2. Can we apply the free fermion approximation to a real metal?

Can we ignore interactions in a real metal? Experiments says yes (free fermion models work very well), but the theoretical answer is much more involving.

2.1. Strong interaction vs. weak interaction

Q: Does interaction get stronger when electron density is higher?

A naive answer: Interaction is proportional to $1/r$, where $r$ is the separation between two electrons. Higher density means that the average separation between electrons is smaller, so higher density means stronger interaction.

In an electron gas, the average distance between electrons $r_s$ can be estimated as

$$\frac{V}{N} = \frac{4\pi}{3} r_s^3$$

(2.1)

where $V/N$ is the average volume occupied by one electron, and the density $n$ is $n = N/V$. Thus

$$r_s = \left(\frac{3V}{4\pi N}\right)^{1/3} = \left(\frac{3}{4\pi n}\right)^{1/3}$$

(2.2)

The average Coulomb interaction one electron feels can be estimated as

$$\frac{E_{int}}{N} \propto \frac{e^2}{r_s} \propto \frac{e^2}{\left(\frac{4\pi}{3} n\right)^{1/3}} \propto n^{1/3}$$

(2.3)

Small $r_s$ (or high density $n$) means stronger interaction.

However, the truth is opposite, because

$$H = H_{\text{KE}} + H_{\text{int}}$$

(2.4)

We need to compare interaction with the kinetic energy to determine whether we have a strongly correlated system or a weakly correlated system. Strong correlation means $H_{\text{int}} \gg H_{\text{KE}}$ and weak correlation means $H_{\text{KE}} \gg H_{\text{int}}$. The total kinetic energy in a Fermi gas is also a function of $r_s$ (or say density)

$$K.E. = 2V \int_{\text{cutoff}} \frac{d^3k}{(2\pi)^3} \frac{k^2}{2m} = 2V \int_0^{k_F} \frac{k^2 dk}{4\pi^2 m} = V \frac{k_F^3}{10\pi^2 m}$$

(2.5)

The particle number is

$$N = 2V \int_{\text{cutoff}} \frac{d^3k}{(2\pi)^3} = 2V \int_0^{k_F} \frac{k^2 dk}{2\pi^2 m} = V \frac{k_F^3}{3\pi^2}$$

(2.6)
So, K.E. per particle
\[
\frac{K.E.}{N} = \frac{V \cdot \frac{4\pi}{10^3m}}{10 m} = \frac{3 k_F^2}{m r_S^2} \propto \frac{1}{m r_S^2}
\] (2.7)

More precisely,
\[
k_F = \left( \frac{3 \pi^2 N}{V} \right)^{1/3}
\] (2.8)

Comparing with \( r_S = \left( \frac{3 V}{4\pi N} \right)^{1/3} = \left( \frac{3}{4\pi n} \right)^{1/3} \)
\[
k_F = \frac{1}{r_S} \left( \frac{9 \pi}{4} \right)^{1/3}
\] (2.9)

So kinetic energy per particle is
\[
\frac{K.E.}{N} = \frac{3 k_F^2}{10 m} = \frac{3}{10} \left( \frac{9 \pi}{4} \right)^{2/3} \frac{1}{m r_S^2}
\] (2.10)

The ratio between K.E. and interaction energy,
\[
\frac{\text{Interaction}}{\text{K.E.}} \propto \frac{e^2}{r_S} \left/ \frac{1}{m r_S^2} \right. = r_S \left/ \frac{1}{m e^2 a_0} \right. = \frac{r_S}{a_0}
\] (2.11)

Here \( a_0 = 1/m e^2 = 0.529 \text{ Å} \). When \( r_S >> a_0 \) (low density), we have a strongly correlated system with the energy of interactions >> K.E. When \( r_S << a_0 \) (high density), we have a weakly correlated systems with K.E.>> interaction.

**Lower density means stronger interaction.**

### 2.1.2. Perturbation theory

In the previous chapter, we showed that the diagrammatic expansion of Feynman is in fact a power-law expansion of interaction strength \( V \). Because \( \frac{\text{Interaction}}{\text{K.E.}} \propto \frac{r_S}{a_0} \), the small parameter in this expansion is in fact \( r_S/a_0 \)

\[
G = G_0 + \sum \frac{r_S}{a_0} + \sum \left( \frac{r_S}{a_0} \right)^2 + \sum \left( \frac{r_S}{a_0} \right)^3 + \ldots
\] (2.12)

If \( r_S << a_0 \) (the high density limit), this expansion converge, i.e. higher order terms are small and can be dropped. In this regime, the free fermion approximation (ignoring interactions) is obviously a good approximation and the error bar is about \( r_S/a_0 \).

