Advanced quantum mechanics (20104301)
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Chapter 5: Fermi gases

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Chapter 5

Fermi gases

Fermi gases play a key role in physics. The most prominent example is that representing electrons in solid state systems, but also star models in astrophysics can be described as Fermi gaes. With small variations, we can also capture atoms in this fashion. For most of this chapter, we will think of a gas of atoms, but it should be clear that the formalism as such smoothely carries over to any other kind of Fermi gas.

5.1 Preliminary remarks

We will start from reconsidering an ideal Fermi gas exhibiting no interaction, but this time with more care. We will see that equipped with our new formalism, we can already come to a number of interesting conclusions. Then we will turn to a model of a gas of electrons featuring a Coulomb interaction. These considerations will also prepare us well for our discussion of superconductivity.

In order to describe an ideal Fermi gas in a container, it is most convenient to make use of *periodic boundary conditions*. This may not be the most natural of all boundary conditions, but it renders Fourier analysis easily available. It should also be clear that for large containers, the boundary conditions do not matter for bulk properties, and hence this seems a meaningful choice. Hence, the following single-particle wave functions seem most suitable,

$$\psi_{p,\sigma}(x,\sigma') = \frac{1}{\sqrt{V}} e^{ipx/\hbar} \delta_{\sigma,\sigma'}, \tag{5.1}$$

where σ, σ' stands for the third component of a spin and

$$p = \frac{2\pi\hbar}{L} n, \tag{5.2}$$

where $n \in \mathbb{Z}^3$ is a vector of integers. To be sure, this is the position-spin representation of the wave function, which is also why we have the Kronecker delta to the right. This quantization property follows from the boundary condition. The volume of the container is $V = L^3$ in three spatial dimension with length of each side of L. Product

like px are to be read as standard scalar products. These eigenfunctions are orthonormal as

$$\int dx \psi^*_{p,\sigma}(x,\sigma')\psi_{p',\sigma''}(x,\sigma''') = \delta_{p,p'}\delta_{\sigma,\sigma'}\delta_{\sigma',\sigma''}\delta_{\sigma'',\sigma'''}. \tag{5.3}$$

Here and in the following, the coordinates $\xi = (x,\sigma)$ are explicitly given in position and spin component. The field operators are now

$$\Psi(x,\sigma) = \sum_p \frac{1}{\sqrt{V}} e^{ipx/\hbar} f_{p,\sigma}, \tag{5.4}$$

where $f_{p,\sigma}$ denote the fermionic annihilation operators for momentum p and spin component σ. The anti-commutation relations between the fermionic field operators are

$$\{\Psi(x,\sigma), \Psi^\dagger(x',\sigma')\} = \delta_{\sigma,\sigma'} \frac{1}{V} \sum_p e^{ip(x-x')/\hbar}. \tag{5.5}$$

Now we have

$$\frac{1}{V} \sum_p e^{ip(x-x')/\hbar} = \sum_n \delta(x - x' + nL). \tag{5.6}$$

Since we are interested what happens inside the box but not in its "replicas", we find the standard fermionic anti-commutation relations.

It is worth hesitating at this point and to considering other quantities in the momentum representation. The number density operator

$$\sum_\sigma \Psi^\dagger(x,\sigma)\Psi(x,\sigma) \tag{5.7}$$

becomes under a Fourier transform to

$$\sum_\sigma \int dx \Psi^\dagger(x,\sigma)\Psi(x,\sigma)e^{-iqx} \tag{5.8}$$

and – making use of Eq. (5.4) – this becomes

$$\sum_\sigma \int dx \frac{1}{V} \sum_p \sum_k e^{-ipx} f^\dagger_{p,\sigma} f_{k,\sigma} e^{-iqx}. \tag{5.9}$$

Exploiting orthonormality, this gives

$$\sum_\sigma \sum_p f^\dagger_{p,\sigma} f_{p+q}. \tag{5.10}$$

This is the Fourier transformed number density operator, different from the number density operator in the momentum representation, which is given by $\sum_\sigma \sum_p f^\dagger_{p,\sigma} f_{p,\sigma}$.

5.2 Ground state of the ideal Fermi gas

It is now the right moment to get back to the Hamiltonian of N non-interacting fermions in a box, expressed in momentum space. This Hamiltonian is given by

$$H = \sum_k \sum_\sigma \frac{(\hbar k)^2}{2M} f^\dagger_{k,\sigma} f_{k,\sigma}. \tag{5.11}$$

Obviously, we only have a kinetic term here, and do not encounter any terms reflecting a physical interaction or external potentials. The *ground state* is now the following: Es handelt sich also lediglich im Terme der kinetischen Energie, ohne Wechselwirkungen oder

Ground state of the ideal Fermi gas: The state vector of the ground state of the non-interacting Fermi gas is given by

$$|\psi_N\rangle = \prod_{p,|p|<k_F} \prod_\sigma f^\dagger_{p,\sigma}|\emptyset\rangle. \tag{5.12}$$

This is the state in which all basis vectors with wave number up to the *Fermi* level are occupied: This is a consequence of the fact that there can only be a single fermion present in each mode. The expectation value of the particle number operator in the momentum representation is given by

$$n_{p,\sigma} = \langle\psi_N|f^\dagger_{p,\sigma} f_{p,\sigma}|\psi_N\rangle = \begin{cases} 1 & |p| \le k_F, \\ 0 & |p| > k_F \end{cases}. \tag{5.13}$$

