Landau's Fermi Liquid Concept to the Extreme: the Physics of Heavy Fermions

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Introductory remarks

Landau's Fermi liquid is the fundamental concept in modern solid state physics and sets the language and notion used to communicate and interpret physical observations in solids. Within the Fermi liquid theory, electrons in solids are described as non-interacting *quasi-particles*, with some of their properties changed as compared to the electrons in free space. Most of you will know the concept of the *effective mass*, which often is sufficient to explain a whole bunch of different experimental findings for a given material. In addition, new "types" of particles, so-called *holes*, appear, and both are needed for a proper understanding of the electronic properties of soilds.

Usually, the electronic properties are captured rather accurately in terms of well-behaved quasi-particles even at elevated temperatures, and interactions only play a role in renormalizing certain correlation functions. However, there are materials, which show (i) extremely strong renormalizations of the properties of electrons and (ii) where the quasi-particles do not survive increasing temperature too much. Furthermore, these creatures are rather sensitive to the tuning of material parameters or other external conditions, and one can frequently encounter *quantum phase transitions*, *quantum critical behavior* and the formation of so-called *non-Fermi liquid phases*. The material class where this behavior is most prominent are the so-called *Heavy Fermions*. You have learned about various experimental facts found in this class in the series of lectures by John Mydosh.

This series of lectures is intended to give you a solid background in the theoretical description of these extreme realizations of Fermi liquids. I will touch - briefly - the breakdown of Fermi liquids in Heavy Fermions, but will mostly concentrate on a proper description of this "simpler" regime. You will learn why Landau's Fermi liquid theory is applicable at all in solids, what are its underlying assumptions and what consequences follow from these assumptions. This will cover the first part of the lecture series. The second is then devoted to the Heavy Fermion behavior. You will meet two basic models used to theoretically describe these systems and learn about there fundamental properties, in particular the Kondo effect, and Noziéres interpretation in terms of a *local Fermi liquid*. Since this is a non-trivial many particle phenomenon, you will also meet a tool to calculate properties numerically, Wilson's Numerical Renormaliztion Group, and learn from it the fundamental ideas behind Heavy Fermion physics. Finally, I will try to make contact to John's lectures again and give you an idea about our current understanding and tools to calculate properties of Heavy Fermion systems.

I will assume that you are familiar with basic concepts in solid state theory and - very important - also some fundamental theoretical concepts, like second quantization and statistical physics. It is also helpful to have an idea what Green's functions in many-body physics are, how to work with them (at least on the levels of equations-of-motion) and what they can tell us.
Finally, there are some books and review articles you may want to read. The list is by no means complete, and I urge you to use the internet to search for more literature, as most is actually contained in normal publications and one has to put together bits and pieces.

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Lecture 1

The homogeneous electron gas

1.1 Basic concetps

The homogeneous electron gas is in connection with solid state physics also sometimes called *jellium model* or *free-electron model* for the solid. One here neglects all structures imposed by the crystal and approximates the lattice by a homogeneous positive background guaranteeing charge neutrality. In addition to neglecting the crystal we also ignore the Coulomb interaction between the electrons. This seems an even more rude approximation at first sight. However, as we will learn later, it is the one that is usually better justified than the assumption of a homogeneous system.

The Hamiltonian for the noninteracting electron gas is simply given by

$$\hat{H}_e = \frac{1}{2m}\sum_{i=1}^{N}\hat{\vec{p}}_i^2 \tag{1.1}$$

$$= \sum_{\vec{k}\sigma}\langle\varphi_{\vec{k}\sigma}|\frac{\hat{\vec{p}}^2}{2m}|\varphi_{\vec{k}\sigma}\rangle\hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}\sigma} \tag{1.2}$$

Since electrons are fermions, the operators $\hat{c}_{\vec{k}\sigma}$ and $\hat{c}^\dagger_{\vec{k}\sigma}$ must fulfill anticommutation relations, i.e. $\{\hat{c}_{\vec{k}'\sigma'}, \hat{c}^\dagger_{\vec{k}\sigma}\} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$. Furthermore, as we are now working with solids, which occupy a finite region in space, we assume that the electrons are confined to a finite but large volume[1] $V = L^3$. A certain mathematical problem arises from the existence of the boundaries, which would require $\Psi(\vec{r} \in \partial V) = 0$ or at least an exponential decay outside the cube. The wave functions are then in principle standing waves, described by either sin or cos functions. For practical purposes it is however more convenient to work with travelling waves described by a complex exponential function. Quite obviously, the type of solution is determined by the existence of boundaries. However, quite often we are not interested in properties at the boundary, but in the *bulk* properties far away from the boundary. These bulk properties can on the other hand not depend on the details of boundary, i.e. we are free to choose convenient boundary conditions in such a situation. This fact has first been observed by Born and von Karmann, who introduced the concept of *periodic boundary conditions* or *Born-von Karman boundary conditions*, which identify the properties at position at $x_i + L$ with those at x_i. For a chain this amounts to closing it into a ring, in two dimensions one ends up with a torus, and so on.

Employing periodic boundary conditions we have

$$\varphi(x,y,z) = \varphi(x+L,y,z) = \varphi(x,y+L,z) = \varphi(x,y,z+L)$$

[1] For simplicity we assume a cube of base length L.

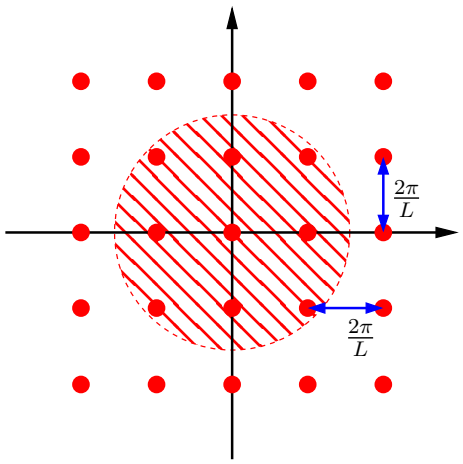
for the wave functions entering (1.2). These conditions lead to discrete $\vec{k}$ vectors which have the components

$$k_i = \frac{2\pi}{L} n_i \quad , \quad n_i \in \mathbb{Z}; .$$

As the set of vectors $\vec{k}$ enumbers all possible inequivalent single-particle states it serves as quantum number. We in addition need the spin as further quantum number, which we denote by σ with $\sigma = \pm 1$. We then have

$$\begin{aligned} \varphi_{\vec{k}\sigma}(\vec{r}) &= \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \\ \langle \varphi_{\vec{k}\sigma} | \frac{\hat{\vec{p}}^2}{2m} | \varphi_{\vec{k}\sigma} \rangle &= \frac{\hbar^2 k^2}{2m} =: \epsilon_{\vec{k}} \quad . \end{aligned}$$

The discrete $\vec{k}$ points form a lattice in $\vec{k}$ space, where each lattice point can accommodate two single-particle states with different spin orientation. The volume per $\vec{k}$ point is just the volume of the elementary cell of the reciprocal lattice, i.e. $(2\pi)^3/V$. Note, however, that we now do not have the restriction that the inequivalent $\vec{k}$ vectors come from the first Brillouin zone as we do not have a crystal with discrete translational symmetry, but free space.



1.2 Ground state properties

In particular, the ground state is obtained by occupying the set $\{\vec{k}_i\}$ of $\vec{k}$ points with the smallest possible energies respecting Pauli's principle, i.e.

$$\langle \Psi_G | \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} | \Psi_G \rangle = \begin{cases} 1, \text{ for } \vec{k} \in \{\vec{k}_i\} \\ 0, \text{ else} \end{cases} \quad .$$

As $\epsilon_{\vec{k}} \propto k^2$, these states can be found within a sphere (*Fermi sphere*) with a certain radius k_F (*Fermi wave vector*) about $\vec{k} = 0$. The value of k_F can be determined from the requirement, that the sum over all occupied states must equal to the number of particles, i.e.

$$N = \sum_\sigma \sum_{k \le k_F}$$

For simplicity we assume that N is even.
How does one evaluate such sums? To this end let me remind you, that the Volume V of the system is very large and consequently the volume per $\vec{k}$ point $d^3k = \frac{(2\pi)^3}{V}$ is very small. Then,

$$\sum_{\vec{k}} \ldots = V \sum_{\vec{k}} \frac{d^3k}{(2\pi)^3} \ldots \overset{V\to\infty}{\to} V \int \frac{d^3k}{(2\pi)^3} \ldots$$

With this observation we find in the thermodynamic limit $V \to \infty$ and $n = N/V$ finite

$$n = \frac{N}{V} = \frac{1}{V} \sum_{\sigma} \sum_{k \le k_F} = \sum_{\sigma} \int_{k \le k_F} \frac{d^3k}{(2\pi)^3} = \frac{1}{4\pi^3} \int_0^{k_F} 4\pi k^2 dk = \frac{1}{3\pi^2} k_F^3 \ ,$$

which leads to

$$\boxed{k_f \ = \ \left(3\pi^2 n\right)^{1/3} \quad (1.3)}$$

as expression for the Fermi wave vector. The corresponding energy

$$\epsilon_{k_F} = \frac{\hbar^2 k_F^2}{2m}$$

is called *Fermi energy* and usually denoted as E_F. We can also calculate the
exercise ground-state energy, which becomes

$$E_0 \ = \ \sum_{\vec{k}, k \le k_F} \sum_{\sigma} \epsilon_{\vec{k}} = \frac{3}{5} N E_F \qquad (1.4)$$

and the energy per particle

$$\varepsilon_0 = \frac{E_0}{N} = \frac{3}{5} E_F \ .$$

With the knowledge of the ground state energy we can start to calculate physical properties. As examples let us determine the pressure P and bulk modulus B_0 of the Fermi gas at $T = 0$. These two quantities are related to the ground state energy through

$$\begin{aligned} P \ &= \ -\left(\frac{\partial E_0}{\partial V}\right)_N \\ B_0 \ &= \ -V \left(\frac{\partial P}{\partial V}\right)_N \ . \end{aligned}$$

exercise As we know the explicit dependency of E_0 on the volume, it is easy to show

$$P = -\frac{3}{5} N \frac{\hbar^2}{2m} \left(-3\pi^2 \frac{N}{V^2}\right) \frac{2}{3} \left(3\pi^2 \frac{N}{V}\right)^{-1/3} = \frac{2}{3} \frac{E_0}{V} = \frac{2}{5} n E_F$$

and

$$B_0 = \frac{5}{3} P = \frac{2}{3} n E_F \ .$$

1.3 Evaluation of $\vec{k}$-sums – Density of States

In the following we will rather often have to deal with expressions of the type

$$\frac{1}{V}\sum_{\vec{k}} F(\epsilon_{\vec{k}}) \ ,$$

where $F(\epsilon_{\vec{k}})$ is some function depending on $\vec{k}$ through the dispersion only. Such a sum can be rewritten as

$$\frac{1}{V}\sum_{\vec{k}} F(\epsilon_{\vec{k}}) = \int_{-\infty}^{\infty} \mathcal{N}(\epsilon) F(\epsilon) d\epsilon \ ,$$

where we have introduce the *density of states* (DOS)

$$\mathcal{N}(\epsilon) := \frac{1}{V}\sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}) \ .$$

Note that this definition also holds for a more general dispersion appearing in a real lattice. Let us calculate the DOS for $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$. From the definition one firstly obtains

$$\mathcal{N}(\epsilon) = \frac{1}{V}\sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}}) = \int_0^{\infty} \frac{4\pi k^2 dk}{(2\pi)^3} \delta(\epsilon - \epsilon_{\vec{k}}) \ . \tag{1.5}$$

To evaluate this expression furher I remind you of the relation

$$\delta(\epsilon - \epsilon_{\vec{k}}) = \sum_{k_i} \frac{1}{|\vec{\nabla}_{\vec{k}} \epsilon_{\vec{k}=\vec{k}_i}|} \delta(k - k_i) \ , \ \ \epsilon - \epsilon_{\vec{k}_i} = 0 \ , \ \ \vec{\nabla}_{\vec{k}} \epsilon_{\vec{k}=\vec{k}_i} \neq 0 \ .$$

In the present case as $\epsilon_{\vec{k}} \geq 0$ we also must have $\epsilon \geq 0$ and hence there exist two roots for a given ϵ, namely $k_0 = \pm\sqrt{\frac{2m\epsilon}{\hbar^2}}$. As also $k \geq 0$ in the integral (1.5), we only need the positive root here. Furthermore, $|\vec{\nabla}_{\vec{k}} \epsilon_{\vec{k}}| = \frac{\hbar^2 k}{m} \neq 0$ for $k \neq 0$ and therefore

$$\begin{aligned} \mathcal{N}(\epsilon) &= \frac{1}{(2\pi)^3} 4\pi k_0^2 \frac{m}{\hbar^2 k_0} = \frac{m}{2\pi^2\hbar^2}\sqrt{\frac{2m\epsilon}{\hbar^2}} \\ &= \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{\epsilon} = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2 k_F^2}\right)^{\frac{3}{2}} k_F^3 \sqrt{\epsilon} \end{aligned}$$

With the definitions of k_f in (1.3) and E_F we finally obtain

$$\boxed{\mathcal{N}(\epsilon) = \frac{3}{4}\frac{n}{E_F}\sqrt{\frac{\epsilon}{E_F}}} \tag{1.6}$$

for the DOS. Some warning: Sometimes the spin factor 2 is included in the definition of the DOS, which then reads $\tilde{\mathcal{N}}(\epsilon) = 2\mathcal{N}(\epsilon) = \frac{3}{2}\frac{n}{E_F}\sqrt{\frac{\epsilon}{E_F}}$. A particularly important value is the DOS at the Fermi energy $\mathcal{N}(E_F)$, which is

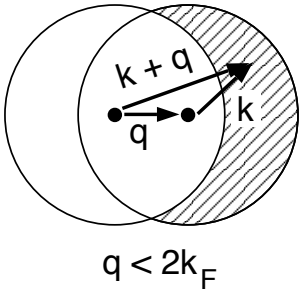
$$\mathcal{N}(E_F) = \frac{3}{4}\frac{n}{E_F} \propto \frac{1}{E_F} \propto m \quad (1.7)$$

This is an important proportionality you should memorize!

