad (196)$$

here we see that the  $i\eta$  plays a role, indeed according to (193) it makes the argument of the logarithm approach the value  $-1$  on the real axis from below or from above according  $\Im c_2(\alpha)$ , so the result turns out to be

$$-i\pi \operatorname{sgn}[\Im c_2(\alpha)] = -i\pi \operatorname{sgn} \left[ N_\alpha - \frac{1}{2} \right] \quad (197)$$

that plugged into the expression (185) gives

$$\frac{i}{2\pi} (-i\pi) \operatorname{sgn} \left( N_\alpha - \frac{1}{2} \right) = \frac{1}{2} \operatorname{sgn} \left( N_\alpha - \frac{1}{2} \right) \quad (198)$$

To this equation we must add the contribution given by the aforementioned asymptotic region, that is the first and last terms of (184) and then sum over the index  $\alpha$  to take the trace and get our expression for the total number of particles.

Such contribution is computed the following: because we are far away from any possible zero in the denominator ( thanks the condition on  $a$  ) we can immediately throw away the  $\eta \rightarrow 0^+$  limit and the  $i\eta$  as well in our computation, then being left with

$$\lim_{\gamma \rightarrow 0^+} \lim_{a \rightarrow +\infty} -\frac{i}{2\pi} \left( \int_{-\infty}^{-a} + \int_a^{+\infty} \right) dw e^{iw\gamma} [\partial_w \log G^{-1}(w)] \quad (199)$$

where we have multiplied by  $-1$  twice to cast the expression in such form. It comes by itself also that the exponential factor now comes into play. Making use of the asymptotic behaviour of  $G(w)$  we can perform the derivative and get

$$\lim_{\gamma \rightarrow 0^+} \lim_{a \rightarrow +\infty} -\frac{i}{2\pi} \left( \int_{-\infty}^{-a} + \int_a^{+\infty} \right) dw e^{iw\gamma} \frac{1}{w} = \frac{1}{2} \quad (200)$$

The last effort is to show why the equation above returns the value  $1/2$ . We have a simple way to do it. It's well known that

$$\lim_{t \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{+\infty} dw e^{iwt} \frac{1}{w - i\eta} = 2\pi i \quad (201)$$

We can take  $a$  to be any fixed positive number and rewrite it as

$$\lim_{t \rightarrow 0^+} \lim_{\eta \rightarrow 0^+} \left( \int_{-\infty}^{-a} + \int_{-a}^a + \int_a^{+\infty} \right) dw e^{iwt} \frac{1}{w - i\eta} = 2\pi i \quad (202)$$

In the middle term we can bring the  $t \rightarrow 0^+$  limit inside the integral and compute it explicitly. Of course the result is

$$\lim_{\eta \rightarrow 0^+} \log \left[ -\frac{(a - i\eta)}{(a + i\eta)} \right] = \quad (203)$$

$$= \lim_{\eta \rightarrow 0^+} \log(-1 + i\eta/a) = i\pi \quad (204)$$

A comparison with (202) then allows to conclude the remainder must be equal to  $i\pi$ . Since this is true for any positive  $a$  and still true when we make  $a$  approach infinity we have proven (200). Putting the pieces together, namely

equation (198) with the latter result, we arrived to our final expression for the total number of particles

$$N = \sum_{\alpha} \frac{1}{2} \{ \text{sgn}(N_{\alpha} - \frac{1}{2}) + 1 \} \quad (205)$$

This result is really interesting. It is exact and holds whenever we setup the theory on a finite lattice, no matter how huge the number of lattice sites is. One can take it to be “just”  $10^{1000000}$  in a cubic box of  $1 m^3$  and still the result is true with no caveat. In my opinion this is important because we know that at those unreal resolutions (and way lower ones anyway) the theory we use surely gets broken by several effects, starting from the special relativity ones but involving GR ones all the same.