Here, the precise value of the Fermi level has not yet been specified. We still have to determine it from the particle number. But this is very easy: For $|p| > k_F$, we have

$$\begin{aligned} f_{p,\sigma}|\psi_N\rangle &= f_{p,\sigma} \prod_{p',|p'|<k_F} \prod_{\sigma'} f^\dagger_{p',\sigma'}|\emptyset\rangle \\ &= \prod_{p',|p'|<k_F} \prod_{\sigma'} f^\dagger_{p',\sigma'} f_{p,\sigma}|\emptyset\rangle = 0. \end{aligned} \tag{5.14}$$

The total particle number is

$$\begin{aligned} N = \sum_{p,\sigma} n_{p,\sigma} &= 2 \sum_{|p|\le k_F} 1 \\ &= 2V \int_0^{k_F} \frac{dp}{(2\pi)^3} = \frac{V k_F^3}{3\pi^2}, \end{aligned} \tag{5.15}$$

And hence[1]

$$k_F^3 = \frac{3\pi^2 N}{V}. \tag{5.18}$$

[1] Here, we have used that

$$\sum_k f(k) = \sum_k \frac{\Delta}{(2\pi/L)^3} f(k) = \left(\frac{L}{2\pi}\right)^3 \int dk f(k), \tag{5.16}$$

This is the desired expression for the Fermi level in the momentum representation. The *Fermi energy* is

$$\varepsilon_F = \frac{(\hbar k_F)^2}{2M}, \tag{5.19}$$

as the energy associated with this Fermi level.

Now what is the particle density in the position representation inside the box? As a function of x this becomes

$$\begin{aligned}\sum_\sigma \langle\psi_N|\Psi^\dagger(x,\sigma)\Psi(x,\sigma)|\psi_N\rangle &= \sum_\sigma \sum_{p,p'} \frac{e^{-ipx}e^{ip'x}}{V}\langle\psi_N|f^\dagger_{p,\sigma}f_{p',\sigma}|\psi_N\rangle \\ &= \sum_\sigma \sum_{p,p'} \frac{e^{-i(p-p')x}}{V}\delta_{p,p'}\langle\psi_N|f^\dagger_{p,\sigma}f_{p',\sigma}|\psi_N\rangle \\ &= \frac{N}{V}. \end{aligned} \tag{5.20}$$

That is no surprise: The density is homogeneous (no point is distinguished), and simply given by the average particle density inside the container with volume V.

The *elementary excitations* of such a ground state are constituted by taking a particle from the Fermi ball and to place is outside the Fermi ball. Such an excited state vector is given by

$$|\phi\rangle = f^\dagger_{k_1,\sigma_2} f_{k_1,\sigma_1}|\psi_N\rangle. \tag{5.21}$$

A particle with spin σ_1 and wave number k_1 is hence exchanged by one with spin σ_2 and wave number k_2. A missing electron has the effect of a positively charged *hole* that in itself can be treated as a fermionic quasi-particle. In fact, we can define

$$a_{k,\sigma} = f^\dagger_{-k,-\sigma}, \tag{5.22}$$

$$a^\dagger_{k,\sigma} = f_{-k,-\sigma}, \tag{5.23}$$

and fine that these *hole operators* again fulfil the anti-commutation relations and can be seen as fermionic quasi-particles.

5.3 Correlations

5.3.1 Fermionic correlation functions

The fermionic correlation function is defined as follows. We can treat it as an auxiliary quantity for the pair correlation function that we will treat in the subsequent section, which is the actually more interesting quantity.

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where

$$\Delta = \left(\frac{2\pi}{L}\right)^3 \tag{5.17}$$

is the volume element in k-space (and of course no differential operator), up to an approximation error that can be made arbitrarily small.

Correlation function: The *correlation function* of a field operator in the ground state

$$G_\sigma(x-x') = \langle\psi_N|\Psi^\dagger(x,\sigma)\Psi(x',\sigma)|\psi_N\rangle \tag{5.24}$$

provides the probability density that the annihilation of a particle at position x' and the creation of a particle at x gives again the original state.

This can at the same time be seen as a transition amplitude of the unnormalized state vector[2] $\Psi(x',\sigma)|\psi_N\rangle$ – the one in which a particle has been omitted at x' – into the (equally unnormalized) state vector $\Psi(x,\sigma)|\psi_N\rangle$ (where a particle is missing at x). We will now consider such as correlation function for our free Fermi gas. We find

$$\begin{aligned} G_\sigma(x-x') &= \langle\psi_N|\sum_{p,p'}\frac{1}{V}e^{-ipx+ip'x'}f^\dagger_{p,\sigma}f_{p',\sigma}|\psi_N\rangle \\ &= \sum_p e^{-ip(x-x')}\langle\psi_N|f^\dagger_{p,\sigma}f_{p',\sigma}|\psi_N\rangle \\ &= \int\frac{dp}{(2\pi)^3}e^{-ip(x-x')}\Theta(k_F-p) \\ &= \frac{1}{(2\pi)^2}\int_0^{k_F}dpp^2\int_{-1}^{1}d\eta e^{ip|x-x'|\eta}, \end{aligned} \tag{5.26}$$

where we have made use of polar coordinates and have substituted the $\cos$. The integration over η gives rise to

$$\frac{e^{ipd}-e^{-ipx}}{ipd} \tag{5.27}$$

with

$$d = |x-x'|. \tag{5.28}$$

Hence, we find

$$\begin{aligned} G_\sigma(x-x') &= \frac{1}{2\pi^2 d}\int_0^{k_F}dpp\sin(pd) \\ &= \frac{1}{2\pi^2 d^3}(\sin(k_Fd)-k_Fd\cos(k_Fd)) \\ &= \frac{3N}{2V}\frac{\sin(k_Fd)-k_Fd\cos(k_Fd)}{(k_Fd)^3}. \end{aligned} \tag{5.29}$$