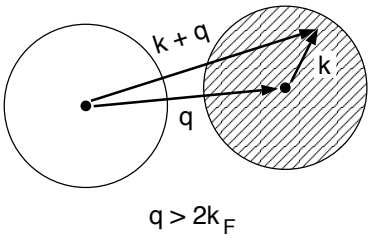
1.4 Excited states of the electron gas

To construct excited states of the noninteracting, free electron gas we have only one possibility, viz taking one electron from a state with $\leq k_F$ and putting it into a state with $k' > k_F$. Let us denote the difference in momentum by $\vec{q} = \vec{k}\,' - \vec{k}$. We now must distinguish two possibilities:

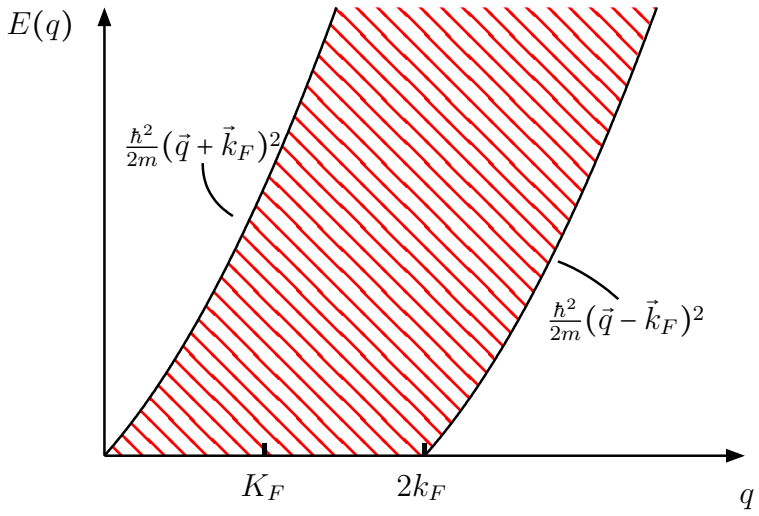
(i) $q \leq 2k_F$:
Not all states inside the Fermi sphere are possible final states for a given $\vec{q}$, but only those that fulfil the requirement $k' = |\vec{k} + \vec{q}| \geq k_F$. Further, as $\vec{k}$ cannot be outside the Fermi sphere, we can restrict k' to $k_F \leq k' \leq |\vec{k}_F + \vec{q}|$ or equivalently $E_F \leq \epsilon_{\vec{k}'} \leq \frac{\hbar^2}{2m}(\vec{q} + \vec{k}_F)^2$.



(ii) $q > 2k_F$:
All states inside the Fermi sphere are possible final states and $|\vec{q} - \vec{k}_F| \leq k' \leq |\vec{q} + \vec{k_F}|$, which is the "Fermi sphere" about the point $\vec{q}$, respectively $E_F < \frac{\hbar^2}{2m}(\vec{q} - \vec{k}_F)^2 \leq \epsilon_{\vec{k}'} \leq \frac{\hbar^2}{2m}(\vec{q} + \vec{k}_F)^2$ for the energies.



Defining the excitation energy as $E(\vec{q}) := \epsilon_{\vec{k}'} - E_F$ we obtain the region where excitations are possible as the shaded area in the figure below.



Until $q = 2k_F$, the excitations are gapless, i.e. the minimal excitation energy $E_{min} = 0$. For $q > 2k_F$, there is a minimum excitation energy $E_{min}(\vec{q}) = \frac{\hbar^2}{2m}(\vec{q} - \vec{k}_F)^2$. The structure of the excitations is such that an electron is transferred from the interior of the filled Fermi sphere to its outside, leaving a hole at $\vec{k}$ in the Fermi sphere. We thus call the excitations of the Fermi sphere *particle-hole pairs*. It is important to understand that this is more than just a name. In fact, the dynamics of the "hole" must be taken into account. The reason is that in the ground state for every $\vec{k}$ occupied there is another occupied state with $-\vec{k}$, which implies that the total momentum $\vec{K} = 0$. An excited state then has an electron in state $\vec{k}'| > k_F$ and a "lonely" electron at $-\vec{k}$ in the Fermi sphere. Therefore the total momentum now is $\vec{K} = \vec{k}' + (-\vec{k}) = \vec{q}$. We thus formally need the electron at $-\vec{k}$. However, the tradition is to rather work with the hole at $+\vec{k}$ instead, which is treated like a particle with charge $+e$ and momentum $-\vec{k}$.

1.5 Finite temperatures

In contrast to $T = 0$, the properties of the Fermi gas at finite temperatures will be influenced by the excited states. One also talks of *thermal excitation of particle-hole pairs* in this connection. To describe the thermal effects, we need the partition function or more precisely the probability for the realization of a certain excited state. Let us take as example the expectation value of the Hamilton operator, which for finite T leads to the internal energy. For our jellium model we then have

$$U(T) = \langle \hat{H}_e \rangle_T = \sum_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} \langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \rangle_T \ .$$

We thus need to evaluate the thermal expectation value $\langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \rangle_T$. The combination of creation and annihilation operator just represents the particle number operator for the state with quantum numbers $\vec{k}$ and σ, and because fermions can occupy each state at most once, $0 \leq \langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \rangle_T \leq 1$ must hold, and we can interpret this expectation value also as *occupation probability* of this particular single-particle state. The result is usually derived in the course on statistical mechanics and reads

$$\langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \rangle_T = f(\epsilon_{\vec{k}}) = \frac{1}{1 + e^{\beta(\epsilon_{\vec{k}} - \mu)}}$$

the famous *Fermi-Dirac* distribution function in Fig. 1.1.

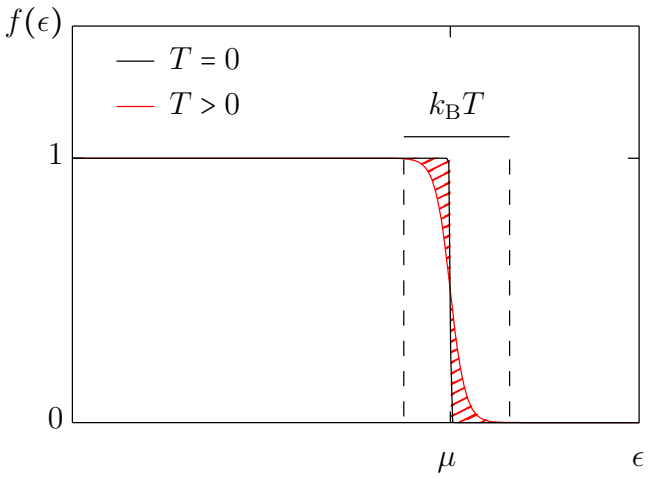


Figure 1.1: Fermi function for $T = 0$ (black line) and $T > 0$ (red line). The states in a region $O(k_B T)$ around the chemical potential is redistributed according to the red shaded area.

The energy now becomes

$$U(T) = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} f(\epsilon_{\vec{k}}) \ .$$

The evaluation of this sum (or integral) is in general pretty cumbersome. However, because $f(\epsilon_{\vec{k}})$ changes appreciably only across a region $O(k_B T)$ one can
exercise approximately evaluate the sum for $k_B T / E_F \ll 1$ using the *Sommerfeld expansion*. The result is

$$u(T, n) = u(0, n) + \frac{\pi^2}{3} (k_B T)^2 \mathcal{N}(E_F) + O(T^4) \quad (1.8)$$

From this result we can calculate the specific heat at constant volume as

$$c_V = \frac{1}{V}\left(\frac{\partial E(T,N)}{\partial T}\right)_{N,V} = \frac{2\pi^2}{3} k_{\mathrm{B}}^2 \mathcal{N}(E_F)\cdot T \ . \quad (1.9)$$

With $\mathcal{N}(E_F) = \frac{3}{4}\frac{n}{E_F}$ this can be cast into

$$c_V(T) = \frac{\pi^2}{2} k_{\mathrm{B}} n \frac{k_{\mathrm{B}} T}{E_F} \propto \frac{T}{E_F} \propto m\cdot T \ .$$

The latter proportionality, i.e. $\frac{c_V}{T} \propto m$, is very important as it opens the road to a phenomenological understanding of the properties of the *interacting* Fermi gas. The quantity

$$\lim_{T\to 0} \frac{c_V(T)}{T} =: \gamma$$

is called *Sommerfeld coefficient of the specific heat.*

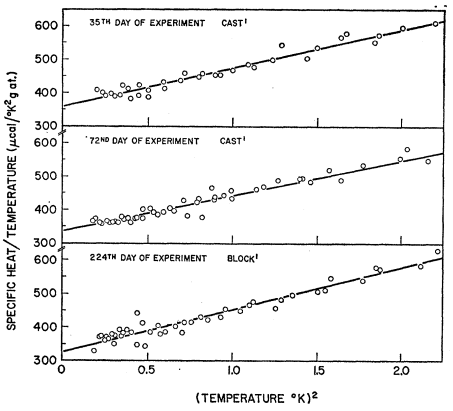


Figure 1.2: Low-temperature specific heat of sodium.

Let us add to this *electronic contribution* the part coming from lattice vibrations (which, as you now, behaves as $c_V = \beta\cdot T^3$) to obtain for the total specific heat of a crystal at low temperatures

$$c_V(T) = \gamma\cdot T + \beta\cdot T^3 \ .$$

Therefore, plotting $\frac{c_V(T)}{T}$ versus T^2 will yield at the same time information about the lattice part (slope) and the electronic part (offset).

Taking into account the fact, that the result (1.9) was derived for non-interacting electrons in free space, it is quite astonishing that one actually finds such a behavior in the experiment for a large number of metals. As an example Fig. 1.2[2] shows experimental data for the specific heat plotted versus T^2 for three different sodium samples.

Another experimental probe is the magnetic response of a system. Electrons carry charge and spin, so they couple in two ways to external magnetic fields. First, through the classical replacement $\vec{p} \to \vec{p} + \frac{e}{c}\vec{A}(\vec{r})$, where $\vec{A}(\vec{r})$ is the vector potential. This term leads to the diamagnetic response, which we will ignore here. The more important contribution comes from the spin, which we inclue

[2]Taken from D.L. Martin, Phys. Rev. **124**, 438 (1961).

via the Pauli term $\hat{H}_{\mathrm{P}} = -\frac{2\mu_{\mathrm{B}}}{\hbar}\hat{\vec{s}}\cdot\vec{B}$. The spin of the an electron in the state $\vec{k}$ can be represented with creation and annihilation operators, and especially the z-component becomes $\hat{s}_{\vec{k},z} = \frac{\hbar}{2}\left(\hat{n}_{\vec{k}\uparrow} - \hat{n}_{\vec{k}\downarrow}\right)$. Assuming a magnetic field in
exercise z-direction, we need to calculate the total magnetization

$$M_z = \frac{2\mu_{\mathrm{B}}}{\hbar}\sum_{\vec{k}}\langle\hat{s}_{\vec{k},z}\rangle_T = \mu_{\mathrm{B}}\sum_{\vec{k}}\langle\hat{n}_{\vec{k}\uparrow} - \hat{n}_{\vec{k}\downarrow}\rangle_T = \ldots = \frac{3}{2}N\frac{\mu_{\mathrm{B}}}{E_F}B_z$$

and hence for the susceptibility

$$\chi_{\mathrm{P}} = \frac{M_z}{B_z} = \frac{3}{2}N\frac{\mu_{\mathrm{B}}}{E_F}$$

The response of the electrons is thus positive, i.e. the Pauli term leads to a *paramagnetic response*. The susceptibility is therefore also referred to as *Pauli paramagnetism*. As for the specific heat, we also find $\chi_{\mathrm{P}} \propto \frac{1}{E_F} \propto m$. It is thus interesting to see what the *Wilson ratio*

$$R_W := \frac{4\pi^2 k_{\mathrm{B}}^2}{3(g\mu_{\mathrm{B}})^2}\frac{\chi_P}{\gamma} \quad . \tag{1.10}$$

is. Inserting the values for γ and χ_{P} for the non-interacting , we obtain $R_W = 1$, which presently does not tell much, except that both specific heat and Pauli susceptibility are driven by the same physics, i.e. the Fermi-Driac distribution of non-interacting particles.

Lecture 2

Fermi liquid theory

2.1 Beyond the independent electron approximation

Up to now we have assumed that the electrons can be treated as non-interacting particles (the so-called *independent electron approximation*). In the following we will discuss some effects of the interaction and in particular how to take them into account. We will not yet include the periodic lattice, but stay within the free electron approximation.

The Hamiltonian of the free electron gas in second quantization reads

$$\hat{H} = \sum_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \frac{1}{2} \sum_{\vec{q}} \sum_{\substack{\vec{k}\,\vec{k}' \\ \sigma\,\sigma'}} V_{\vec{q}}\, \hat{c}^\dagger_{\vec{k}+\vec{q}\sigma} \hat{c}^\dagger_{\vec{k}'-\vec{q}\sigma'} \hat{c}_{\vec{k}'\sigma'} \hat{c}_{\vec{k}\sigma} \tag{2.1}$$

where

$$V_{\vec{q}} = \frac{4\pi}{V} \frac{e^2}{q^2}$$

is the Fourier transform of the Coulomb interaction. At first, the term $\vec{q} = 0$ seems to be troublesome. However, it can be shown that it is cancelled by the positive background charge ensuring charge neutrality.

exercise

A first attempt to capture the effects of the interaction is within a Hartree-Fock treatment. Within this approximation one finds

$$\begin{aligned} \hat{H} \to \hat{H}_{\mathrm{HF}} &= \sum_{\vec{k}\sigma} E_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \\ E_{\vec{k}} &= \epsilon_{\vec{k}} - \sum_{\vec{q}} V_{\vec{q}} f(E_{\vec{k}+\vec{q}}) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi} k_F F\left(\frac{k}{k_F}\right) . \end{aligned}$$

The function

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|$$

is called *Lindhard function*. Its graph is shown in the left panel of Fig. 2.1, and

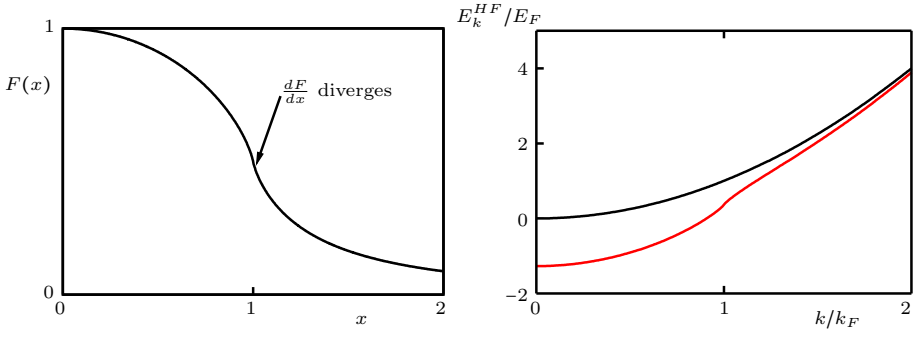


Figure 2.1: Lindhard function and Hartree-Fock dispersion.