For example think that, regardless being fantasy according to the present knowledge, the Schwarzschild radius of a black hole with the mass of a single electron would be something like  $10^{-57}$  meters. So it is quite simple to believe that whatever may be described with the many-body theory is taken into account by our model. This tells us, comparing with the previous proofs we have seen, that the “volume” where  $G(k, \mu) > 0$  equals expression (205), giving us a new key to interpret the Luttinger-Ward theorem: whenever the interactions, lowering the occupation inside the Fermi Surface and raising it outside, do not change its value more than  $1/2$ , we can use  $G(k, \mu) > 0$  to specify the total number of particles. This fact by its own seems to suggest that the diagrammatic theory we discussed so long is valid whenever such “ $\frac{1}{2}$ -bound” holds, and this is seemingly a pretty nice result.

#### 6.4 A wye way for future investigations

In trying to put together the pieces that make up the Luttinger-Ward theorem, I ran into the fact that the adiabatic evolution of chapter 4 invoked to justify, to mention one, the emergence of Landau effective Hamiltonian can be used twofold:

- take the non-interacting ground state in a very remote past  $t'$ , evolve it adiabatically to the present time and stick in it a bare excitation carrying momentum  $k$

$$\frac{1}{R} a_k^{\dagger} U_{\eta}(0, t') |E^0_{gs}\rangle$$

- take the non-interacting ground state in a very remote past  $t'$ , stick in it a bare excitation carrying momentum  $k$  and only then evolve it

adiabatically to the present time

$$\frac{1}{R} U_{\eta}(0, t') a_k^{\dagger} |E_{gs}^0\rangle$$

where  $\frac{1}{R}$  is the appropriate necessary normalization factor, different in the two cases. This possibility is interesting since it tells us, thanks the Gell-Mann & Low theorem, that if we can prove that the limit  $\eta \rightarrow 0$  exists in practice we can assure it is possible to map the set of bare excitations made of exact eigenstates of the free Hamiltonian into another set of what should reasonably called the “dressed” ones, again made up of exact eigenstates and this time of the interacting theory. This suggests that all these states will be the analogue of their non-interacting counterpart, so it wouldn't be mysterious that they make out a ball in  $k$ -space with exactly the same volume that the Fermi Surface encloses in the free theory.

# Conclusions

In this thesis we have seen a considerable amount of interesting and often apparently disparate ingredients of the many-body theory. To them we have devoted lengthy - but hopefully meaningful and not overly boring - discussions, in order to elucidate why they have to be put together in the same cauldron to point out the importance, as well as to widen the comprehension, of the Luttinger-Ward theorem. We did it with the conviction to give a very little but non-vanishing contribution to all that has been said and written in the latter half century about this challenging theorem and its proof. The time is come to draw our conclusions.

To this end it comes natural to summarize for the last time the steps we performed developing this thesis, with the matured comprehension of the connections between the many arguments involved and the questions - emerged in very same development - that still have to be addressed.

The thesis begun with the historical proof given by Luttinger and Ward where we have clarified that the presence of a discontinuity in  $n(k)$  is just accessory and that the essence of it lays on the conservation of the volume where the propagator at the chemical potential is positive, opening our eyes on the proper definition of the Fermi Surface for a system of interacting electrons.

Then we spent a whole chapter to relate the validity of the theorem to the diagrammatic of  $\log(Z)$ , making evident how the validity of one interlinks with the other. The expansion involved and its relation with Gell-Mann & Low theorem made us focus on quasi-particles and Fermi-liquids since both emerge as effects of the adiabatic continuity that ranging in very different regimes allows to connect the free and interacting theories: we deepened these macro-areas of condensed matter physics in the chapter three and four.

Then we went back to focus again on Luttinger-Ward theorem in a novel fashion, presenting in chapter five a couple of recent proofs and some intriguing arguments that shed a renewed light on it without sparing the emergence of new questions, also showing that the range of applicability of this uttermost theorem is yet poorly understood and will certainly reserve many surprises in the years to come.

The trail ends then arriving to chapter six where, apart devising a possible future investigation motivated by the same very same purpose of the whole thesis, I give my two cents to the piggy bank of the literature concerning the subject of it, with the belief that, at least a very little, they will matter

too the day someone will finally find out the right approach to break it and offer the world its treasure.

In the end I wish to report my personal opinion saying that my feeling is Luttinger-Ward theorem truly grounds on something we don't really understand yet, and if it will be dealt with having patience and humbleness by those who will encounter it along their road, as many did from its very birth until today, it will throw us to a whole new approach to a lot of areas of mathematics and physics.

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