That is to say, the correlation function oscillates with a characteristic period of $1/k_F$. This may be not so much of a surprise, as this is the only scale present in momentum space. What is more, it decays to zero for large distances. The zeros in d are given by the solutions of $\tan(x) = x$.

[2] We will in a minute find that

$$\langle\psi_N|\Psi^\dagger(x,\sigma)\Psi(x,\sigma)|\psi_N\rangle = \frac{N}{2V}. \tag{5.25}$$

5.3.2 Fermionic pair correlation function

Due to the Pauli principle, even non-interacting Fermions of the same spin are in a way correlated with each other[3]. The Pauli principle forbibs that two fermions occupy the same orbital. This hard constraint is inherited by an interesting effect in the position representation. They have an effective tendency to repel each other, so that the probability of finding them in the same place is small. The Coulomb interaction (different from this), which is also repulsive, strengthens this effect even more. For the moment being, we will consider non-interacting fermions, and will only later consider particles under the additional effect of the Coulomb interaction.

There are several options to meaningfully characterized such correlations. One is by means of the pair correlation function. Let us assume we remove a particle at x from $|\psi_N\rangle$, in order to get the $N-1$ particle state vector

$$|\phi(x,\sigma)\rangle = \Psi(x,\sigma)|\psi_N\rangle. \tag{5.30}$$

Its density distribution is given by

$$\begin{aligned}\langle\phi(x,\sigma)|\Psi^\dagger(x',\sigma)\Psi(x',\sigma)|\phi(x,\sigma)\rangle &= \langle\psi_N|\Psi^\dagger(x,\sigma)\Psi^\dagger(x',\sigma')\Psi(x',\sigma')\Psi(x,\sigma)|\psi_N\rangle \\ &= \left(\frac{N}{2V}\right)^2 g_{\sigma,\sigma'}(x-x'). \end{aligned}\tag{5.31}$$

This expression defines the *pair correlation function*. It is the probability density to find a particle at x and at the same time also at x'. It can be helpful to express the pair correlation function in Fourier space. This is given by

$$\begin{aligned}\left(\frac{N}{2V}\right)^2 g_{\sigma,\sigma'}(x-x') &= \frac{1}{V^2}\sum_{k,k'}\sum_{q,q'} e^{-i(k-k')r-i(q-q')r'} \\ &\times \langle\psi_N|f^\dagger_{k,\sigma}f^\dagger_{q,\sigma'}f_{q',\sigma}f_{k',\sigma}|\psi_N\rangle. \end{aligned}\tag{5.32}$$

Let us consider two special cases separately.

- In the first case, we have that $\sigma \neq \sigma'$. That is to say, the spin component is different. Then $k = k'$ and $q = q'$ must be true to get a non-vanishing contribution. We find

$$\left(\frac{N}{2V}\right)^2 g_{\sigma,\sigma'}(x-x') = \frac{1}{V^2}\frac{N}{2}\frac{N}{2}, \tag{5.33}$$

  and hence simply

$$g_{\sigma,\sigma'}(x-x') = 1, \tag{5.34}$$

  completely regardless of the distance. This is a consequence of the rather obvious observation that fermionic particles with a different spin are not subject to the Pauli principle. Hence, they take no notice of each other.

[3] Even though they are not entangled, as one would say in the precise wording of quantum information theory.

- There is a second case, however. Here, we have that $\sigma = \sigma'$. Then there are in turn two possibilities: Either $k = k', q = q'$ or $k = q', q = k'$. We now find that

$$\begin{aligned}\langle\psi_N|f^\dagger_{k,\sigma}f^\dagger_{q,\sigma}f_{q',\sigma}f_{k',\sigma}|\psi_N\rangle &= \delta_{k,k'}\delta_{q,q'}\langle\psi_N|f^\dagger_{k,\sigma}f^\dagger_{q,\sigma}f_{q,\sigma}f_{k,\sigma}|\psi_N\rangle \\ &+ \delta_{k,q'}\delta_{q,k'}\langle\psi_N|f^\dagger_{k,\sigma}f^\dagger_{q,\sigma}f^\dagger_{k,\sigma}f_{q,\sigma}|\psi_N\rangle \\ &= (\delta_{k,k'}\delta_{q,q'} - \delta_{k,q'}\delta_{q,k'}) \\ &\times \langle\psi_N|f^\dagger_{k,\sigma}f_{k,\sigma}f^\dagger_{q,\sigma}f_{q,\sigma}|\psi_N\rangle.\end{aligned}$$

  Since $(f_{k,\sigma})^2 = 0$ it must be true at the same time that $k \neq q$, and so we get

$$\left(\frac{N}{2V}\right)^2 g_{\sigma,\sigma}(x-x') = \frac{N^2}{4V^2} - (G_\sigma(x-x'))^2. \tag{5.35}$$

  With the help of the above correlation function – and this is where it comes into play – we find in terms of the normalized distance $e = k_F|x-x'|$ the expression

$$g_{\sigma,\sigma}(x-x') = 1 - \frac{3}{e^6}\left(\sin(e) - e\cos(e)\right)^2. \tag{5.36}$$

Interestingly, the probability to find two fermions with the same spin nearby with distances smaller than$1/k_F$ is small. The suppression of $g_{\sigma,\sigma}$ on these length spaces is called *exchange hole* or *correlation hole*. If we already find a particle at x , then the conditioned probability to find another particle at the same location is reduced.