the Hartree-Fock dispersion $E_{\vec{k}}$ as red curve in the right panel in comparison to

the non-interacting dispersion included as black line. Note that we have eliminated the "classical" charge-density interaction by using charge neutrality, i.e. the renormalization of the dispersion is due to so-called *exchange contributions* only and hence a pure effect of Pauli's principle!
The exchange contribution to the Hartree-Fock energy can be rewritten as

$$\begin{aligned}\sum_{\vec{q}} V_{\vec{q}} f(E_{\vec{k}+\vec{q}}) &= \int_V d^3r \, \frac{e}{r} \rho^{xc}_{\vec{k}}(\vec{r}) \\ \rho^{xc}_{\vec{k}}(\vec{r}) &= -\frac{e}{V} \sum_{k' \le k_F} e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} \quad .\end{aligned}$$

The object $\rho^{xc}_{\vec{k}}(\vec{r})$ is called *exchange charge density* and is non-local even for the homogeneous electron gas. It can be evaluated to

$$\rho^{xc}_{\vec{k}}(\vec{r}) = -\frac{3en}{2} \frac{e^{ikr}}{(k_F r)^3} \left[k_F r \cos(k_F r) - \sin(k_F r)\right] \quad .$$

A more intuitive quantity is the total exchange charge density obtained from summing $\rho^{xc}_{\vec{k}}(\vec{r})$ over $k \le k_F$. The result is

$$\langle \rho^{xc}_{\vec{k}}(\vec{r}) \rangle := \frac{1}{V} \sum_{k \le k_F, \sigma} \rho^{xc}_{\vec{k}}(\vec{r}) = -\frac{9ne}{2} \frac{1}{(k_F r)^6} \left[k_F r \cos(k_F r) - \sin(k_F r)\right]^2 \quad .$$

It describes the *average change of the charge density induced by an electron at the origin in a distance r due to Pauli's principle.* Again it must be emphasized that this is a purely quantum mechanical phenomenon! This exchange charge density oscillates in a characteristic manner. These oscillations are caused by the existence of a sharp Fermi surface and called *Friedel oscillations.*
For large r the exchange charge density $\langle \rho^{xc}_{\vec{k}}(\vec{r}) \rangle$ goes to zero $\propto r^{-4}$. For small r, on the other hand, we can expand the different parts and obtain

$$\begin{aligned}\langle \rho^{xc}_{\vec{k}}(\vec{r} \to 0) \rangle &\approx -\frac{9en}{2} \frac{1}{(k_F r)^6} \left[k_F r - \frac{1}{2}(k_F r)^3 - k_F r + \frac{1}{6}(k_F r)^3\right]^2 \\ &= -\frac{1}{2} en \quad .\end{aligned}$$

Thus, in the vicinity of a given electron, the "effective" charge density seen by another electron is $\rho_{eff} = \rho_0 + \langle \rho^{xc}_{\vec{k}}(\vec{r} \to 0) \rangle \approx en - \frac{1}{2}en = \frac{1}{2}en$! This characteristic reduction of the effective charge density is called *exchange hole.* In Hartree-Fock theory one considers only contributions among one spin species. If one takes into account the Coulomb correlations beyond Hartree-Fock, one obtains due to the presence of the other spin species a further *correlation hole* $-\frac{1}{2}en$, i.e. the effective *electronic* charge density in the vicinity of a given electron is actually reduced to zero! Thus, in practice, every electron can be thought of being "dressed" with an *exchange-correlation hole* it has to carry along during

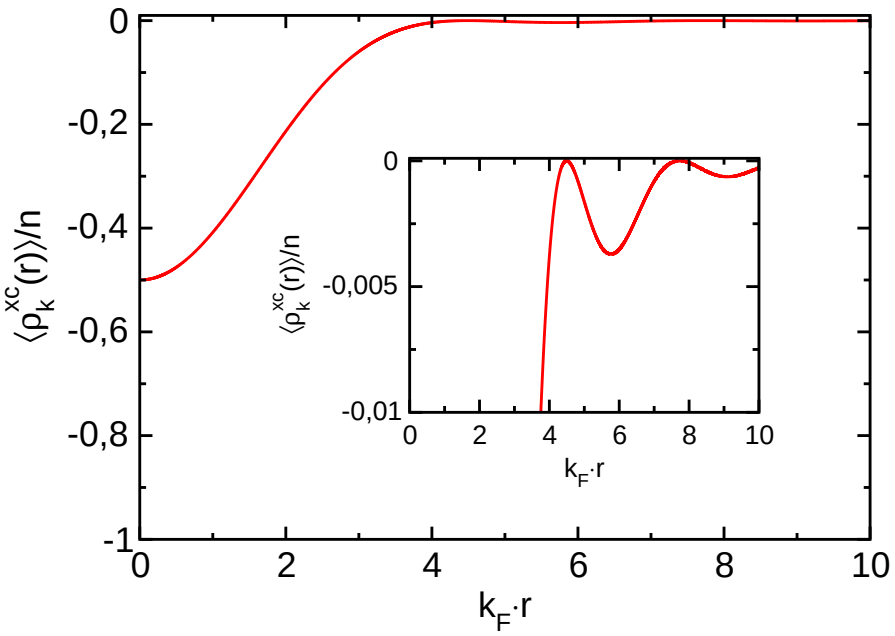


Figure 2.2: Exchange charge density $\langle\rho_{\vec{k}}^{xc}(\vec{r})\rangle/n$ as function of $k_F \cdot r$.

its motion. Such a parcel will of course hinder the motion, and to an "outsider" the electron will appear as having a larger mass. In this sense it will no longer be the electron we know from free space, but some modified creature one calls *quasi electron* or more general *quasi particle*.

The concept of quasi-particles is a very common and powerful one. In fact, all "particles" you know (electrons, quarks, hadrons, mesons, photons, ...) are actually quasi-particles, because we never see them as completely isolated individuals, but always in an interacting environment which usually completely modifies their properties.

2.2 Landau's Fermi liquid theory

The properties of the noninteracting electron gas can be summarized as follows: It has a specfic heat $c_V(T) = \gamma T$ with a temperature independent Sommerfeld constant γ, a magnetic Pauli susceptibility $\chi_P(T)$ =const. and a bulk modulus $B_T(T)$ =const. for $k_\mathrm{B}T \ll E_F$. As already noted, another interesting quantity is the Wilson ratio

$$R_W := \frac{4\pi^2 k_\mathrm{B}^2}{3(g\mu_\mathrm{B})^2}\frac{\chi_P}{\gamma} \quad . \tag{2.2}$$

For the noninteracting electron gas we have $R_W = 1$.

The astonishing *experimental* observation now is that for many metallic solids at low temperature one again finds the same behavior for the electronic con-

tributions to specific heat, susceptibilty and bulk modulus, together with a Wilson ratio R_W =O(1). It thus seems that in spite of the long-ranged and strong Coulomb repulsion among the electrons the low-temperature properties can be well approximated by ignoring the Coulomb interaction.

A partial solution to this puzzle is provided by inspecting the response of the electron gas to an external charge or electrostatic potential. With standard arguments from electrostatics such an external charge will, due to the mobility of the electrons, lead to a total charge density $\rho(\vec{r}) = \rho^{\text{ext}}(\vec{r}) + \rho^{\text{ind}}(\vec{r})$ and a total electrostatic potential $\Phi(\vec{r}) = \Phi^{\text{ext}}(\vec{r}) + \Phi^{\text{ind}}(\vec{r})$, which are related through Poisson's equation. For a homogeneous and isotropic system, the total and external potential are related via a dielectric function according to

$$\Phi(\vec{r}) = \int d^3r\, \varepsilon(\vec{r} - \vec{r}\,')\Phi^{\text{ext}}(\vec{r}\,') \ .$$

After a spatial Fourier transformation this relation becomes

$$\Phi^{\text{ext}}(\vec{q}) = \varepsilon(\vec{q})\, \Phi(\vec{q}) \ .$$

In Fourier space the Poisson equations for the external and total charge have the form[1] $q^2\, \Phi^{\text{ext}}(\vec{q}) = 4\pi\, \rho^{\text{ext}}(\vec{q})$ and $q^2\, \Phi(\vec{q}) = 4\pi\, \rho(\vec{q})$. Together with $\rho^{\text{ext}} = \rho - \rho^{\text{ind}}$ one can identify

$$\varepsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \frac{\rho^{\text{ind}}(\vec{q})}{\Phi(\vec{q})} \ .$$

Thus, what we need is a relation between the total potential and the induced charge density.

To this end we try to approximately solve the Schrödinger equation for our test charge in the presence of the total electrostatic potential, i.e.

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi_i(\vec{r}) - e\Phi(\vec{r})\psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r}) \ .$$

To proceed we assume that $\Phi(\vec{r})$ (and consequently also $\rho(\vec{r})$) varies only little over atomic length scales as shown in Fig. 2.3, i.e. we assume that $|\vec{\nabla}^2 \Phi| \ll |\vec{\nabla}^2 \psi_i|$ and $\Phi(\vec{r}) \approx \Phi(\vec{R})$ within the small but macroscopic volume element ΔV. In this case we can approximate the solution of the Schrödinger equation by plane waves with a position dependent dispersion

$$\epsilon_{\vec{k}}(\vec{R}) = \frac{\hbar^2 k^2}{2m} - e\Phi(\vec{R}) \ .$$

This dispersion leads to a position dependent particle density

$$n(\vec{R}) = \frac{1}{V} \sum_{\vec{k}} f\left(\epsilon_{\vec{k}}(\vec{R})\right)$$

[1] Remember: $\vec{\nabla}^2 \xrightarrow{\text{FT}} -q^2$.

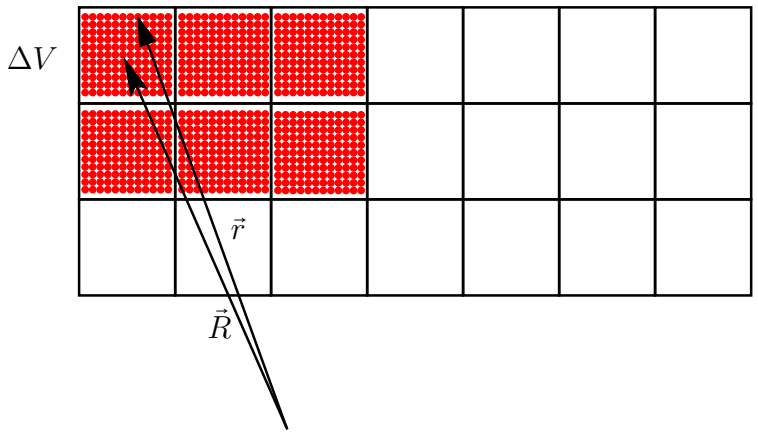


Figure 2.3: Macroscopic versus microscopic structure

and a corresponding charge density $\rho(\vec{R}) = -en(\vec{R})$. The induced charge density then becomes $\rho^{\rm ind}(\vec{R}) = -en(\vec{R}) + en_0$, where

$$n_0 = \frac{1}{V}\sum_{\vec{k}} f\left(\frac{\hbar^2 k^2}{2m}\right) \ .$$

We then obtain from a Taylor expansion with respect to ϕ

$$\begin{aligned}\rho^{\rm ind}(\vec{R}) &= -e\frac{1}{V}\sum_{\vec{k}}\left[f\left(\frac{\hbar^2k^2}{2m} - e\Phi(\vec{R})\right) - f\left(\frac{\hbar^2k^2}{2m}\right)\right] \\ &= -e^2\frac{\partial n_0}{\partial\mu}\Phi(\vec{R}) + {\rm O}(\Phi^2) \ .\end{aligned}$$

After Fourier transformation with respect to $\vec{R}$ we insert this into the formula for the dielectric function to obtain the *Thomas-Fermi dielectric function*

$$\begin{aligned}\varepsilon(\vec{q}) &= 1 + \frac{4\pi e^2}{q^2}\frac{\partial n}{\partial\mu} \\ &= 1 + \left(\frac{q_{TF}}{q}\right)^2 \qquad (2.3) \\ q_{TF}^2 &= 4\pi e^2\frac{\partial n}{\partial\mu} \qquad (2.4)\end{aligned}$$

with the *Thomas-Fermi wave vector* q_{TF}. Note that we have neglected all contributions from *short length scales*, i.e. possible modifications for *large wave vectors*.

As a special case let us calculate the effective potential of a point charge Q with

$$\Phi^{\rm ext}(\vec{q}) = \frac{4\pi Q}{q^2}$$

to obtain

$$\Phi(\vec{q}) = \frac{1}{\varepsilon(\vec{q})}\frac{4\pi Q}{q^2} = \frac{4\pi Q}{q^2 + q_{TF}^2} \ .$$

Note that $\Phi(\vec{q})$ now is finite for $\vec{q} \to 0$. Furthermore, transformed into real space, we find

$$\Phi(\vec{r}) = \frac{Q}{r} e^{-q_{TF} r}$$

for the potential, i.e. a short ranged Yukawa potential. We may even evaluate the expression for q_{TF} for $k_{\mathrm{B}}T \ll E_F$ to obtain

$$\frac{q_{TF}^2}{k_F^2} = \frac{4}{\pi}\frac{1}{k_F a_B} = \mathrm{O}(1) \ .$$

Thus $q_{TF} \approx k_F$, and the range of $\Phi(\vec{r})$ is only sizeable over distances a_B.
This peculiar property of the electron gas is called *screening* and very efficiently cuts off the range of the Coulomb interaction, even among the electrons themselves.[2] Nevertheless, the remaining short-ranged effective repulsion still poses a problem, because in its presence a single-particle state $|n_{\vec{k}\sigma}\rangle$ is not an eigenstate of the system, but will evolve in time under the action of the total Hamiltonian. In general, one can identify a time scale τ, the *lifetime*, after which the state $|n_{\vec{k}\sigma}(t)\rangle$ has lost all "memory" of its initial form.
After this discussion we can now give an operational definition, under what conditions it makes sense at all to talk of electrons: When $\tau \to \infty$ or at least $\tau \gg$ relevant time scales, the state $|n_{\vec{k}\sigma}(t)\rangle \approx |n_{\vec{k}\sigma}(0)\rangle$ is called *quasi-stationary*. We thus need an idea of the lifetime τ of a single-particle state in the presence of the Coulomb interaction. To this end we put an electron in a state close to the Fermi surface, i.e. with an energy $\epsilon_{\vec{k}} > E_F$. This electron can interact with a second electron just below the Fermi energy, leading to an excited state where the two electrons must have energies just above the Fermi energy (Pauli principle). If we denote with $\epsilon_i = \epsilon_{\vec{k}_i} - E_F$ the energies relative to the Fermi energy, energy conservation requires $\epsilon_3 + \epsilon_4 = \epsilon_1 - |\epsilon_2| \geq 0$ or $|\epsilon_2| \leq \epsilon_1$. Therefore, the fraction of electrons in the Fermi volume, that can actually interact with an additional electron with energy slightly above the Fermi energy, can be estimated as

$$\begin{aligned}
\delta_i &\approx \frac{\text{volume of Fermi sphere in } [-\epsilon_1, 0]}{\text{volume of Fermi sphere}} \\
&= \frac{V(E_F) - V(E_F - \epsilon_1)}{V(E_F)} = 1 - \frac{V(E_F - \epsilon_1)}{V(E_F)} \\
&= 1 - \left(\frac{E_F - \epsilon_1}{E_F}\right)^{3/2} \approx \frac{3}{2}\frac{\epsilon_1}{E_F} \ll 1 \ ,
\end{aligned}$$

