Chapter 6

The Jellium Model

Imagine we want to describe the electronic properties of a Na crystal. Each atom donates one electron to the bulk, while all the others remain tightly bound. Therefore we treat one electron per atom explicitly and represent the Na$^+$ ions as positively charged point particles at (fixed) lattice sites. To simplify the discussion we now assume these positive charges to be smeared out homogeneously over the whole crystal (jellium model). Then the Hamiltonian becomes

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k,\sigma} a_{k,\sigma} + \frac{1}{2V} \sum_{k, k', \sigma, \sigma'} V(q) a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma},$$  \hspace{1cm} (6.1)

where $\hat{v}(q) = \frac{e^2}{iq\pi}$ is the Fourier transform of the Coulomb interaction and $\varepsilon_k = \frac{(\hbar k)^2}{2m}$. The missing term $q = 0$ has been exactly compensated by the terms involving the ionic background (see exercises).

6.1 Ground state energy

Hartree-Fock approximation

In general the Hartree-Fock approximation consists in assuming a trial ground state

$$|\Psi_0\rangle = a^\dagger(\varphi_1) a^\dagger(\varphi_2) \ldots a^\dagger(\varphi_N)|0\rangle.$$  \hspace{1cm} (6.2)

Subsequently, the best set of single-particle wave functions $\varphi_i$ is determined by minimizing the expectation value of the Hamiltonian

$$E(\{\varphi_i\}) = \langle \Psi_0 | H | \Psi_0 \rangle$$  \hspace{1cm} (6.3)

with respect to $\varphi_i$, $i = 1, \ldots, N$. For the translationally invariant jellium model it is natural to choose plane waves and to make the Ansatz

$$|\Psi_0\rangle = \prod_{k, \sigma, k < k_F} \left( a^\dagger_{k, \sigma} \right) |0\rangle,$$  \hspace{1cm} (6.4)

i.e., all single-particle levels with $\varepsilon_k < \varepsilon_F$ are occupied and all levels with $\varepsilon_k > \varepsilon_F$ are empty.
The expectation value of the kinetic energy is

$$
\sum_{k, \sigma} \varepsilon_k \langle \Psi_0 | a^\dagger_{k, \sigma} a_{k, \sigma} | \Psi_0 \rangle = \sum_{k, \sigma} \varepsilon_k .
$$

(6.5)

For the Coulomb interaction we have to evaluate the term

$$
\langle \Psi_0 | a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} | \Psi_0 \rangle .
$$

(6.6)

We note that all four wave vectors have to be smaller than \( k_F \), otherwise this term vanishes. Moreover, either \( k + q = k' \) and \( k' - q = k' \) (i.e., \( q = 0 \)) or \( k + q = k' \), \( \sigma = \sigma' \) and \( k' - q = k, \sigma = \sigma' \). The first case leads to the so-called Hartree or direct Coulomb term, but since the term with \( q = 0 \) does not occur in Eq. (6.1) the Hartree term vanishes. Or more precisely: the Hartree term is compensated by the positively charged background. Indeed, here we have a product of operators all at time \( t = 0 \) so that there is no \( T \) symbol and the variational state \( | \Psi_0 \rangle \) is just the Fermi sea. Applying Wick’s theorem in the form (5.18)

$$
\langle \Psi_0 | a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} | \Psi_0 \rangle
\begin{align*}
&= a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} + a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} + a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} \\
&= a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} + a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} + a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} \\
\end{align*}
$$

The first term vanishes because

\[
\begin{align*}
& a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} = \langle \Psi_0 | a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} | \Psi_0 \rangle = 0 \\
& a^\dagger_{k', \sigma'} a_{k, \sigma} = \langle \Psi_0 | a^\dagger_{k', \sigma'} a_{k, \sigma} | \Psi_0 \rangle = 0.
\end{align*}
\]

The contractions in the second are

\[
\begin{align*}
a^\dagger_{k'-q, \sigma'} a_{k, \sigma} &= \langle \Psi_0 | a^\dagger_{k'-q, \sigma'} a_{k, \sigma} | \Psi_0 \rangle = f_{\sigma'} \delta k' - q, k = f_{\sigma'} \delta q_0 \\
a^\dagger_{k+q, \sigma} a_{k, \sigma} &= \langle \Psi_0 | a^\dagger_{k+q, \sigma} a_{k, \sigma} | \Psi_0 \rangle = f_{k, \sigma} \delta q_0.
\end{align*}
\]

This is the direct contribution to the energy which vanishes because the mode \( q = 0 \) is omitted in the Jellium Hamiltonian (6.1).