This effect is a consequence of the fermionic anticommutation relations and no effect resulting from a genuine interaction – even if the net effect is similar. Again, fermions with the same spin act as if they intended to repel each other, even in the absence of an interaction, but with the same effect. For bosons, this is different: They tend to "bunch". In the lecture, I have explained how this can be measured with thermal light. In fact, the effectively repulsive effect for fermions plays a key role in physics: Surely in the understanding of properties of materials – in fact even when showing the stability of matter. But is also determines properties of stars, to name just two examples.

5.4 Systems with Coulomb interaction

We now turn to describing fermionic systems exhibiting a Coulomb interaction. The Hamiltonian of a system of fermions interacting with a *Coulomb interaction* is in second quantization given by an expression of the following form:

Hamiltonian of electrons with Coulomb iteraction:

$$\begin{aligned} H &= \sum_{k,\sigma} \frac{\hbar^2 k^2}{2M} f^\dagger_{k,\sigma} f_{k,\sigma} \\ &+ \frac{e^2}{2V} \sum_{k,k',q,\sigma,\sigma',q\neq 0} \frac{4\pi}{q^2} f^\dagger_{k+q,\sigma} f^\dagger_{k'-q,\sigma} f_{k',\sigma'} f_{k,\sigma}. \end{aligned} \tag{5.37}$$

The first term is the known kinetic term. The second one captures the interaction. We have left out the term corresponding to $q = 0$. Why have we done that? To start with, it would surely diverge. But we also do not have to take it into account, making use of an argument of the following sort: This part is being compensated by the positively charged background, e.g., by the positive ions in a solid state system. We will now set out to derive this Hamiltonian from a microscopic model. Its Hamiltonian is given by

$$H = H_{\text{El}} + H_{\text{Ion}} + H_I, \tag{5.38}$$

capturing the dynamics of the electrons, the positively charged background, and the interactions. We will see that because of the long-ranged character of the Coulomb interaction the individual terms will diverge in the limit of large systems: The sum, however, is perfectly well-defined and non-divergent. In order to deal with these divergences, it can be helpful to define a cutoff $\mu > 0$ that should not worry us too much. We will in the last step investigate the limit of a small cutoff. In this way, we can more easily discuss the terms individually.

The Hamiltonian of the positively charged *ions* is given by

$$H_{\text{Ion}} = \frac{1}{2} e^2 \int dx dx' \frac{n(x) n(x')}{|x - x'|} e^{-\mu |x - x'|}. \tag{5.39}$$

Here, $n(x) = N/V$ simply is constant density. $\mu > 0$ is the mentioned cutoff. We hence have

$$H_{\text{Ion}} = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 V 4\pi \int_0^\infty ds s e^{-\mu s}, \tag{5.40}$$

obviously simply a number. The interactions of the electrons with the positively charged background is

$$H_I = -e^2 \sum_{j=1}^{N} \frac{N}{V} \int dx \frac{e^{-\mu(x - x_j)}}{|x - x_j|}, \tag{5.41}$$

where $\{x_j : j = 1, \ldots, N\}$ are the positions of the electrons. These are in principe one-body operators. But making use of translational invariance, we again find that this again gives rise to a number,

$$H_I = -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}. \tag{5.42}$$

Finally, the actual Hamiltonian of interest of the electrons is

$$H_{\rm El} = \sum_{j=1}^{N} \frac{p_j}{2M} + \frac{e^2}{2} \sum_{j,k=1,j\neq k}^{N} \frac{e^{-\mu|x_j - x_k|}}{|x_j - x_k|}. \tag{5.43}$$

The thermodynamic limit is the limit of $N \to \infty$ and $V \to \infty$, where N/V is held constant. We begin with the terms of ions

$$H_{\rm Ion} = \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}. \tag{5.44}$$

In the limit $\mu \to 0$ this term diverges, which again only manifests that in the thermodynamic limit because of the long-ranged nature of the interaction every ion will eventually interact with any other. Note that the interaction between ions and electrons is given by Gl. (5.42). The Hamiltonian hence is

$$H = -\frac{e^2}{2} N^2 V^{-1} 4\pi \mu^{-2} + H_{\rm El}, \tag{5.45}$$

and we can again turn to the electronic contribution, the one we are actually interested in. We will now express it in second quantization. The kinetic term is as usual

$$T = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2M} f^\dagger_{k,\sigma} f_{k,\sigma}. \tag{5.46}$$

To identify the interaction term in second quantization is obviously somewhat more tedious. The coordinates are $\xi = (p, \sigma)$, with single-body wave functions

$$\psi_{p,\sigma}(x, \sigma') = \frac{1}{\sqrt{V}} e^{ipr/\hbar} \delta_{\sigma,\sigma'}. \tag{5.47}$$