[2] This is not a trivial statement, but must (and can) be actually proven by inspecting the interaction energy between two electrons.

where we used $V(\epsilon) \sim k^3 \sim \epsilon^{3/2}$. In particular, for $\epsilon_1 \to 0$ the phase space for interactions vanishes, i.e. for the state ϵ_1 the liftime $\tau \to \infty$. As for the final states after the interaction process $0 \leq \epsilon_3 + \epsilon_4 \leq \epsilon_1$ must hold and $\epsilon_1 \to 0$, we may approximately assume $\epsilon_3 \approx \epsilon_4 \approx \epsilon_1/2$,and hence find as phase space fraction for final states of the interaction process

$$\delta_f \approx \frac{3}{2}\frac{\epsilon_3}{E_F} \sim \frac{\epsilon_1}{E_F} \ .$$

Taking together, the total phase space for an interaction process becomes

$$\delta \sim \left(\frac{\epsilon_1}{E_F}\right)^2 \ .$$

If we take finite temperature into account, the Fermi surface becomes "soft" in a region $\mathrm{O}(k_\mathrm{B}T)$ around the Fermi energy, and the previous estimate must be modified to

$$\delta \sim a\left(\frac{\epsilon_1}{E_F}\right)^2 + b\left(\frac{k_\mathrm{B}T}{E_F}\right)^2 \ .$$

Using Fermi's golden rule, we can estimate the decay rate or equivalently the inverse lifetime of an additional electron placed into a state close to the Fermi surface according to

$$\frac{1}{\tau} \sim \delta\,|V(\vec{q})|^2 \sim \left(\frac{k_\mathrm{B}T}{E_F}\right)^2 |V(\vec{q})|^2 \ ,$$

where $\vec{q}$ denotes a typical momentum transfer due to the interaction. For the bare Coulomb interaction one then finds $\frac{1}{\tau} \sim \frac{T^2}{q^2}$, which is indetermined in the limit $T \to 0$ and $q \to 0$. However, for the screened Coulomb interaction we have $\frac{1}{\tau} \sim \frac{T^2}{q^2+q_{TF}^2}$, i.e. $\tau \sim 1/T^2 \to \infty$ as $T \to 0$.

> For non-singular interactions, the concept of single-particle states remains valid in a quasi-stationary sense for energies at the Fermi surface and low temperatures.

Based on this observation, Landau 1957 made the suggestion that the low-energy excitations of the interacting Fermi gas can be described by quasi-stationary single-particle states $|n_{\vec{k}}(t)\rangle$ that evolve adiabatically[3] from corresponding states $|n_{\vec{k}}^{(0)}\rangle$ of the noninteracting Fermi gas. However, because these quasi-stationary states are not true eigenstates of the interacting system, one cannot use the notion of "electrons" in association with them any more. Thus

[3] i.e. one switches on the interaction from $t = -\infty$ to $t = 0$ sufficiently slow (for example as $e^{\eta t}$) and assumes that the state always is uniquely indentifyable with $|n_k(t = -\infty)\rangle$.

Landau further suggested to call the interacting Fermi system with these properties a *Fermi liquid* and the objects described by the quasi-stationary states *quasi electrons* or more general *quasi particles*. For these quasi particles Landau proposed the following axioms:

- Quasi particles have a spin $s = \hbar/2$, i.e. are Fermions.
- Quasi particles interact (Landau quasi particles).
- The number of quasi particles equals the number of electrons (uniqueness).

In particluar the last axiom means that the particle density $n = N/V$ and consequently $k_F = \left(3\pi^2 n\right)^{3/2}$ remains unchanged. This observation can be rephrased as

> The volume of the Fermi body is not changed by non-singular interactions (Luttinger theorem).

Let us discuss the consequences of the concepts of quasi particles. First, we note that for the noninteracting electron gas we have a distribution function $f(\epsilon_k) \equiv n^{(0)}_{k\sigma}$, the Fermi function. With this function we can write the ground state energy of the system as

$$E_{GS} = \sum_{\vec{k}\sigma} \epsilon_k \, n^{(0)}_{k\sigma} \quad ,$$

while for the system in an excited state we will in general have a different distribution n_k and

$$E = \sum_{\vec{k}\sigma} \epsilon_k \, n_{k\sigma} \quad .$$

In particular, if we add or remove one electron in state k_0, we have $\delta n_{k\sigma} := n_{k\sigma} - n^{(0)}_{k\sigma} = \pm\delta_{k,k_0}$ and $\delta E = E - E_{GS} = \epsilon_{k_0}\delta_{k,k_0}$. Therefore

$$\frac{\delta E}{\delta n_{k\sigma}} = \epsilon_k \quad .$$

As the quasi particles are objects that evolve in one-to-one correspondence from the free particles of the electron gas, we add another axiom for the interacting system, namely

- There exists a *distribution function* $n_{\vec{k}\sigma}$ such that the energy of the system can be written as a functional $E[n_{\vec{k}\sigma}]$ of this function. In particular, there exists a *gound-state distribution function* $n^{(0)}_{\vec{k}\sigma}$ with $E_{GS} = E[n^{(0)}_{\vec{k}\sigma}]$. The low-energy excitations are characterised by deviations $\delta n_{\vec{k}\sigma} = n_{\vec{k}\sigma} - n^{(0)}_{\vec{k}\sigma}$,

$|\delta n_{\vec{k}\sigma}| \ll 1$ from the ground state distribution and a corresponding change of energy

$$\delta E[n_{\vec{k}\sigma}] = E[n_{\vec{k}\sigma}] - E_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} \delta n_{\vec{k}\sigma} + \frac{1}{2} \sum_{\vec{k}\sigma} \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'} \delta n_{\vec{k}\sigma} \delta n_{\vec{k}'\sigma'} + \dots \tag{2.5}$$

in the sense of a Volterra expansion (= Taylor expansion for functionals).

From the first term in this expression we can define in correspondence to the structure of the noninteratcing electron gas the *energy of a quasi particle* as

$$\boxed{\epsilon[n_{\vec{k}\sigma}] \quad := \quad \frac{\delta E[n_{\vec{k}\sigma}]}{\delta n_{\vec{k}\sigma}}}$$

If $\epsilon[n_{\vec{k}\sigma}] \equiv \epsilon_{\vec{k}\sigma} > E_F$, we talk of a *quasi particle*, in the other case of a *quasi hole*. The convention is to drop the word "quasi" and talk of particles and holes, always keeping in mind that these notions are meant in the sense of Landau's axioms.

The determination of the distribution function, based on general thermodynamic principles and the expansion (2.5), is somewhat tedious. The final result, however, looks quite intuitive and reasonable. It reads

$$n_{\vec{k}\sigma} = \left[1 + \exp\left\{\beta(\epsilon_{\vec{k}\sigma} - \mu)\right\}\right]^{-1}$$

and formally looks like the Fermi function. In reality it however is a very complicated implicit equation, as $\epsilon_{\vec{k}\sigma} = \epsilon[n_{\vec{k}\sigma}]$ is a (usually unknown) functional of the distribution function.

Let us now concentrate on the ground state, where we have $\epsilon^{(0)}_{\vec{k}\sigma} := \epsilon[n^{(0)}_{\vec{k}\sigma}]$. We can then define a *group velocity* for the particles in the usual way as $\vec{v}_{\vec{k}\sigma} := \vec{\nabla}_{\vec{k}} \epsilon^{(0)}_{\vec{k}\sigma}$. To keep things simple we procced without external magnetic field, ignore spin-orbit coupling and assume an isotropic system. In this case everything depends on k only, and in particular $\vec{v}_{\vec{k}\sigma} = v_k \frac{\vec{k}}{k}$. For[4] $k = k_F$ we now *define*

$$\boxed{\begin{array}{lcl} v_{k_F} & =: & \dfrac{\hbar k_F}{m^*} \\ \epsilon^{(0)}_k & =: & \mu + \hbar v_F \,(k - k_F) \quad . \end{array}}$$

[4]Remember: k_F is the same as for the noninteracting system!

The constant m^* introduced in this way is called *effective mass of the particles*. Having an explicit form for the dispersion, we can now also calculate the density of states as

$$\begin{aligned}\mathcal{N}(\epsilon) &= \frac{1}{V}\sum_{\vec{k}}\delta(\epsilon_k^{(0)}-\mu-\epsilon)\\ &= \int\frac{d^3k}{(2\pi)^3}\delta(\epsilon_k^{(0)}-\mu-\epsilon) = \frac{1}{\hbar v_F}\int\frac{k^2dk}{2\pi^2}\,\delta(k-k_0)|_{k_0=k_F+\epsilon/(\hbar v_F)}\\ &= \frac{1}{2\pi^2\hbar v_F}\left(k_F+\frac{\epsilon}{\hbar v_F}\right)^2 \quad .\end{aligned}$$

The convention is such that $\epsilon = 0$ represents the Fermi energy. In particular, for the density of states at the Fermi energy one then finds

$$\boxed{\mathcal{N}(0) = \frac{k_f^2}{2\pi^2\hbar v_F} = \frac{m^*k_F}{2\pi^2\hbar^2} = \frac{m^*}{m}\mathcal{N}^{(0)}(E_F) \quad .}$$

The second term in the expansion (2.5) defines the *quasi particle interaction*

$$f_{\vec{k}\sigma;\vec{k}'\sigma'} := \frac{\delta^2 E[n_{\vec{k}\sigma}]}{\delta n_{\vec{k}\sigma}\delta n_{\vec{k}'\sigma'}} \quad .$$

An obvious question is how important this part actually is. To this end let us consider a variation in the ground state energy

$$\begin{aligned}\delta E &= \delta\epsilon - \mu\delta n\\ &= \sum\vec{k}\sigma\left(\epsilon_{\vec{k}\sigma}^{(0)}-\mu\right)\delta n_{\vec{k}\sigma} + \frac{1}{2}\sum_{\vec{k}\sigma}\sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}\sigma}\delta n_{\vec{k}'\sigma'} + \ldots\end{aligned}$$

As we are interested in low energy excitations, we have $|\epsilon_{\vec{k}\sigma}^{(0)} - E_F| \ll E_F$ and may assume

$$\frac{\epsilon_{\vec{k}\sigma}^{(0)} - E_F}{E_F} \propto \delta n_{\vec{k}\sigma}$$

to leading order, respectively $(\epsilon_{\vec{k}\sigma}^{(0)} - E_F)\delta n_{\vec{k}\sigma} = \mathrm{O}(\delta n^2)$. On the other hand, the "interaction term" is $\mathrm{O}(\delta n^2)$ by construction, and thus of the same order. Consequently, both terms are actually important for the consistency of the theory. Therefore, we will in general have to deal with a *renormalised particle energy*

$$\epsilon_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}^{(0)} + \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} \quad .$$

Due to isotropy and without spin-orbit interaction the interaction can only depend on the relativ orientation of $\vec{k}$ and $\vec{k}'$ respectively σ and σ'. Moreover,

for Fermions all the action is concentrated to within a small shell around the Fermi energy, and thus $\vec{k}\cdot\vec{k}\,' \approx k_F^2\cos\vartheta$. We can then define

$$\begin{aligned} f^S_{kk'} &:= f_{\vec{k}\uparrow;\vec{k}\,'\uparrow} + f_{\vec{k}\uparrow;\vec{k}\,'\downarrow} \text{ spin-symmetric interaction,} \\ f^A_{kk'} &:= f_{\vec{k}\uparrow;\vec{k}\,'\uparrow} - f_{\vec{k}\uparrow;\vec{k}\,'\downarrow} \text{ spin-antisymmetric interaction.} \end{aligned}$$

As $f^\alpha_{kk'}$ depends only on $\cos\vartheta$, we can further expand it into Legendre polynomials according to

$$f^\alpha_{kk'} = f^\alpha_{k,\cos\vartheta} = \sum_{l=0}^{\infty} f^\alpha_l P_l(\cos\vartheta)$$

and finally obtain

$$\boxed{f_{\vec{k}\sigma;\vec{k}\,'\sigma'} = \frac{1}{2V\mathcal{N}(0)}\sum_{l=0}^{\infty}\left(F^S_l + \sigma\cdot\sigma'\,F^A_l\right)P_l(\cos\vartheta)\ . \quad (2.6)}$$

The quantities $F^\alpha_l := V\mathcal{N}(0)f^\alpha_l$ are called *Landau parameters*. Note that by definition they are dimensionless.
We now are ready to calculate physical quantities.

1. Let us start with the specific heat, which is defined via

$$c_V = \frac{1}{V}\left(\frac{\partial E}{\partial T}\right)_{N,V} = \frac{1}{V}\sum_{\vec{k}\sigma}\left[\epsilon^{(0)}_{\vec{k}\sigma} + \sum_{\vec{k}\,'\sigma'} f_{\vec{k}\sigma;\vec{k}\,'\sigma'}\delta n_{\vec{k}\,'\sigma'}\right]\frac{\partial n_{\vec{k}\sigma}}{\partial T}\ .$$

   As the second part is by construction of at least $\mathrm{O}(\delta n)$ =$\mathrm{O}(T)$, we can stick to the first as $T\to 0$. This leads to[5]

$$\boxed{\begin{aligned} c_V &= \gamma T \\ \gamma &= \frac{\pi^2}{3}k_B^2\mathcal{N}(0) = \frac{m^*}{m}\gamma^{(0)}\ . \end{aligned}}$$

2. A second interesting quantity is the *compressibility* defined as

$$\kappa := -\frac{1}{V}\frac{\partial V}{\partial p}\ ,\quad p = -\frac{\partial E_{GS}}{\partial V}\ .$$

   With some manipluations this can be cast into the form

$$\boxed{\kappa = \frac{1}{n^2}\frac{\partial n}{\partial \mu}}$$

[5]The calculation is identical to the one for the electron gas.

This result is again quite reasonable, as the compressibility is something that tells us how easy it is to make the system more dense or how easy it is to add particles to the system. Both are related to the density n, and a change in particle number is regulated by the chemical potential.