For the last term, which is the exchange contribution, we have

$$
\begin{align*}
& a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} \\
&= - a^\dagger_{k+q, \sigma} a^\dagger_{k'-q, \sigma'} a_{k', \sigma'} a_{k, \sigma} \\
&= - f_{k', \sigma'} \delta k+q, k' \delta \sigma \sigma' f_{k, \sigma} \delta k'-q, k \delta \sigma' \\
&= - f_{k', \sigma'} f_{k, \sigma} \delta k'-k, q \delta \sigma'.
\end{align*}
$$

This yields the Fock or exchange term

$$
- \frac{1}{2V} \sum_{k, k', \sigma, \sigma'} \hat{V}(k' - k),
$$

(6.7)

where the minus sign originates from the “wrong” ordering of operators in Eq. (6.6). The total energy per particle (in the limit \( V \to \infty \), \( n = \frac{N}{V} = \text{constant} \)) is obtained by adding the kinetic energy (6.5) and the exchange term (6.7)

$$
\frac{E}{N} = \frac{1}{n} \left\{ 2 \int_{k < k_F} \frac{d^3k}{(2\pi)^3} \varepsilon_k - \int_{k < k_F} \frac{d^3k}{(2\pi)^3} \int_{k < k_F} \frac{d^3k'}{(2\pi)^3} \int_{k < k_F} \frac{d^3k'}{(2\pi)^3} \varepsilon_0 |k - k'|^2 \right\}.
$$

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The integrals can be explicitly calculated and one finds

$$ E/N = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} - \frac{3e^2 k_F}{16\pi^2 \varepsilon_0}. \quad (6.8) $$

The density can be parametrized in terms of the dimensionless parameter $r_s$,

$$ n = \frac{k_F^3}{3\pi^2} = \frac{1}{4\pi} (r_s a_0)^3, \quad (6.9) $$

where $a_0$ is the characteristic length for the Coulomb interaction, the Bohr radius,

$$ a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{me^2}. \quad (6.10) $$

Eq. (6.8) can then be written as

$$ E/N = R_y \left( 2.21 r_s^{-2} - 0.916 r_s^{-1} \right), \quad (6.11) $$

where $R_y = \frac{me^4}{2(4\pi \varepsilon_0 \hbar^2)^2}$ is the Rydberg constant. The expression (6.11) has a minimum at $r_s \approx 4.8$, in remarkable agreement with the experimental values of simple metals (3.93 for Na, 4.86 for K). However, at the minimum the absolute value of the exchange energy is twice the kinetic energy, which renders the variational state, an eigenstate of the kinetic energy operator, questionable.

### Beyond Hartree-Fock

A systematic expansion of the ground state energy in powers of $e^2$, derived by Gell-Mann and Brückner in 1957, gives (see Section 5.1 of Mahan’s book for a very detailed discussion)

$$ E/N = R_y \left[ 2.21 \, r_s^{-2} - 0.916 \, r_s^{-1} + 0.0622 \log r_s ight. \
0.096 + 0 \, r_s \left] \quad (6.12) \right] $$

It indicates that $r_s$ is the expansion parameter. Therefore the Hartree-Fock approximation can only be trusted for large densities where the kinetic energy dominates. Such densities can be reached in dense plasmas or white dwarfs, but not for electrons in metals.

In the small-density limit the Coulomb interaction dominates and the system becomes unstable with respect to the formation of a Wigner crystal (Wigner 1934). A simple variational state of such a crystal would be of the form of Eq. (6.2) where the $\varphi_i$ are Wannier functions associated with the sites of the crystal lattice. Evidence for a Wigner crystal has been found for electrons on the surface of liquid helium (Grimes and Adams 1979). For a two-dimensional electron liquid the crystallization is expected to occur at $r_s = 37 \pm 5$ (Tanatar and Ceperley 1989), where $r_s$ is related to the areal density $n$ as $\pi r_s^2 = \frac{1}{n_{00}}$. Recently, some evidence for such a transition has been reported for GaAs/AlGaAs heterostructures.