Let us recap what we need to compute the interaction Hamiltonian in second quantization. These are, for the interaction contribution V_2 of the Hamiltonian in first quantization, terms of the form

$$\begin{aligned} \langle \psi_{k_1,\sigma_1}, \psi_{k_2,\sigma_2} | V_2 | \psi_{k_3,\sigma_3}, \psi_{k_4,\sigma_4} \rangle &= \frac{e^2}{V^2} \int dx_1 dx_2 e^{-ik_1 x_1} \delta_{\sigma_1,\sigma_3} e^{-ik_2 x_2} \delta_{\sigma_2,\sigma_4} \\ &\times \frac{e^{-\mu|x_1 - x_2|}}{|x_1 - x_2|} e^{ik_3 x_1} e^{ik_4 x_2}. \end{aligned} \tag{5.48}$$

Turning to new position coordinates of the absolute position $x = x_2$ and the relative distance $y = x_1 - x_2$ we get

$$\begin{aligned} \langle \psi_{k_1,\sigma_1}, \psi_{k_2,\sigma_2} | V_2 | \psi_{k_3,\sigma_3}, \psi_{k_4,\sigma_4} \rangle &= \frac{e^2}{V^2} \int dx e^{-i(k_1 + k_2 - k_3 - k_4)x} \\ &\times \int dy e^{i(k_3 - k_1)y} \frac{e^{-\mu y}}{y} \delta_{\sigma_1,\sigma_3} \delta_{\sigma_2,\sigma_4} \\ &= \frac{e^2}{V} \delta_{\sigma_1,\sigma_3} \delta_{\sigma_2,\sigma_4} \delta_{k_1+k_2,k_3+k_4} \frac{4\pi}{(k_1 - k_3)^2 + \mu^2}. \end{aligned} \tag{5.49}$$

The Kronecker deltas result from the orthogonality of the spin wave functions. Therefore, the Hamiltonian becomes

$$\begin{aligned} H &= -\frac{1}{2}\frac{e^2N^2}{V}\frac{4\pi}{\mu^2} + \sum_{k,\sigma}\frac{\hbar^2k^2}{2M}f^\dagger_{k,\sigma}f_{k,\sigma} \\ &+ \frac{e^2}{2V}\sum_{k_1,\sigma_1}\sum_{k_2,\sigma_2}\sum_{k_3,\sigma_3}\sum_{k_4,\sigma_4}\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\delta_{k_1+k_2,k_3+k_4} \\ &\times \frac{4\pi}{(k_1-k_3)^2+\mu^2}f^\dagger_{k_1,\sigma_1}f^\dagger_{k_2,\sigma_2}f_{k_4,\sigma_4}f_{k_3,\sigma_3}. \end{aligned} \tag{5.50}$$

We will now see how we can get gid of μ in the Hamiltonian, making use of the charge neutrality. It makes a lot of sense to again change the coordinates, after all, we are perfectly free to make use of any coordinates we would like to use,

$$k_1 = k+q, \tag{5.51}$$
$$k_2 = p-q, \tag{5.52}$$
$$k_3 = k, \tag{5.53}$$
$$k_4 = p. \tag{5.54}$$

Now always $k_1+k_2 = k_3+k_4$, and $\hbar(k_1-k_3) = \hbar q$ is the momentum that is being transferred in a two-body interaction. In these coordinates, the last term of (5.50) becomes

$$\frac{e^2}{2V}\sum_{k,p,q}\sum_{\sigma_1,\sigma_2}\frac{4\pi}{q^2+\mu^2}f^\dagger_{k+q,\sigma_1}f^\dagger_{p-q,\sigma_2}f_{p,\sigma_2}f_{k,\sigma_1}, \tag{5.55}$$

again using Kronecker deltas. It makes a lot of sense to chop this expression in parts, specifically in contributions with $q\neq 0$ and those with $q=0$, that is,

$$\begin{aligned} &\frac{e^2}{2V}{\sum_{k,p,q}}'\sum_{\sigma_1,\sigma_2}\frac{4\pi}{q^2+\mu^2}f^\dagger_{k+q,\sigma_1}f^\dagger_{p-q,\sigma_2}f_{p,\sigma_2}f_{k,\sigma_1} \\ &+ \sum_{k,p}\sum_{\sigma_1,\sigma_2}\frac{4\pi}{\mu^2}f^\dagger_{k,\sigma_1}f^\dagger_{p,\sigma_2}f_{p,\sigma_2}f_{k,\sigma_1}. \end{aligned} \tag{5.56}$$

Here $\sum'$ refers to the sum in which the term $q=0$ has been omitted. The second term, that is, the one belonging to $q=0$, becomes

$$\begin{aligned} &\frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{k,p,\sigma_1,\sigma_2}f^\dagger_{k,\sigma_1}f^\dagger_{p,\sigma_2}f_{p,\sigma_2}f_{k,\sigma_1} \\ =\ &\frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{k,p,\sigma_1,\sigma_2}\left(f^\dagger_{k,\sigma_1}f_{k,\sigma_1}\left(f^\dagger_{p,\sigma_2}f_{p,\sigma_2}-\delta_{k,p}\delta_{\sigma_1,\sigma_2}\right)\right) \\ =\ &\frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{k,p,\sigma_1,\sigma_2}n_{k,\sigma_1}\left(n_{p,\sigma_2}-\delta_{k,p}\delta_{\sigma_1,\sigma_2}\right) \\ =\ &\frac{e^2}{2V}\frac{4\pi}{\mu^2}\left(N^2-N\right), \end{aligned} \tag{5.57}$$

where we have used that we have exactly N particles: We can therefore replace the number operators by the actual particle number, the respective eigenvalue of the particle number. They become numbers, the leading terms of which, linear in N^2, precisely cancel each other. The term

$$-\frac{e^2}{2V}\frac{4\pi}{\mu^2}N \tag{5.58}$$

That is to say, if we take the limits in the order of first taking $N, V \to \infty$ and then $\mu \to 0$, then the we get exacty the above Hamiltonian of electrons with Coulomb interaction. We are done.