We thus have to calculate

$$\delta n = \frac{1}{V}\sum_{\vec{k}\sigma} \delta n_{\vec{k}\sigma} \ .$$

From the definition of the quasi particle energy we can now infer

$$\delta n_{\vec{k}\sigma} = \frac{\partial n_{\vec{k}\sigma}}{\partial(\epsilon_{\vec{k}\sigma} - \mu)}(\delta\epsilon_{\vec{k}\sigma} - \delta\mu)$$

or

$$\delta n = \frac{1}{V}\sum_{\vec{k}\sigma}\left(-\frac{\partial n_{\vec{k}\sigma}}{\partial \epsilon_{\vec{k}\sigma}}\right)(\delta\mu - \delta\epsilon_{\vec{k}\sigma}) \ .$$

Now the quasi particle interaction becomes important. The change in the energy is given by

$$\delta\epsilon_{\vec{k}\sigma} = \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} \ .$$

Furthermore, as we vary the chemical potential, the resulting variations are better isotropic and spin independent. We therefore can conclude that from the Landau parameters only F_0^S can play a role, i.e. with the definition (2.6)

$$\delta\epsilon_{\vec{k}\sigma} = \frac{F_0^S}{2V\mathcal{N}(0)}\sum_{\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} = \frac{F_0^S}{2\mathcal{N}(0)}\delta n \ .$$

Collecting all terms one arrives at

$$\delta n = \left(\delta\mu - \frac{F_0^S}{2\mathcal{N}(0)}\delta n\right)\frac{1}{V}\sum_{\vec{k}\sigma}\left(-\frac{\partial n_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}\sigma}}\right) \ .$$

The $\vec{k}$ sum can be cast into an integral yielding

$$\frac{1}{V}\sum_{\vec{k}\sigma} = \left(-\frac{\partial n_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}\sigma}}\right)\int d\epsilon\,\mathcal{N}(\epsilon)\left(-\frac{\partial n(\epsilon)}{\partial\epsilon}\right) \xrightarrow{T=0} 2\mathcal{N}(0) \ .$$

We therefore find

$$\delta n = 2\mathcal{N}(0)\delta\mu - F_0^S\delta n \ \Leftrightarrow \ \frac{\delta n}{\delta\mu} = \frac{\mathcal{N}(0)}{1+F_0^S} \ .$$

For the noninteracting system one can do an equivalent calculation, which leads to t compressibility $\kappa^{(0)}$ and with the relation between the density of states of the Fermi liquid and the noninteracting gas we arrive at the final expression

$$\boxed{\kappa = \frac{1}{n^2}\frac{2}{\mathcal{N}(0)}1 + F_0^S = \frac{m^*/m}{1+F_0^S}\kappa^{(0)}}$$

The important things are, that we again find a renormalisation $\propto m^*/m$ with respect the as for the specific heat. The novel aspect however is that a further renormalisation occurs due to the quasi particle interactions. In fact, dependeing on the sign of F_0^S, this can lead to a sizeable change in κ. Moreover, if $F_0^S \leq -1$, the above expression leads to a divergence of κ or a negative sign. This immediately tells us that the Fermi liquid is instable and the whole concept of quasi particles breaks down.

3. From the Fermi gas we know already that the susceptibility is another important quantity. To calculate it we apply a small external field $\vec{B} = b\vec{e}_z$ and obtain

$$\delta\epsilon_{\vec{k}\sigma} = -g\mu_B b\sigma\frac{\hbar}{2} + \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} \quad .$$

Again we use

$$\delta n_{\vec{k}\sigma} = \left(-\frac{\partial n_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}\sigma}}\right)(\delta\mu - \delta\epsilon_{\vec{k}\sigma})$$

and observe that $\delta\mu$ cannot depend on the sign of b. Hence, $\delta\mu \propto b^2$, which we can ignore $\delta\mu$ in leading order in b. Therefore, $\delta n_{\vec{k}\sigma} \propto \delta\epsilon_{\vec{k}\sigma}$ and then $\delta n_{\vec{k}\uparrow} = -\delta n_{\vec{k}\downarrow}$. For a given σ the quasi particle interaction part then becomes

$$\sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} = \sum_{\vec{k}'}\left(f_{\vec{k}\sigma;\vec{k}'\sigma} - f_{\vec{k}\sigma;\vec{k}'\bar{\sigma}}\right)\delta n_{\vec{k}'\sigma} = \frac{F_0^A}{\mathcal{N}(0)}\delta n_\sigma \quad .$$

Note that here naturally F_0^A comes into play.

With this result we have

$$\begin{aligned}
\delta n_\sigma &= \frac{1}{V}\sum_{\vec{k}}\delta n_{\vec{k}\sigma} = -\frac{1}{V}\sum_{\vec{k}}\left(-\frac{\partial n_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}\sigma}}\right)\delta\epsilon_{\vec{k}\sigma} \\
&= -\left(-g\mu_B b\sigma\frac{\hbar}{2} + \frac{F_0^A}{\mathcal{N}(0)}\delta n_\sigma\right)\mathcal{N}(0) \\
\delta n_\sigma &= g\mu_B b\sigma\frac{\hbar}{2}\frac{\mathcal{N}(0)}{1+F_0^A} \quad .
\end{aligned}$$

For the difference of up and down changes one then obtains

$$\delta n_\uparrow - \delta n_\downarrow = \frac{g\mu_B\hbar}{2}\frac{\mathcal{N}(0)}{1+F_0^A}\,b$$

and with the magnetization given by $m = \frac{g\mu_B\hbar}{2}(n_\uparrow - n_\downarrow)$ the expression for the susceptibility becomes

$$\chi_P = \frac{\partial m}{\partial b} = \left(\frac{g\mu_B\hbar}{2}\right)^2 \frac{\mathcal{N}(0)}{1+F_0^A} = \frac{m^*/m}{1+F_0^A}\chi_P^{(0)}$$

As for the compressibility, we again observe two distinct contributions to the renormalisation with respect to the noninteracting electron gas: One from the effective mass and a second from the quasi particle interactions. If we calculate now the Wilson ratio (2.2), we find

$$R_W = \ldots = \frac{1}{1+F_0^A} \quad .$$

It is thus important to note that the Fermi gas value $R_W = 1$ can easily be changed to values of the order $1 \ldots 10$ by the quasi particle interactions. Furthermore, we again have to require $F_0^A > -1$ in order for the Fermi liquid concept to be valid. Otherwise we will in general observe a magnetic instability.

4. Let us now ask how the effective mass is related to the true electron mass. This can be achieved by invoking Galileian invariance, i.e. according to Noether the conservation of the momentum of center of mass.

   Let us assume we change the momentum of an electron by $\vec{k} \to \vec{k} + \delta\vec{k}$. The change in quasi particle energy induced by this "kick" is then

$$\delta\epsilon_{\vec{k}\sigma} = \vec{\nabla}_{\vec{k}}\epsilon_{\vec{k}\sigma}\delta\vec{k} + \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta n_{\vec{k}'\sigma'} \quad .$$

   We now restrict to $T = 0$ and an isotropic system and use

$$\begin{aligned}
\vec{\nabla}_{\vec{k}}\epsilon_{\vec{k}\sigma} &\approx \vec{\nabla}_{\vec{k}}\epsilon^{(0)}_{\vec{k}\sigma} = \hbar^2\frac{k_F}{m^*}\frac{\vec{k}}{k} \\
\delta n_{\vec{k}\sigma} &= -\vec{\nabla}_{\vec{k}} n_{\vec{k}\sigma}\delta\vec{k} \\
&= -\frac{\partial n_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}\sigma}}\vec{\nabla}_{\vec{k}}\epsilon_{\vec{k}\sigma}\delta\vec{k} \\
&\approx \delta\left(\epsilon_{\vec{k}\sigma} - \mu\right)\frac{\hbar^2\vec{k}\cdot\delta\vec{k}}{m^*} \quad .
\end{aligned}$$

   On the other hand, Galilein invariance enforces that for real particles

$$\delta\epsilon_{\vec{k}\sigma} = \frac{\hbar^2\vec{k}\cdot\delta\vec{k}}{m} \quad .$$

   Now we invoke the fact that there must be a one-to-one correspondence between real particles and quasi particles, i.e.

$$\frac{\hbar^2\vec{k}\cdot\delta\vec{k}}{m} \stackrel{!}{=} \frac{\hbar^2\vec{k}\cdot\delta\vec{k}}{m^*} + \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma;\vec{k}'\sigma'}\delta\left(\epsilon_{\vec{k}'\sigma'} - \mu\right)\frac{\hbar^2\vec{k}'\cdot\delta\vec{k}}{m^*}$$

For $T = 0$, we now can replace $\vec{k} \cdot \delta\vec{k} \to k_F \frac{\vec{k}}{k} \cdot \delta\vec{k}$ and $\vec{k}\,' \cdot \delta\vec{k} \to k_F \frac{\vec{k}'}{k'} \cdot \delta\vec{k} = \cos\vartheta' \frac{\vec{k}}{k} \cdot \delta\vec{k}$. The latter is achieved by choosing a proper axis of reference in the sum on $\vec{k}\,'$. We thus have to evaluate

$$\sum_{l=0}^{\infty} F_0^S \int \frac{d\Omega'}{4\pi} P_l(\cos\vartheta') \cos\vartheta' = \frac{F_1^S}{3} = \frac{1}{3}\delta_{l,1}$$

and finally

$$\boxed{\frac{m^*}{m} = 1 + \frac{1}{3}F_1^S}$$

Again, we see that we have a stability criterion, namely $F_1^S > -3$ in order to have meaningful results. In general, the criterion is $F_l^S > -(2l+1)$ respectively $F_l^A > -(2l+1)$.

When one of these criteria is violated, i.e. for one specific $l \geq 0$ one has $F_l^{S,A} \leq -(2l+1)$, one finds an *instability of the Fermi liquid* towards an ordered phase with some order parameter respecting the particular symmetry. For example, if $F_0^A \to -1$, we expect a magnetically ordered phase (ferromagntism), while for $F_0^S \to -1$ charge separation occurs.

Note that these instabilities occur from within the Fermi liquid phase and usually do not destroy the quasi-particles, their physical properties rather are based on these quasi-particles. There are other situations when interactions actually prevent quasi-particles from forming. For example, as discussed in the motivation of Landau's concept, if an interaction channel becomes singular, it can prevent the Fermi liquid from forming. A particular example are interacting Fermions in one dimension, where interactions always lead to singular scattering processes and no Fermi liquid forms. The actual low-energy properties are of bosonic nature (spin- and charge-density waves), and the corresponding low-energy model is the so-called Tomonaga-Luttinger model. Systems that share its properties have been named *Luttinger liquids* by D. Haldane in the early 1980's. One-dimensional systems are hard to find and the unambiguous experimental observation of a Luttinger liquid is still pending. Systems, that do not obeye the Fermi liquid paradigms are however common nowadays, and John Mydosh has given you an abundance of examples in the Heavy Fermion compounds (see also the review [8]).

A problem in a theoretical description of these *non-Fermi liquids* found in Heavy Fermions is that up to now no real microscopic model has been found that

produces at least for a certain class of compounds the observed experiments. Moreover, before one can even think of trying to set up a model one must first understand the Fermi liquid phase, in particular its origin and what type of physical parameters can lead to its destruction. This is the aim of my lecture: To give you an idea of the fundamental physical concepts underlying the Heavy Fermi liquid and how stable it is.

Up to now we discussed the Fermi liquid at $T = 0$ or for $T \to 0$. How about the behavior at finite T? For the independent electron gas, the relations were valid up to $O(T^2)$, the corrections can be calculated from higher order terms in the Sommerfeld expansion. A similar procedure is possible here, too. However, because the quasi-particle distribution function is not a simple Fermi function any more, one can expect that corrections arise. The calculations are involved, and the final results are

$$\gamma(T) = \gamma(0) - \begin{cases} g_3 T^2 \ln T & \text{for } d = 3 \\ g_2 T & \text{for } d = 2 \end{cases}$$

for the Sommerfeld coefficient and

$$\chi_P(T) = \chi_P(0) - \begin{cases} c_3 T^2 & \text{for } d = 3 \\ c_2 T & \text{for } d = 2 \end{cases}$$

for the Pauli susceptibility. Note the characteristic non-analytic temperature dependence in the Sommerfeld coefficient. This is a consequence of residual interactions and absent in the independent electron gas. It has been neasured, for example in ^3He.

There are a lot of further consequences (see for example [8]) one can draw from the Landau picture, most of which do not need any further parameters than the effective mass and the first Landau parameters. As there is an abundance in experiments in agreement with the predictions of Landau Fermi Liquid theory for many materials, it is one of the best founded and experimentally verified theories in condensed matter physics.

Nevertheless, a *microscopic* foundation based on the Hamiltonian of a solid is yet another story. Using the tools of many-particle physics, one can actually show that under certain conditions the Fermi liquid picture can be derived [2, 5]. Although this is a particularly interesting calculation, we won't be able to follow it here. Let me just note for later reference that a very important quantity in the game is the *single-particle Green's function*

$$G_{\vec{k}\sigma}(z) := \text{Laplacetransform}\left[i\langle [\hat{c}_{\vec{k}\sigma}(t), \hat{c}^\dagger_{\vec{k}\sigma}(0)] \rangle \right]$$

where the time dependence has to be calculated in Heisenberg picture. Especially interesting is the imaginary part

$$A_{\vec{k}\sigma}(\omega) := -\frac{1}{\pi}\Im m G_{\vec{k}\sigma}(\omega + i0^+)$$

where 0^+ denotes an infinitesimal positive number. $A_{\vec{k}\sigma}(\omega)$ is called *spectral function* and its $\vec{k}$-sum

$$\mathcal{N}(\omega) = \frac{1}{V}\sum_{\vec{k}} A_{\vec{k}\sigma}(\omega)$$

the *(local) density of states* (DOS). Both are, although presently only abstract objects, also accessible by experiment, namely with photoemmission – angle-resolved (ARPES) for $A_{\vec{k}\sigma}(\omega)\cdot f(\omega)$ and angle integrated (PES) for $N(\omega)\cdot f(\omega)$, where $f(\omega)$ is Fermi's function.