If \( r_S >> a_0 \) (the low density regime), one should use interactions the non-perturbed Hamiltonian and treat the kinetic energy as perturbation. There, to the leading order, we can set the kinetic energy to zero. The ground state is easy to find. Because electrons want to say as far away from each other as possible to reduce the interaction energy, in 2D, they just form a close pack structure (a triangular lattice). This state is known as a Wigner crystal. Please notice that it is NOT a crystal of atoms. It is a crystal made by electrons, and the lattice back ground is irrelevant here.

**Reality:** In typical metals, \( 2 < r_S/a_0 < 6 \). Neither too small, nor too large. We can not ignore interactions, neither can be ignore the kinetic energy.

With such a strong interaction, we cannot ignore interactions. So let’s go to the first order and see what we get.

### 2.2. Hartree-Fock approximation

The first order perturbation theory here is known as the Hartree-Fock approximation. In this section, we compute the first order perturbation theory using quantum field theory we learned in the previous chapter. The final conclusion of this section is, after we include the first order corrections, the theory is even worse. In fact, when we compare theoretical results with experimental data, the free fermion theory works much better, and the Hartree-Fock approximation generates wrong results. This is due to the special property of \( 1/r \) interactions.
2.2.1. Coulomb interaction in the momentum space

What is the Coulomb interaction in the k-ω space, \( V(q, i \Omega_n) \)?

\[
V(r) = \frac{e^2}{r}
\]  

(2.13)

Define \( U(r) = \frac{e}{r} \), which is the potential induced by a point charge \( e \). Maxwell told us that

\[
\nabla^2 U(r) = -4 \pi e \delta(r)
\]  

(2.14)

In q-space

\[
-q^2 U(q) = -4 \pi e
\]  

(2.15)

Therefore,

\[
U(q) = 4 \pi \frac{e}{q^2}
\]  

(2.16)

Notice that \( V(r) = e U(r) \), so \( V(q) = e U(q) \)

\[
V(q) = \frac{4 \pi e^2}{q^2}
\]  

(2.17)

This is our \( V(q, i \Omega_n) \).

\[
V(q, i \Omega_n) = V(q) = \frac{4 \pi e^2}{q^2}
\]  

(2.18)

**Note 1:** \( V(q, i \Omega_n) \) is independent of \( i \Omega_n \). This is because that Coulomb interaction is instantaneous (a good approximation in non-relativistic systems).

**Note 2:** \( V(q) \) is a singular function at \( q \to 0 \).

2.2.2. Hartree-Fock approximation

Consider these diagrams

\[
\begin{aligned}
1' & \quad 1
+ \begin{array}{c}
\text{\includegraphics[width=1cm]{diagram}}
\end{array}

\begin{array}{c}
\text{\includegraphics[width=1cm]{diagram}}
\end{array}

+ 1' & \quad 1
\end{aligned}
\]  

Using Dyson’s equation, we find that

\[
G^{HF}(k, i \omega_n) = \frac{1}{\omega - \epsilon(k) - \Sigma^{HF}(k, i \omega_n)}
\]  

(2.19)

where

\[
\Sigma^{HF}(k, i \omega_n) = \quad \begin{array}{c}
\text{\includegraphics[width=1cm]{diagram}}
\end{array} + \quad \begin{array}{c}
\text{\includegraphics[width=1cm]{diagram}}
\end{array}
\]  

\[
= \pi \int \frac{d q}{(2 \pi)^d} \frac{1}{\beta} \sum_{q \Omega} V(0, 0) G^{00}(q, i \Omega_n) - \int \frac{d q}{(2 \pi)^d} \frac{1}{\beta} \sum_{q \Omega} G^{00}(k + q, i \omega_n + i \Omega_n) V(q, i \Omega_n)
\]  

(2.20)

The first term (the Hartree term) is a constant, independent of \( k \) and \( \omega_n \). This term just shift the single particle energy \( \epsilon(k) \) by a constant, which has no physical impact. The second term (the Fock term) is more important.

\[
\Sigma_F(k, i \omega_n) =
\]  

\[
= \quad \begin{array}{c}
\text{\includegraphics[width=1cm]{diagram}}
\end{array}
\]  

\[
= -\int \frac{d q}{(2 \pi)^d} \frac{1}{\beta} \sum_{q \Omega} G^{00}(k + q, i \omega_n + i \Omega_n) V(q, i \Omega_n) = -\int \frac{d q}{(2 \pi)^d} \frac{1}{\beta} \sum_{q \Omega} G^{00}(k + q, i \Omega_n) V(q, i \Omega_n - i \omega_n)
\]  

(2.21)
Here, in the last step, we redefine \( i\Omega_n \) as \( i\Omega_n \rightarrow i\omega_n \).