5.4.1 Perturbation theory and stability of Fermi gases

The trouble is, there is no exact solution of this Hamiltonian: It is not a quadratic polynomial in the fermionic operators and hence no "non-interacting Hamiltonian". This is no surprise, as it is set up to capture the Coulomb interaction. Let us remind ourselves that the number of problems in quantum physics that have an exact solution is pretty small: It consists of free fermions and bosons, some stabilizer and spin models, and highly structured problems such as Bethe-solvable models. What we can make use of, needless to say, are ideas of perturbation theory. We will now compute the first order correction of the energy density. We start from the ground state vector of free Fermi gases,

$$|\psi_N\rangle = \prod_{p\leq k_F}\prod_{\sigma} f^\dagger_{p,\sigma}|\emptyset\rangle = \left(\prod_{p=0}^{k_F} f^\dagger_{p,\uparrow}\right)\left(\prod_{p=0}^{k_F} f^\dagger_{p,\downarrow}\right)|\emptyset\rangle \tag{5.59}$$

We consider the kinetic terms as the leading term and treat the interaction as a small perturbation, one that we treat in perturbation theory. The kinetic term already is diagonal, and hence we get

$$\begin{aligned}
E^{(0)} &= \langle\psi_N|\sum_{k,\sigma}\frac{\hbar^2k^2}{2M}f^\dagger_{k,\sigma}f_{k,\sigma}|\psi_N\rangle \\
&= \frac{\hbar^2}{2M}\sum_{k,\sigma}\theta(k_F-k) \\
&= \frac{\hbar^2}{2M}2\frac{V}{(2\pi)^3}\int dk k^2\theta(k_F-k) \\
&= \frac{\hbar^2}{M}\frac{V}{(2\pi)^3}4\pi\frac{1}{5}k_F^5 \\
&= \frac{3\hbar^2k_F^2}{10M}N \\
&= \frac{3}{5}\varepsilon_F N \\
&= \frac{e^2}{2a_0}\frac{1}{r_s^2}\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}N.
\end{aligned} \tag{5.60}$$

So the zeroth order contribution to the energy that only includes the kinetic term becomes

$$E^{(0)} = \frac{e^2}{2a_0}\frac{2.21}{r_s^2}N. \tag{5.61}$$

Here we have made use of the fact that

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_0^3} = \frac{3}{4\pi a_0^3 r_s^3}. \tag{5.62}$$

Here, r_0 is the radius of a ball with a volume that corresponds to the volume per particle. This is not an uncommon type of argument. One treats the systems as if they were balls filling a certain volume. The number

$$a_0 = \frac{\hbar^2}{Me^2} \tag{5.63}$$

is the *Bohr-radius*, and

$$r_s = \frac{a_0}{r_0}. \tag{5.64}$$

This number captures the density of the Fermi gas.

We can now turn to discussing the contribution of the interaction. In first order of perturbation theory the change in energy is just the expectation value of the perturbingg Hamiltonian. We hence get

$$E^{(1)} = \frac{e^2}{2V}{\sum_{k,k',q,\sigma,\sigma'}}' \frac{4\pi}{q^2}\langle\psi_N|f^\dagger_{k+q,\sigma}f^\dagger_{k'-q,\sigma'}f_{k',\sigma'}f_{k,\sigma}|\psi_N\rangle. \tag{5.65}$$

The sum $\sum'$ again means that the term with $q = 0$ has been omitted. The only term for which each annihilation operator is compensated by a creation operator (as only then we get a non-vanishing contribution), is linear in

$$\delta_{\sigma,\sigma'}\delta_{k,k'+q}f^\dagger_{k+q,\sigma}f^\dagger_{k,\sigma'}f_{k+q,\sigma'}f_{k,\sigma}. \tag{5.66}$$

This energy contribution hence becomes

$$\begin{aligned} E^{(1)} &= -\frac{e^2}{2V}{\sum_{k,q,\sigma}}' \frac{4\pi}{q^2}n_{k+q,\sigma}n_{k,\sigma} \\ &= -\frac{e^2}{2V}\sum_\sigma{\sum_{k,q}}' \frac{4\pi}{q^2}\theta_(k_F - |q+k|)\theta(f_K - k) \\ &= -\frac{3\pi e^2 V}{(2\pi)^6}\int dk\theta(k_F-k)\int dk'\frac{1}{|k-k'|}\theta(k_F-k'). \end{aligned} \tag{5.67}$$

This is an interesting expression. We compute here the overlap of two Fermi balls with relative distance q. Now we have

$$-\frac{4\pi e^2}{(2\pi)^3}\int dk'\frac{1}{|k-k'|^2}\theta(k_F-k) = -\frac{2e^2}{\pi}k_F F\left(\frac{k}{k_F}\right), \tag{5.68}$$

where the function $F : \mathbb{R}^+ \to \mathbb{R}^+$ is defined as

$$F(y) = \frac{1}{2} + \frac{1-y^2}{4y} \log \left| \frac{1+y}{1-y} \right|. \tag{5.69}$$