Using the tools of many-particle theory, one can calculate several interesting properties from the spectral function respectively DOS, for example the momentum distribution function

$$n_{\vec{k}\sigma} = \langle \hat{c}^\dagger_{\vec{k}\sigma}\,\hat{c}_{\vec{k}\sigma}\rangle = \int_{-\infty}^{\infty} d\omega\, A_{\vec{k}\sigma}(\omega)\,\frac{1}{1+e^{\beta\omega}}$$

A more accessible form for the Green's function is obtained with *Dyson's equation* as

$$G_{\vec{k}\sigma}(z) = \frac{1}{z + \mu - \epsilon_{\vec{k}} - \Sigma_{\vec{k}\sigma}(z)}$$

with an unknown function $\Sigma_{\vec{k}\sigma}(z)$, the *self-energy*. This function contains all information about interactions and is in general hard to calculate. However, in the vicinity of the Fermi energy $z = 0$ and $\vec{k} = \vec{k}_F$ one can in some cases expand it in a Taylor series

$$\Sigma_{\vec{k}\sigma}(z) = \Sigma_{\vec{k}\sigma}(0) + z\,\left.\frac{\partial\Sigma_{\vec{k}\sigma}(z)}{\partial z}\right|_{z=0} + z^2\,\left.\frac{\partial^2\Sigma_{\vec{k}\sigma}(z)}{\partial z^2}\right|_{z=0} + \dots$$

For a Fermi liquid, the derivatives have the following properties, assuming $z = \omega + i0^+$ with $\omega \in \mathbb{R}$:

$$\begin{aligned} \Sigma_{\vec{k}\sigma}(0) &\in \mathbb{R} \\ \left.\frac{\partial\Sigma_{\vec{k}\sigma}(z)}{\partial z}\right|_{z=0} &\leq 0 \\ \left.\frac{\partial^2\Sigma_{\vec{k}\sigma}(z)}{\partial z^2}\right|_{z=0} &= -i\,\eta \text{ with } \eta > 0 \end{aligned}$$

One can obtain these results from inspecting the lowest-order contribution to the self-energy, which for the imaginary part reads (abbreviating $f(\epsilon_{\vec{k}}) \equiv f_{\vec{k}}$)

$$\Im m\Sigma_{\vec{k}\sigma}(\omega) \propto -\sum_{\vec{k}_1\vec{q}} |V(\vec{q})|^2\; f_{\vec{k}_1}\left(1 - f_{\vec{k}+\vec{q}}\right)\cdot\left(1 - f_{\vec{k}_1-\vec{q}}\right)\,\delta(\omega - (\epsilon_{\vec{k}+\vec{q}} + \epsilon_{\vec{k}_1-\vec{q}} - \epsilon_{\vec{k}_1}))$$

When we use the arguments from the motivation of Landau's theory, we again arrive at

$$\Im m\Sigma_{\vec{k}\sigma}(\omega) \propto -\left[\omega^2 + (\pi k_{\mathrm{B}}T)^2\right]$$

Since one can intepret $\Im m\Sigma_{\vec{k}\sigma}(\omega)$ as scattering rate and hence as inverse life-time, we thus have just reproduced in a more formal manner our initial result about the life-time of single-particle states in an interacting Fermi system.
Inserting the results for the self-energy into the equation for the Green's function, and introducing the abbreviations

$$\begin{aligned} Z_{\vec{k}_F} &= 1 - \left.\frac{\partial\Sigma_{\vec{k}_F\sigma}(z)}{\partial z}\right|_{z=0} \geq 1 \\ \tilde{\epsilon}_{\vec{k}} &:= \frac{1}{Z_{\vec{k}_F}}\epsilon_{\vec{k}} \\ \tilde{\mu} &= \frac{1}{Z_{\vec{k}_F}}\left(\mu - \Sigma_{\vec{k}_F\sigma}(0)\right) \end{aligned}$$

one obtains

$$\boxed{G_{\vec{k}\sigma}(z) = \frac{1}{Z_{\vec{k}_F}}\,\frac{1}{\omega + \tilde{\mu} - \tilde{\epsilon}_{\vec{k}} + i\,\eta\cdot\omega^2}} \qquad (2.7)$$

Note that the Fermi wave vector $\vec{k}_F$ is implicitely defined via

$$0 = \mu - \epsilon_{\vec{k}_F} - \Sigma_{\vec{k}_F\sigma}(0)$$

Close to the Fermi energy $\omega = 0$, the imaginary part becomes small and hence the Green's function becomes a simple pole with a weight $Z^{-1}_{\vec{k}_F}$. For the independent electron gas, the Green's function has the form

$$G^{(ni)}_{\vec{k}\sigma}(z) = \frac{1}{\omega + \mu - \epsilon_{\vec{k}} + i\,0^+}$$

and the interacting Green's function is of similar structure. The weight of the pole is however $Z^{-1}_{\vec{k}_F} < 1$, i.e. the interacting Green's function does not describe a real particle, but a particle-like object which contains only a fraction of the real particle. Hence we call the excitation described by this Green's function a quasi-particle and the factor Z^{-1} *quasi-particle weight*. Finally, close to the Fermi wave vector, we may expand $\epsilon_{\vec{k}}$ in a Taylor series as

$$\epsilon_{\vec{k}} \approx \mu + \frac{\hbar k_F}{m}\left|\vec{k} - \vec{k}_F\right|$$

and hence

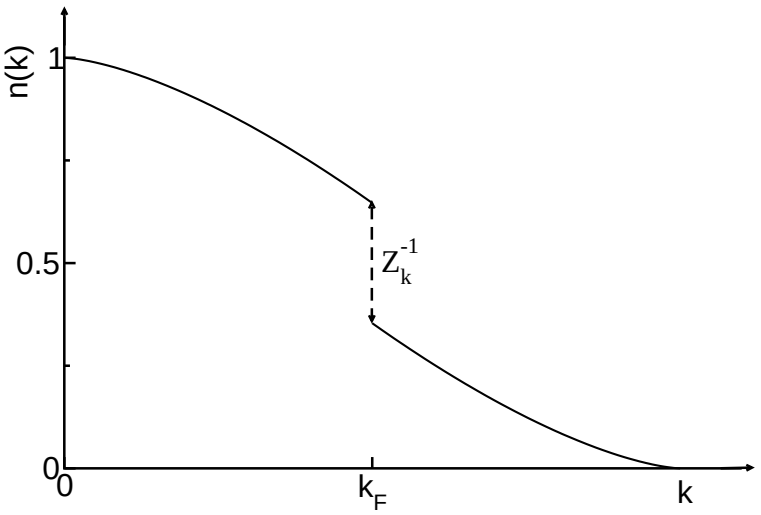
$$\tilde{\epsilon}_{\vec{k}} \approx \tilde{\mu} + \frac{\hbar k_F}{Z_{\vec{k}_F}\cdot m}\left|\vec{k} - \vec{k}_F\right|$$

From Landau's phenomenological theory we however know that $m^* = Z_{\vec{k}_F} \cdot m$ must hold, hence one also calls $Z_{\vec{k}_F}$ the *mass renormalization*. Note that we introduced a generalization of Landau's concept: The renormalizations can be $\vec{k}$-dependent.

With the approximate form (2.7) for the Green's function, one can show that the momentum distribution function $n_{\vec{k}\sigma}$ at $T = 0$ has a jump at $\vec{k}_F$, namely

$$n_{\vec{k}\searrow\vec{k}_F,\sigma} - n_{\vec{k}\nearrow\vec{k}_F,\sigma} = \frac{1}{Z_{\vec{k}_F}}$$

The behavior is shown in the figure below. Note that no statement can be



made about the curvature and actual values, except that for $\vec{k} \to 0$ we will have $n(\vec{k}) \to 1$.

To summarize, the fingerprints of a Fermi liquid from a microscopic point of view are:

- At $T = 0$, one has a jump in the momentum distribution, with a height < 1 which is the inverse effective mass of the Fermi liquid.
- The single particle self-energy in the Fermi liquid regime close to the Fermi surface has the properties

  $$\Sigma_{\vec{k}\sigma}(\omega + i0^+) \approx \Sigma_{\vec{k}_F\sigma}(0) - Z_{\vec{k}_F}\omega - i\eta_{\vec{k}_F} \cdot (\omega^2 + \pi^2 k_B^2 T^2)$$

  with $Z_{\vec{k}_F}$, $\eta_{\vec{k}_F} > 0$.

Lecture 3

Heavy Fermions

3.1 Introductory remarks

In the lecture series by John Mydosh, you have learned about the Kondo effect as a phenomenon that shows up in diluted magnetic alloys. It leads to a series of very characteristic fingerprints like the resistivity minimum and a logarithmic increase towards low temperatures or a Curie-like susceptibility with a negative offset, which becomes a constant with unusually large value at low temperature. There furthermore exists a characteristic temperature, the *Kondo temperature* T_{K}, below which these features occur, and which actually can serve as an energy scale with all properties depending on the ratio T/T_{K}, $\omega/k_{\mathrm{B}}T_{\mathrm{K}}$, etc. only.

These properties were well-known in the early seventies already, and models that showed similar behavior, the *single-impurity Anderson model* (SIAM) or the *single-impurity Kondo model* (SIKM) have been established in the early sixties already (see e.g. [4] for an overview; an older article, which gives a nice account of the understanding in the mid-seventies is G. Gruner, and A. Zawadowski, *Magnetic impurities in non-magnetic metals*, Rep. Prog. Phys. **37**, 1497 (1974)).

In the late seventies and early eighties, another class of systems fascinated the solid-state community: Based on Cerium, or later also Uranium, several compounds where discovered, that could be characterized as Fermi liquids, but they showed extremely enhanced Landau parameters. One could find effective masses that were in excess of $1000m_e$ respectively Sommerfeld coefficients larger than $1J/\mathrm{Mol}K^2$, whereas normal metals have values in the range of $mJ\mathrm{Mol}K^2$. Due to the extremely large effective mass, one coined the name Heavy Fermions (HF) for these compounds. The class of materials became even more exciting, when Steglich discovered superconductivity in the HF compound $CeCu_2Si_2$. This discovery was the more exciting, as (i) usually compounds with open d or f-shells which form local moments do not become superconducting that easily, and (ii) the heavy quasi-particles obviously were the ones that are forming the Cooper pairs, as is evident from the jump in the specific heat (see e.g. F. Steglich, *Superconductivity and magnetism in heavy-Fermion compounds*, J. Phys. Soc. Jpn. **74**, 167 (2005)). Even more fascinating, sometimes the superconducting phase is either close or even coexisting with an antiferromagnetic phase, with magnetic moments strongly reduced from the expected bare values of a Cerium $4f$ moment. Finally, during the past 15 years many HF compounds where found to be close to a *quantum critical point*, exhibiting rather peculiar features as function of temperature.

3.2 Connection of Heavy Fermions and Kondo effect

Since HF compounds contain open f-shells and hence local magnetic moments, a connection of the HF behavior and the Kondo effect in dilute magnetic alloys is suggestive. Are there any further hints that make this connection at least in the Fermi liquid phase more manifest? For a variety of Cerium compounds one is in

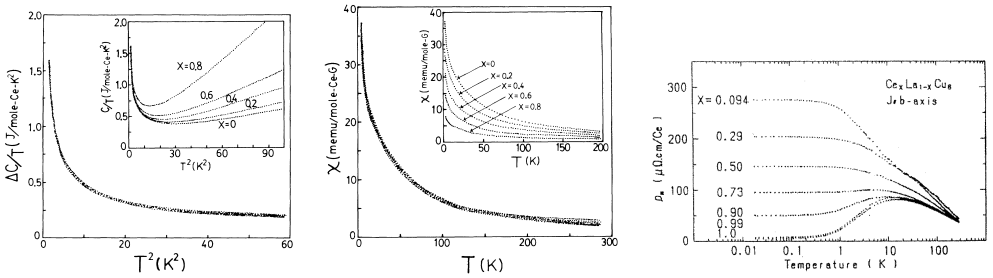


Figure 3.1: Scaling of physical properties for (La,Ce)Pb_3 respectively (La,Ce)Pb_3 (C.L. Lin, A. Wallash, J.E. Crow, T. Mihalisin, and P. Schlottmann, Phys. Rev. Lett. **58**, 1232 (1987); Y. Onuki, T. Komatsubara, J. Magn. Magn. Mater **63-64** 281 (1987)).

the fortunate situation that one can alloy them with Lanthanum, which does not have a localized f-electron. If there is a one-to-one correspondence between the HF state at full Cerium concentration and the Kondo effect at dilute, one should actually observe a scaling when going from the pure Lanthanum compound to the full Cerium. This is indeed the case, as becomes apparent from the experiments on (La,Ce)Al_3 respectively (La,Ce)Cu_6 shown in Fig. 3.1. Thus, at least as far as the Fermi liquid phase of HF compounds is concerned, the latter seem to behave like a collection of Kondo impurities and for an understanding of this phase it is obviously necessary to understand the properties of diluted magnetic impurities in metals.

As already John Mydosh told you in his lectures, there are two fundamental models that are used to theoretically describe magnetic impurities in metals [4]. The first is the single-impurity Anderson model

$$\hat{H}_{\mathrm{SIAM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_\sigma \left(\epsilon_f + \frac{U}{2} \hat{f}^\dagger_{\bar{\sigma}} \hat{f}_{\bar{\sigma}} \right) \hat{f}^\dagger_\sigma \hat{f}_\sigma + \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} \left[V_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{f}_\sigma + \mathrm{h.c.} \right]$$

and the second the single-impurity Kondo model

$$\hat{H}_{\mathrm{SIKM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} - \sum_{\vec{k}_1,\vec{k}_2} \sum_{\sigma_1,\sigma_2} J_{\vec{k}_1\vec{k}_2} \hat{\vec{S}}_f \cdot \vec{\tau}_{\sigma_1\sigma_2} \hat{c}^\dagger_{\vec{k}_1\sigma_1} \hat{c}_{\vec{k}_2\sigma_2}$$

In both models, the first term describes a band of independent fermionic (quasi-) particles with a dispersion $\epsilon_{\vec{k}}$. These "conduction electrons" are coupled to

some set of local degrees of freedom. For the Anderson model, a localized level hosting Fermions, too; for the Kondo model we have only a quantum mechanical spin $\hat{\vec{S}}$. The important aspect in the Anderson model is that if two particles are occupying this local level, one has to pay a penality $U > 0$, which is a caricature of the Coulomb repulsion. Finally, the local subsystem talk to the band electrons through a hybridization $V_{\vec{k}}$ respectively an exchange interaction $J_{\vec{k}_1\vec{k}_2}$. In the following, we will always assume $V_{\vec{k}} \equiv V$ respectively $J_{\vec{k}_1\vec{k}_2} \equiv J$.
You have already learned that the Anderson model is a complicated beast, because in Hartee-Fock approximation one finds an unphysical phase transition, which somehow has to be removed by "higher-order" processes in a perturbational sense. Likewise, the Kondo Hamiltonian leads, in low-order perturbation theory (see lectures buy John Mydosh or the book by A. Hewson [4]) to logarithmically divergent contributions. This is the so-called *Kondo problem*.
Before we try to understand some of the physics better, let us discuss an interesting limiting case for the Kondo model, viz the limit $|J| \to \infty$. One has to distinguish two cases. For one, one can have $J \to +\infty$. In this case, the spin-flip part in the exchange interaction becomes inoperative, and one can replace it by the Ising variant. Under this circumstance, the action of the spin-exchange is more or less a simple potential scattering for the conduction electrons with a strong elastic potential. The situation is different when $J \to -\infty$. Then, the system can get most out of the exchange interaction by forming a singlet between the local spin and some conduction electron at the impurity site. This becomes a *bound state* and the said conduction electron, together with the local spin, is removed from the system altogether. If one asks what the local density of states for the band-electrons *at the impurity site* then will be, the answer is quite simple: It must be zero, because the bound state has just removed the corresponding states.