### 2.3. Frequency sum

\[
\Sigma_{\mathbf{k}}(i, \omega_n) = -\int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\beta} \sum_{\omega} G^{(0)}(k + \mathbf{q}, i\Omega_n) V(q, i\Omega_n - i\omega_n)
\]  

(2.22)

The sum of frequency here \( \sum_{\omega} \) sums over all fermionic Matsubara frequencies (because \( i\Omega_n \) is the frequency of a fermionic Green’s function \( G^{(0)} \)). In general, if we consider an arbitrary function \( f(i\Omega_n) \) and sums over all fermionic Matsubara frequencies, we get

\[
\sum_{\omega} f(i\Omega_n) = \sum_{\omega} f \left( \frac{2n + 1}{\beta} \pi - i\mu \right)
\]  

(2.23)

Q: How should we compute the sum?

#### 2.3.1. Cauchy’s residue theorem

For a complex function \( f(z) \), there is a very famous and very important integral formula, known as Cauchy’s residue theorem. We can use this formula to compute the frequency sum. Let’s consider a complex function \( f(z) \) and a contour on the complex plane. We assign a direction for the contour \( \mathcal{C} \) and compute the integral \( \oint_{\mathcal{C}} f(z) \). Here, the integral is computed along the direction of \( \mathcal{C} \).

**Inside and outside:** a contour separate the complex plane into two regions: inside and outside. If we follow the direction of the contour, the region on the right hand side of the contour is called “inside” and the other side is “outside”. Notice that if we flip the direction of the contour \( \mathcal{C} \), we flip inside and outside.

**Here, we emphasize that inside and outside are relative concepts. The inside of \( \mathcal{C} \) is the same as the outside of \(-\mathcal{C}\).**

Assume that inside/outside the contour \( \mathcal{C} \), \( f(z) \) is an analytic function except for some discrete singularity points \( z_m \), at which \( f(z_m) \to \infty \). At each singularity point, we write \( f(z) \) as a power series.

\[
f(z) = \ldots + \frac{a_{-n}}{(z - z_m)^n} + \ldots + \frac{a_{-1}}{z - z_m} + a_0 + a_1(z - z_m) + \ldots + a_n(z - z_m)^n + \ldots
\]  

(2.24)

The value of \( a_{-1} \) is known as the residue at \( z_m \), \( \text{Res}(f, z_m) \). Another way to define the residue is

\[
\text{Res}(f, z_m) = \lim_{z \to z_m} (z - z_m) f(z)
\]  

(2.25)

One can prove that

\[
\oint_{\mathcal{C}} f(z) = 2\pi i \sum_{z_m \text{ inside } \mathcal{C}} \text{Res}(f, z_m)
\]  

(2.26)

and this is known as the Cauchy’s residue theorem. We can do the same thing for contour \(-\mathcal{C}\) (flip the direction of \( \mathcal{C} \))

\[
\oint_{-\mathcal{C}} f(z) = 2\pi i \sum_{z_m \text{ inside } -\mathcal{C}} \text{Res}(f, z_m)
\]  

(2.27)

Notice that \( \oint_{\mathcal{C}} f(z) = -\oint_{-\mathcal{C}} f(z) \) and inside of \(-\mathcal{C}\) is just outside of \( \mathcal{C} \),

\[
\oint_{\mathcal{C}} f(z) = -2\pi i \sum_{z_m \text{ outside } \mathcal{C}} \text{Res}(f, z_m)
\]  

(2.28)

This proves one conclusion, which we will use later

\[
\sum_{z_m \text{ inside } \mathcal{C}} \text{Res}(f, z_m) = -\sum_{z_m \text{ outside } \mathcal{C}} \text{Res}(f, z_m)
\]  

(2.29)

This singularity points are known as the poles, and thus Cauchy told us that \( \oint_{\mathcal{C}} f(z) \) are purely determined by the residue at the poles.

#### 2.3.2. Residue of the Fermi distribution function

Now consider the Fermi distribution function,