This means that the energy contribution becomes

$$\begin{aligned} E^{(1)} &= -\frac{e^2 k_F V}{\pi} \int_{k<k_F} \frac{dk}{(2\pi)^3} \left(1 + \frac{k_F^2 - k^2}{2kk_F} \log \left| \frac{k_F + f}{k_F - f} \right| \right) \\ &= -N \frac{3}{4} \frac{e^2 k_F}{\pi} \\ &= -\frac{e^2}{2a_0 r_s} \left(\frac{9\pi}{4} \right)^{1/3} \frac{3N}{2\pi} \\ &= -\frac{e^2}{2a_0} \frac{0.916}{r_s} N \end{aligned} \tag{5.70}$$

Thus, the first two terms are in the perturbation theory for the energy density given by

$$\frac{E}{V} = \frac{e^2}{2a_0} \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + O(1) \right). \tag{5.71}$$

The first term is that of the kinetic energy, the second the exchange term. This is an important result in that it shows that the contribution of the potential energy becomes a small perturbation when $r_s \to 0$, so in the limit of high density. The leading term in the interaction energy of electron gases of high density can indeed be described in perturbation theory. This is remarkable in the light of the facts that the interaction potential is neither small (remember that the particles are close and hence the Coulomb interaction strongest) nor short-ranged (but actually infinitely-ranged). But still, in this regime the interaction is found to be a small perturbation of the kinetic energy. The second term that captures the exchange energy is negative. The microscopic Hamiltonian has contributions of direct interaction and exchange terms. The direct term corresponds to the term with $q = 0$, and cancels with

$$H_{\text{Ion}} + H_I. \tag{5.72}$$

All that remains, therefore, is the negative exchange energy. The system is stable. We should not forget, however, that this stability and the cancellation of the $q = 0$ term is a consequence of the presence of a positive background. If one would put negatively charged electrons in a container, the system would be all but stable.

These expressions provide roughly the correct energy densities for the electron gas of metals. Most importantly, it captures the right behaviour, in that the energy density takes a minimum for some value of $r_s > 0$ and one hence arrives at a stable bound system.
[4]

[4]Der nächste Term divergiert aber logarithmisch: Wir erhalten

$$\frac{E}{N} = \frac{e^2}{a_0 r_s^2} \left(a + b r_s + c r_s^2 \log r_s + d r_s^2 + o(r_s^2) \right), \tag{5.73}$$

wobei $a, b, c, d \in \mathbb{R}$ Konstanten sind. Die genaue Berechung von c und d ist nicht einfach, aber in nichtnumerischer Weise mit elementaren Methoden möglich.

Another limit that we would like to briefly discuss is the limit $r_s \to \infty$. This is a limit that Wigner discussed first [**?**]. One can show that in principle, even smaller energy densities are possible if electrons are arranged in a *Wigner crystal*. One finds for large r_s the expression

$$\frac{E}{N} = \frac{e^2}{2a_0}\left(-\frac{1.79}{r_s} + \frac{2.64}{r_s^{3/2}} + O(r_s^{5/2})\right), \tag{5.74}$$

an expression that provides a good approximation for $r_s \gg 10$. It is indeed true that the Wigner crystal has a lower energy density as the fluid. Then the kinetic energy becomes negligible over the electrostatic energy of classical charged particles. Ions in a Penning trap show a very similar behaviour.

5.4.2 Impact of the Coulomb interaction on electron levels

As a final remark we will investigate the impact of the Coulomb interaction on the energy levels

$$\varepsilon_0(k) = \frac{(\hbar k)^2}{2M} \tag{5.75}$$

of the electrons. To recap, the Hamiltonian of an electron gas with interaction reads

$$\begin{aligned} H &= \sum_{k,\sigma} \frac{\hbar^2 k^2}{2M} f^\dagger_{k,\sigma} f_{k,\sigma} \\ &+ \frac{e^2}{2V} \sum_{p,k',q,\sigma,\sigma',q\neq 0} \frac{4\pi}{q^2} f^\dagger_{p+q,\sigma} f^\dagger_{k'-q,\sigma} f_{k',\sigma'} f_{p,\sigma}. \end{aligned} \tag{5.76}$$

We will now ask the question how the impact of the interaction could possibly be. We will do this in an unorthodox fashion, yet a simple one. We will consider a time evolution and see what the influence of interaction is. We will resort to an approximate treatment of the time evolution of fermionic operators. Again, this may look a bit weird, but quickly leads to a result.