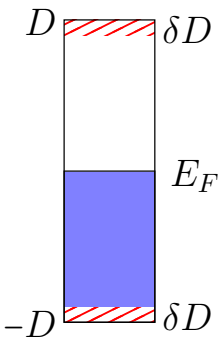
3.3 Some fundamental results

After these prelimiaries, let us try to understand what these limits have to do with the actual physics of the Kondo model, and what the Kondo and Anderson Hamiltonian have to do with each other. Let us begin with the first point. We will use an argument based on the analysis by P.W. Anderson.[1] The idea goes as follows: We start with the original Kondo Hamiltonian and "remove" the states at high energies by some procedure. This will in general lead to a theory, where the removed high-energy states generate new interactions. An

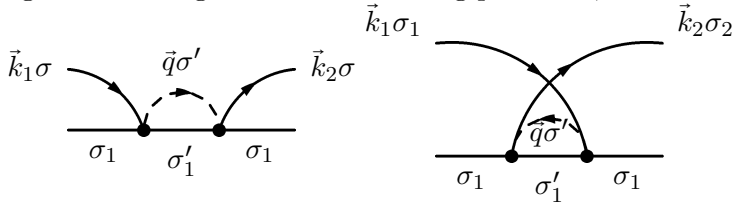
[1] *Poor man's scaling*, P.W. Anderson, Journal of Physics C: Solid State Physics **3**, 2436 (1970).

idea of the general structure can be obtained by reading papers on functional renormalization. We now *require* that the interactions generated are of the same form as the original ones, but with renormalized values. If we succeed, we can continue with this procedure until we reach the Fermi energy and have then the effective low-energy model at our hand.

To be precise, we assume that the energies of the band states are originally located within an interval $[-D, D]$ around the Fermi energy. We now reduce this interval to $[-D + \delta D, D - \delta D]$ and try to incorporate the states in the intervals $[-D, -D + \delta D]$ respectively $[D - \delta D, D]$ in effective interactions of a Kondo model living on the reduced interval, see for example the sjketch to the right.



This procedure can be fomrally be carried through by inspecting the following classes of scattering processes,



where the full lines with arrow denote band electrons from $[-D + \delta D, D - \delta D]$ and the dashes lines with arrows the ones from the "high energy states". There are several possible processes: Those that preserve the spin across the vertices and those that produce spin-flips. The former are due to action of $\hat{S}_z$ on both vertices, the latter if at least one vertex has an operator $\hat{S}^{\pm}$ associated with it. The internal momentum has to be chosen such that the integration only goes over energies $|\epsilon| \in [D - \delta D, D]$. For example, if we take the left process with $\hat{S}^+$ at the left and $\hat{S}^-$ at the right vertex, the energy in the dashed internal line is $\epsilon_{\vec{q}} \approx D$ and evaluation of the diagram leads to

$$\frac{J_\perp^2}{E - D + \epsilon_{\vec{k}_1}} |\delta D| \, \hat{S}^- \hat{S}^+ \, \hat{c}^\dagger_{\vec{k}_1\sigma_1} \hat{c}_{\vec{k}_1\sigma_1}$$

while its exchange part on the right contributes

$$\frac{J_\perp^2}{E - D - \epsilon_{\vec{k}_2}} |\delta D| \, \hat{S}^+ \hat{S}^- \, \hat{c}^\dagger_{\vec{k}_2\sigma_2} \hat{c}_{\vec{k}_2\sigma_2}$$

Note that we must allow for the exchange interaction to become anisotropic, because otherwise we cannot recast the resulting interactions into the form of the Kondo model. We thus are actually forced to study a more general Kondo

model with

$$J \to \begin{pmatrix} J_z & 0 & 0 \\ 0 & J_\perp & 0 \\ 0 & 0 & J_\perp \end{pmatrix}$$

One can construct altogether eight different of such processes. To map the resulting scattering matrix elements back to a Kondo-like Hamiltonian, one puts E and $\epsilon_{\vec{k}_i}$ onto the Fermi energy, and obtains with the requirement $J_\alpha \to J_\alpha + \delta J_\alpha$ the following set of differential equations (for a more detailed derivation see Anderson's original paper or [4])

$$\begin{aligned} \frac{dJ_\perp}{d\ln D} &= 2\mathcal{N}_F\, J_z J_\perp \\ \frac{dJ_z}{d\ln D} &= 2\mathcal{N}_F\, J_\perp^2 \end{aligned}$$

Note that by construction $\delta D < 0$!

This set of differential equations has the integral $J_\perp^2 - J_z^2 = c$. Let us start with the case $J_z > 0$, which corresponds to the *ferromagnetic* Kondo model. Since the equation for J_z contains $J_\perp^2 > 0$ on the right hand side, J_z will decrease and at some point hit $J_z = 0$. What actually happens depends now on the magnitude

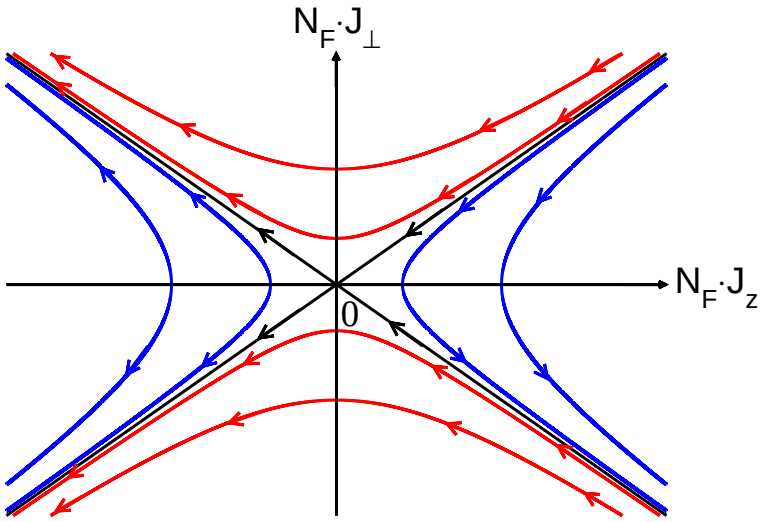


Figure 3.2: Sketch of the low of the coupling constants for the Kondo model from Anderson's poor man's scaling analysis.

and sign of $J_\perp$. If $0 < J_\perp < J_z$, the couplings $J_\perp$ will also scale to zero, and hence the effective low energy model for $J > 0$ is a model with the spin decoupled from the conduction states; this situation is called *weak-coupling fixed point*. If however $J_\perp < 0$, or $0 < J_z < J_\perp$, then $J_\perp$ scales toward ∞ and "drags" J_z along

towards $-\infty$. The low energy model in this case, as well as for the case $J_z < 0$, is the one with $J \to -\infty$, and hence an *antiferromagnetic Kondo model* with infinitely strong exchange interaction. This situation is therefore called *strong-coupling fixed point*. Note that however small $|J|$ is, as long as it is negative (antiferromagnetic coupling), it will inevitably scale to the strong coupling fixed point! The full flow of the coupling constants in the different regimes is shown in Fig. 3.2.

The physics of the strong coupling fixed point, on the other hand, is the formation of a bound state and a renormalized Fermi liquid for the band electrons, as discussed before. One can even define an energy scale $\bar{D} = k_\mathrm{B} T_\mathrm{K}$ where the value for say the renormalized $\mathcal{N}_F \cdot J_z$ exceeds a certain value and the flow predicted by the low-order equations becomes meaningless. This "Kondo temperature" is given by

$$T_\mathrm{K} \propto \exp\left[-\frac{1}{\mathcal{N}_F \cdot |J|}\right]$$

where $J < 0$ denotes the initial value of the exchange interaction. This is just the usual functional dependence of the Kondo temperature known from other approaches.

Still, we are left with two rather different models and we must decide somehow which one to use. Fortunately, there exists the work by Schrieffer and Wolff,[2] where it is shown that both models are actually equivalent. The most fortunate aspect however is, that this equivalence holds precisely in the most interesting physical regime. This happens pretty rarely in the theory of such complex systems.

Let us write the Anderson Hamiltonian as

$$\hat{H}_\mathrm{SIAM} = \hat{H}_0 + \hat{V}$$

where $\hat{H}_0$ collects the Hamiltonians of the conducution electrons and and the local f-level, and $\hat{V}$ denotes the hybridization between these subsystems. The actual mapping of Anderson's model to the Kondo model can be achieved by a canonical transformation

$$\hat{H}_\mathrm{SIKM} = e^{\hat{S}} \hat{H}_\mathrm{SIAM} e^{-\hat{S}}$$

where we require that $\hat{V} = [\hat{H}_0, \hat{S}]$. With this requirement, we remove the direct term $\hat{V}$ from the transformed Hamiltonian, i.e. the leading order in the hybridization now is $\mathrm{O}(V^2)$. The following $\hat{S}$ has the desired property:

$$\hat{S} = V \sum_{\vec{k}\sigma} \left[\frac{1 - \hat{n}_{f,-\sigma}}{\epsilon_{\vec{k}} - \epsilon_f} + \frac{\hat{n}_{f,-\sigma}}{\epsilon_{\vec{k}} - \epsilon_f - U} \right] \hat{c}^\dagger_{\vec{k}\sigma} \hat{f}_\sigma - \mathrm{h.c.}$$

[2] J.R. Schrieffer and P.A. Wolff, Phys. Rev. **149**, 491 (1966).

The next non-vanishing term of $O(V^2)$ in the expansion has a rather complicated structure at first sight. In addition to the conduction electron term, there appears

$$\hat{H}_{\text{ex}} = -\sum_{\vec{k}_1\vec{k}_2} \frac{J_{\vec{k}_1,\vec{k}_2}}{4} \left(\sum_{\sigma\sigma'} \hat{f}^\dagger_\sigma \vec{\tau}_{\sigma\sigma'} \hat{f}_{\sigma'}\right) \cdot \left(\sum_{\sigma\sigma'} \hat{c}^\dagger_{\vec{k}_1\sigma} \vec{\tau}_{\sigma\sigma'} \hat{c}_{\vec{k}_2\sigma'}\right)$$

with

$$J_{\vec{k}_1,\vec{k}_2} = V^2 \left[\frac{1}{\epsilon_{\vec{k}_1} - \epsilon_f - U} + \frac{1}{\epsilon_{\vec{k}_2} - \epsilon_f - U} - \frac{1}{\epsilon_{\vec{k}_1} - \epsilon_f} - \frac{1}{\epsilon_{\vec{k}_2} - \epsilon_f}\right]$$

a potential scattering term

$$\hat{H}_{ps} = \sum_{\vec{k}_1\vec{k}_2\sigma} \left[W_{\vec{k}_1,\vec{k}_2} + \frac{1}{2} J_{\vec{k}_1,\vec{k}_2} \hat{n}_{f,\sigma}\right] \hat{c}^\dagger_{\vec{k}_1\sigma} \hat{c}_{\vec{k}_2\sigma}$$

with

$$W_{\vec{k}_1,\vec{k}_2} = \frac{V^2}{2} \left[\frac{1}{\epsilon_{\vec{k}_1} - \epsilon_f} + \frac{1}{\epsilon_{\vec{k}_2} - \epsilon_f}\right]$$

a renormalized interaction

$$\hat{H}'_0 = \sum_{\vec{k}\sigma} \left[W_{\vec{k},\vec{k}} + \frac{1}{2} J_{\vec{k},\vec{k}} \hat{n}_{f,-\sigma}\right] \hat{n}_{f,\sigma}$$

and a term that changes the occupancy of the f-orbital by two. We are interested in the regime, where the f-occupancy $\langle \hat{n}_f \rangle = 1$, hence this term is of no importance. Similarly, the interaction and potential scattering terms are negligible or even zero. Thus, in this order and under the above assumption we are left with the first term only, which is precisely the Kondo interaction. Note that $\langle \hat{n}_f \rangle = 1$ enforces $\epsilon_f = -U/2 < 0$ and $\epsilon_f + U = U/2 > 0$. One can thus be even more specific and state that the present second order will be a good approximation to the Anderson Hamiltonian, provided that

$$\pi \mathcal{N}_F V^2 = \Gamma_0 \ll |\epsilon_f|,\ \epsilon_f + U$$

This slightly generalized version also allows for $\epsilon_f \neq -U/2$, i.e. $\langle \hat{n}_f \rangle \neq 1$. However, the derivation makes only sense if we at least assume that $|\langle \hat{n}_f \rangle - 1| \ll 1$. The final step now is to restrict all band energies to the Fermi surface, i.e. simply set $\epsilon_{\vec{k}_i} = 0$. Then, the exchange interaction becomes

$$J = -2V^2 \left[\frac{1}{\epsilon_f + U} - \frac{1}{\epsilon_f}\right] = -\frac{2V^2 U}{|\epsilon_f|(\epsilon_f + U)}$$

and particularly for the particle-hole symmetric case $\epsilon_f = -U/2$ we arrive at

$$J = -\frac{8V^2}{U} < 0$$

As this is an antiferromagnetic exchange interaction, Anderson's model in the *Kondo limit* or *strong coupling limit* therefore exhibits the Kondo effect, and one can even give an estimate for the Kondo temperature, namely

$$T_{\rm K} \propto \exp\left[-\frac{U}{8\mathcal{N}_F V^2}\right] = \exp[\left[-\frac{\pi U}{8\Gamma_0}\right]$$

That this is indeed true, and that even the prefactor is identical, we have learned in the tutorials.

3.4 The local Fermi liquid

Let us now turn to actual results for the Anderson respectively Kondo model. As far as the low-temperature or low-energy properties are concerned, we now know that both are identical. Hence, I only make a distinction when it becomes necessary. In Fig. 3.3 I show the behavior of several thermodynamic quantities,

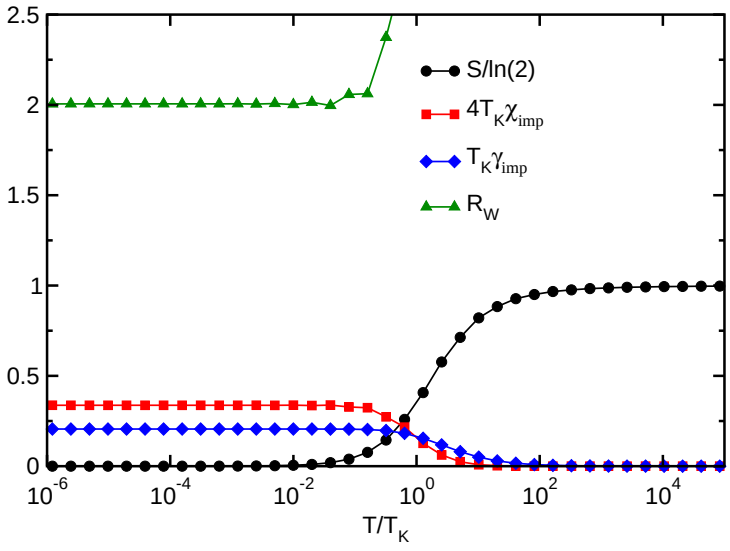


Figure 3.3: Entropy, local spin susceptibility and Sommerfeld coefficient for the SIAM as function of $T/T_{\rm K}$. The triangles are the Wilson ratio.

namely the entropy, the local magnetic susceptibility mutliplied by $T_{\rm K}$ and the Sommerfeld coefficient, also scaled by $T_{\rm K}$. The latter are both of order one, i.e. they show an enhancement relative to the non-interacting model (try and calculate these quantities) by a common factor $T_{\rm K}^{-1}$. Within a Fermi liquid picture this means that the effective mass is $m^* \propto T_{\rm K}^{-1}$. Furthermore, the Wilson ratio R_W has the value $R_W = 2$ as $T \to 0$, hence both γ and χ are enhanced due to the same physical processes. The additional enhancement of χ points toward a Landau parameter $F_0^A = -\frac{1}{2} > -1$, i.e. enhanced magnetic correlations in the

Fermi liquid. This is, up to now, consistent with our expectation from a Landau Fermi liquid. The only disturbing thing is that we only have an impurity system here. P. Nozières was the first to view such behavior as generalizations of the standard Fermi liquid theory for lattice models and coined the name *local Fermi liquid* for it. Let us see if our other "fingerprints" are present, too. To this end we need the self-energy of the local Green's function for the f-electrons. For a value $U = 10\pi\Gamma_0$ we see the result in Fig. 3.5. Quite obvioulsy, there is

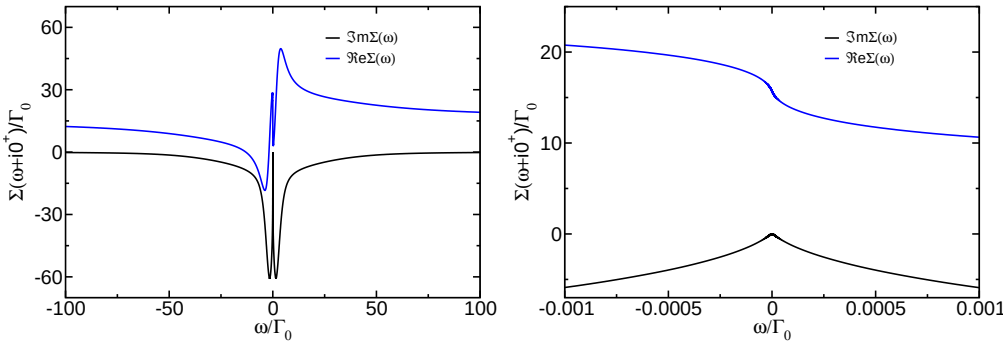


Figure 3.4: Self-energy (real and imaginary part) of the SIAM for $U = 10\pi\Gamma_0$ as function of ω/Γ_0. Left: Overall view. Right: Magnified view around $\omega = 0$.

a strong energy dependence to the self-energy, and in the blow-up in the right panel one sees a nice parabolic structure at low energies in the imaginary part. The real part definitely has a negative slope around $\omega = 0$, but to what extent it shows a linear behavior is not really evident. To this end we magnify the real part around the Fermi energy even more, and obtain Fig. **??**. Indeed, we have a nice linear behavior for $\omega \to 0$, and a linear fit gives a nice agreement in this region. The slope here is -49370, i.e. we expect an effective mass $m^* = 49371$ or a Kondo scale $T_K \approx 2 \cdot 10^{-5}\Gamma_0$. You may want to compare this with estimates for T_K you have obtained from say entropy.

This discussionshows nicely, that the Kondo model or Anderson model in the Kondo regime indeed can provide a Fermi liquid with extremely enhanced Fermi liquid parameters or extremely small energy scales. From this point of view, we can indeed expect that using a model based on these impurity systems for the Heavy Fermions can actually provide a good description, at least as far as the Fermi liquid phase is concerned.

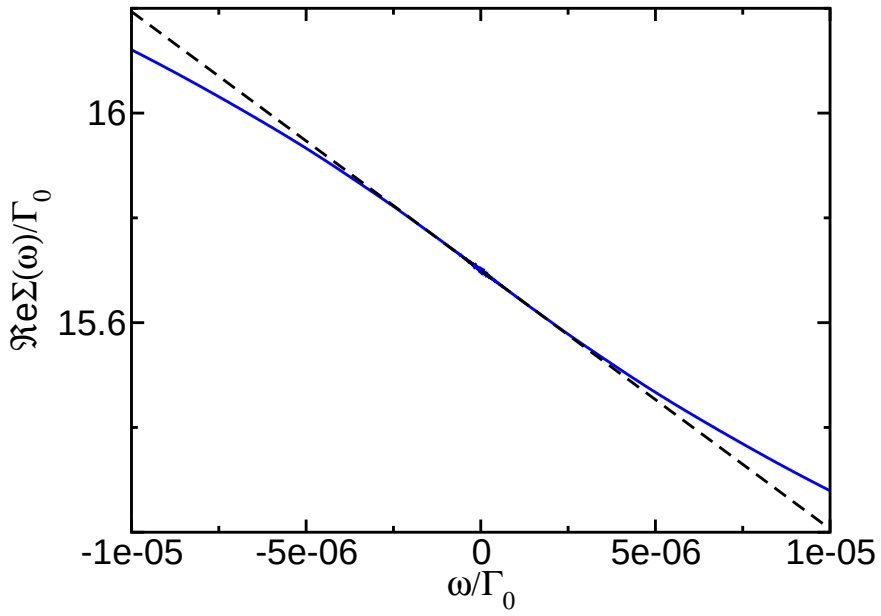


Figure 3.5: Real part of the self-energy close to $\omega = 0$. The dashed line is a linear fit to the linear regime around $\omega = 0$.

3.5 Heavy Fermions - a first attempt

Based on the previous discussion, what is a proper model for a theoretical description of Heavy Fermion compounds? A reasonable extension of the SIAM is obviously the model

$$\hat{H}_{\mathrm{PAM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_{i\sigma} \left(\epsilon_f + \frac{U}{2} \hat{f}^{\dagger}_{i\bar{\sigma}} \hat{f}_{i\bar{\sigma}} \right) \hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma} + \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} \left[V_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{f}_{\vec{k}\sigma} + \mathrm{h.c.} \right]$$

known as *periodic Anderson model* (PAM). The index i denotes the site $\vec{R}_i$ on a suitable lattice. A similar periodic extension of the Kondo model is

$$\hat{H}_{\mathrm{KLM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} - J \sum_{i} \sum_{\sigma_1,\sigma_2} \hat{\vec{S}}_i \cdot \vec{\tau}_{\sigma_1\sigma_2} \hat{c}^{\dagger}_{i\sigma_1} \hat{c}_{i\sigma_2}$$

This model is usually referred to as *Kondo lattice model* (KLM) respectively *periodic Kondo model* (PKM). Again, the index i labels the site in the lattice. In contrast to the SIAM or SIKM, we do not have an exact or even reliable numerical solution for the periodic versions. Over the past 20 years, some simple approximate methods have been developed. A particular simple and at least for $T = 0$ rather accurate method is the so-called *slave-boson mean-field theory*. This theory works easiest in the limit $U \to \infty$ of the PAM. One introduces for

each site $\vec{R}_i$ a boson $\hat{b}_i$ and writes the PAM in the limit $U = \infty$ as[3]

$$\hat{H}_{\text{PAM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_{i\sigma} \epsilon_f \hat{f}^\dagger_{i\sigma} \hat{f}_{i\sigma} + \frac{V}{\sqrt{N}} \sum_{\vec{k}\sigma} \left[\hat{c}^\dagger_{\vec{k}\sigma} \hat{b}^\dagger_i \hat{f}_{\vec{k}\sigma} + \text{h.c.} \right]$$

together with a constraint

$$\sum_\sigma \hat{f}^\dagger_{i\sigma} \hat{f}_{i\sigma} + \hat{b}^\dagger_i \hat{b}_i = 1$$

As long as we obeye this constraint on the operator level, one can indeed show that the PAM and the slave-boson model are equivalent. A simple version now is to replace $\hat{b}_i \to b \in \mathbb{R}$. and introduce the constraint in the Hamiltonian via a Lagrange multiplier, which acts as an effective chemical potential. The Hamiltonian then reads

$$\begin{aligned} \hat{H}^{MF}_{\text{PAM}} = & \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_{i\sigma} \epsilon_f \hat{f}^\dagger_{i\sigma} \hat{f}_{i\sigma} + \frac{bV}{\sqrt{N}} \sum_{\vec{k}\sigma} \left[\hat{c}^\dagger_{\vec{k}\sigma} \hat{f}_{\vec{k}\sigma} + \text{h.c.} \right] \\ & -\lambda \left(\sum_{i\sigma} \hat{f}^\dagger_{i\sigma} \hat{f}_{i\sigma} + Nb^2 - 1 \right) \end{aligned}$$

This Hamiltonian is a single-particle one an can be diagonalized immediately. The result is that one obtains (i) a renormalized position $\tilde{\epsilon}_f = +b^2$ for the f-level and (ii) a rescaling of the hybridization $V \to bV$. The mean-field parameter b is given by $b = W \cdot \exp\left[-\frac{\pi|\epsilon_f|}{2\Gamma_0}\right]$, where $\Gamma_0 = \pi \mathcal{N}_F V^2$ as before. On can now interpret the objects described by the operators $\hat{f}^{(\dagger)}_{i\sigma}$ as local quasiparticles and can then for example calculate the band-structure for the model. The generic result is shown in Fig. 3.6. One finds a rather characteristic structure, namely hybridized bands close to the Fermi energy, with a gap of order T_{K} between them. Note that this picture remains true for the more elaborate slave-boson verisons for finite U, too, and that then for the particle-hole symmetric case a full gap occurs at the Fermi level. This situation is conventionally referred to as *Kondo insulator*.

We are now nearly at the end of the possible discussions without a more elaborate many-body technique. One particularly interesting feature, however, must still be discussed, namely the question of magnetism in Heavy Fermions. Since this quite frequently occurs in real compounds and especially often also drives quantum critical begavior, understanding its origin is a rather important task. There exisits a very simple argument due to Doniach (see for example Hewson [4]). Namely, as is well known, the presence of local moments in a metal gives rise to the sol-called $RKKY$ interaction. This interaction is due to the response

[3] There also exist versions for finite U, but they are more complicated and would go beyond the scope of this lecture.

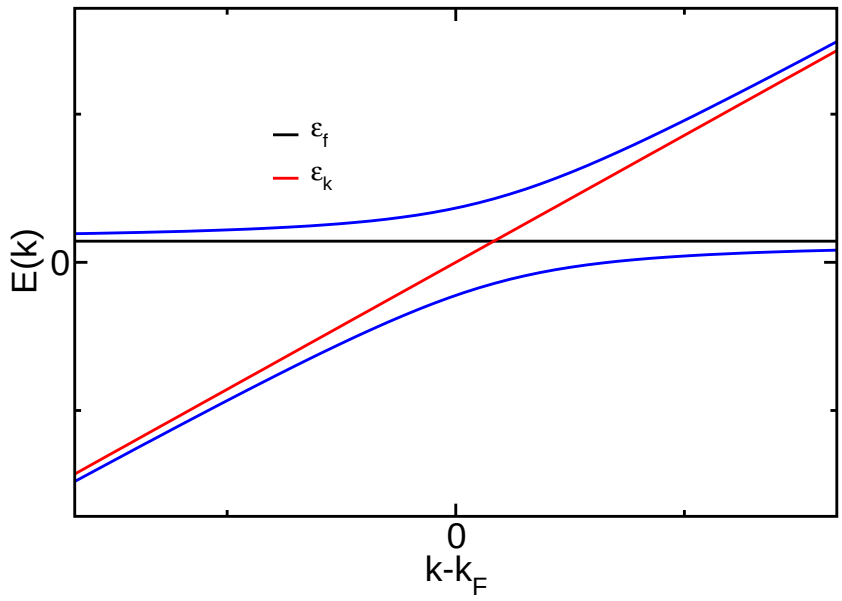


Figure 3.6: Bandstructure of the PAM in the slave-boson mean-field approximation. Note that the f-level is the effective one, shifted above the Fermi energy. The hybridization then leads to the picture of hybridized bands, with a gap between these bands across the effective f-level position. If this position is shifted to $\omega = 0$, a gap of width T_K arises, i.e. one finds a *Kondo insulator*.

of the electron gas and is proportional to J^2, because for two moments involved in the interaction process we have one factor of J coupling it to the conduction electrons. This interaction tries to stabilize magnetism (the sign depends on the band filling and can be both antiferro- and feromagnetic), and the energy scale in a mean-field estimate is proportional to the exchange constant $T_N \propto K \propto J^2$. The formation of a magnetic ground state however needs the presence of local moments. These are however screened by Kondo effect, which has a temperature scale $T_\mathrm{K} \propto e^{-1/(\mathcal{N}_F|J|)}$, assuming an antiferromagnetic Kondo exchange. Thus, for small J, the Kondo screening is exponentially suppressed and magnetism will win, while for large J Kondo will eventually screen the moments before magnetism sets in. From this argument it follows, that there should exist a critical J_c,at which magnetism vanishes. This is a quantum phase transition!

You may wonder whether this can be achieved experimentally. The answer is yes, namely by pressure. Increasing pressure will actually increase the overlap of wave functions, hence the hybridization, and thus increase J. A system where a transition from an antiferromagnet to a heavy Fermi liquid through external pressure has been observed is actually $CeCu_{6-x}Au_x$ with $x > 0.1$ [8].

Any attempt to approximately solve either the Kondo or the Anderson model in their periodic versions thus should be able to reproduce theses two effects: The formation of a heavy Fermi liquid with hybridized bands near the Fermi energy and the Doniach competition between magnetism of local moments and the Kondo screening.

3.6 DMFT treatment of the periodic Kondo model

Slides will be provided later!