We consider the evolution of fermionic operators in the Heisenberg picture, that is

$$\begin{aligned} \frac{\partial}{\partial t} f_{k,\sigma}(t) &= \frac{i}{\hbar}\left[\sum_{k',\sigma'} \varepsilon_0(k') f^\dagger_{k',\sigma'} f_{k',\sigma'}, f_{k,\sigma}\right] \\ &= -\frac{i}{\hbar}\sum_{k',\sigma'} \varepsilon_0(k')\{f^\dagger_{k',\sigma'}, f_{k,\sigma}\} f^\dagger_{k',\sigma'}, \end{aligned} \tag{5.77}$$

which immediately leads to

$$\frac{\partial}{\partial t} f_{k,\sigma}(t) = -\frac{i}{\hbar}\varepsilon_0(k) f_{k,\sigma}(t). \tag{5.78}$$

We define the time dependent correlation function $G_{k,\sigma}$ as

$$G_{k,\sigma}(t) = \langle \psi_N | f_{k,\sigma}(t) f^\dagger_{k,\sigma} | \psi_N \rangle. \tag{5.79}$$

The multiplication with $f^\dagger_{k,\sigma}(t)$ delivers the evolution equation for $G_{k,\sigma}$ as

$$\frac{\partial}{\partial t}G_{k,\sigma}(t) = -\frac{i}{\hbar}\varepsilon_0(k)G_{k,\sigma}(t). \tag{5.80}$$

It solution is

$$G_{k,\sigma}(t) = e^{-i\varepsilon_0(k)t/\hbar}(-n_{k,\sigma}+1), \tag{5.81}$$

since

$$\langle\psi_N|f_{k,\sigma}(0)f^\dagger_{k,\sigma}(0)|\psi_N\rangle = -n_{k,\sigma}+1. \tag{5.82}$$

The is the result without taking the Coulomb interaction into account. Doing so gives rise to

$$\frac{\partial}{\partial t}f_{k,\sigma}(t) = \frac{i}{\hbar}\left(\varepsilon_0(k)f_{k,\sigma} - \frac{1}{V}\sum_{p,q\neq 0,\sigma'}\frac{4\pi e^2}{q^2}f^\dagger_{p+q,\sigma'}f_{k+q,\sigma}f_{p,\sigma'}\right). \tag{5.83}$$

This expression results in the equation of motion of the correlation function as

$$\begin{aligned}\frac{\partial}{\partial t}G_{k,\sigma}(t) &= -\frac{i}{\hbar}\Big(\varepsilon_0(k)G_{k,\sigma}(t) \\ &- \frac{1}{V}\sum_{p,q\neq 0,\sigma'}\frac{4\pi e^2}{q^2}\langle\psi_N|f^\dagger_{p+q,\sigma'}(t)f_{k+q,\sigma}(t)f_{p,\sigma'}(t)f^\dagger_{k,\sigma}(0)|\psi_N\rangle\Big).\end{aligned} \tag{5.84}$$

An annoying observation is that on the right hand side, we no longer find the correlaton function, but also terms that contain the correlation functions in higher orders. We make use of the assumption that these expressions can be approximately written as products of lower correlators. Such truncations of infinite hierarchies are not uncommon in physics (in fact, to mention that is the secret reason for including this chapter). One basically makes a Gaussian assumption, referring to the feature that moments factor as if one had encountered a Gaussian distribution. This is good enough for our purposes, but not exact (and a rigorously minded person will ask for bounds to the errors made, which can be provided). We will here be not too pedantic, however. We will therefore assume that

$$\begin{aligned}&\langle\psi_N|f^\dagger_{p+q,\sigma'}(t)f_{k+q,\sigma}(t)f_{p,\sigma'}f^\dagger_{k,\sigma}(0)|\psi_N\rangle \\ \approx\ &\langle\psi_N|f^\dagger_{p+q,\sigma'}(t)f_{k+q,\sigma}(t)|\psi_N\rangle\langle\psi_N|f_{p,\sigma'}(t)f^\dagger_{k,\sigma}(0)|\psi_N\rangle \\ =\ &\delta_{\sigma,\sigma'}\delta_{p,k}\langle\psi_N|f^\dagger_{p+q,\sigma'}(t)f_{p+q,\sigma}(t)|\psi_N\rangle\langle\psi_N|f_{k,\sigma'}(t)f^\dagger_{k,\sigma}(0)|\psi_N\rangle\end{aligned} \tag{5.85}$$

Under this assumption – and we will now remove the $\approx$ symbols and will make use of equality signs, knowing that this is an approximation – we get the close equation of motion

$$\begin{aligned}\frac{\partial}{\partial t}G_{k,\sigma}(t) &= -\frac{i}{\hbar}\Big(\varepsilon_0(k)G_{k,\sigma}(t) \\ &- \frac{1}{V}\sum_{q\neq 0}\frac{4\pi e^2}{q^2}n_{k+q,\sigma}\Big)G_{k,\sigma}(t).\end{aligned} \tag{5.86}$$

We can read off the following expression

$$\varepsilon(k) = \frac{(\hbar k)^2}{2M} - \frac{1}{V}\sum_{k'} \frac{4\pi e^2}{|k-k'|} n_{k',\sigma}. \tag{5.87}$$

The change in ε is therefore

$$\begin{aligned}
\Delta\varepsilon(k) &= -\int \frac{dk}{(2\pi)^3} \frac{4\pi e^2}{|k-k'|} \theta(k_F - k') \\
&= -\frac{e^2}{\pi} \int_0^{k_F} ds s^2 \int_{-1}^{1} dt \frac{1}{k^2 + s^2 - 2kst} \\
&= -\frac{e^2}{\pi k} \int_0^{k_F} ds s \log \left| \frac{k+s}{k-s} \right| \\
&= -\frac{2e^2 k_F}{\pi} F\left(\frac{k}{k_F}\right),
\end{aligned} \tag{5.88}$$

where F is exactly the above function that we had encountered in (5.69). The energy levels are hence closer compared to the free Fermi gas.