

Theoretical Condensed Matter Physics
September 15, 2021

5 System of Interacting Electrons

5.1 Jellium model of metals

For ionic crystal with ion density $n = N/V$, its electronic Hamiltonian in second quantized form is

$$H = H_e + H_{ii} + H_{ie} + H_{ee} \quad (5.1)$$

where

$$H_e = \sum_s \int d^3r \psi_s^\dagger(r) \frac{p^2}{2m} \psi_s(r) \quad (5.2)$$

$$H_{ii} = \frac{1}{2} \int d^3R \int d^3R' n(R)n(R') \frac{e^2}{|R - R'|} \quad (5.3)$$

$$H_{ie} = - \sum_s \int d^3r \int d^3R \psi_s^\dagger(r) n(R) \frac{e^2}{|r - R|} \psi_s(r) \quad (5.4)$$

$$H_{ee} = \frac{1}{2} \sum_{ss'} \int d^3r \int d^3r' \psi_s^\dagger(r) \psi_{s'}^\dagger(r') \frac{e^2}{|r - r'|} \psi_{s'}(r') \psi_s(r) \quad (5.5)$$

The dynamics of ionic lattices is ignored within Born-Oppenheimer approximation. Let us apply the plane wave expansion of the electronic state function operator $\psi_s(r)$ as

$$\psi_s(r) = \frac{1}{\sqrt{V}} \sum_k c_{k,s} e^{ik \cdot r} \quad (5.6)$$

Then we have from above

$$\begin{aligned} H_e &= \sum_{kk',s} c_{k,s}^\dagger c_{k',s} \frac{1}{V} \int d^3r e^{-ik \cdot r} \left(\frac{-\hbar^2}{2m} \nabla^2 \right) e^{ik' \cdot r} \\ &= \sum_{kk',s} \frac{\hbar^2 k^2}{2m} c_{k,s}^\dagger c_{k',s} \underbrace{\frac{1}{V} \int d^3r e^{-i(k-k') \cdot r}}_{=\delta_{kk'}} = \sum_{k,s} \frac{\hbar^2 k^2}{2m} c_{k,s}^\dagger c_{k,s} \end{aligned} \quad (5.7)$$

$$H_{ii} = \frac{1}{2} N^2 \int d^3R \int d^3R' \frac{e^2}{|R - R'|} = \frac{1}{2} N^2 V(0) \quad (5.8)$$

where the ions are assumed to be uniform distribution, like a jelly.

$$\begin{aligned}
H_{ie} &= - \sum_{kk',s} c_{k,s}^\dagger c_{k',s} \underbrace{\frac{1}{V} \int d^3r \int d^3R \frac{n(R)e^2}{|r-R|} e^{i(k-k')\cdot r}}_{f_{kk'}} \\
&= \sum_{kk',s} f_{kk'} c_{k,s}^\dagger c_{k',s}
\end{aligned} \tag{5.9}$$

$$\begin{aligned}
H_{ee} &= \frac{1}{2V} \sum_{ss'} \sum_{kk'k''k'''} V(q) c_{k''',s}^\dagger c_{k'',s'}^\dagger c_{k',s'} c_{k,s} \\
&\quad \times \underbrace{\frac{1}{V} \int d^3r e^{-i(k'''-k-q)\cdot r}}_{\delta_{k'''=k+q}} \underbrace{\frac{1}{V} \int d^3r' e^{-i(k''-k'+q)\cdot r}}_{=\delta_{k''=k'-q}} \\
&= \frac{1}{2V} \sum_{k,k',q,s,s'} V(q) c_{k+q,s}^\dagger c_{k'-q,s'}^\dagger c_{k',s'} c_{k,s}
\end{aligned} \tag{5.10}$$

after we have applied the Fourier transformation of the potential

$$V(r-r') = \frac{1}{V} \sum_q V(q) e^{iq\cdot(r-r')}, \quad V(r-r') = \frac{e^2}{|r-r'|} \rightarrow V(q) = \frac{4\pi e^2}{q^2}$$

Next let us calculate the quantum expectation of these Hamiltonian with electronic ground state

$$|\Omega\rangle = \prod_s \prod_{k \leq k_F} c_{k,s}^\dagger |0\rangle, \tag{5.11}$$

$$\langle \Omega | c_{k,s}^\dagger c_{k,s} | \Omega \rangle = n_{k,s} = \begin{cases} 1, & 0 < k \leq k_F \\ 0, & k > k_F \end{cases} \tag{5.12}$$

Then we have

$$E_{kin} = \sum_{k,s} \frac{\hbar^2 k^2}{2m} \langle \Omega | c_{k,s}^\dagger c_{k,s} | \Omega \rangle = \sum_{k,s} \frac{\hbar^2 k^2}{2m} n_{k,s} \tag{5.13}$$

and

$$E_{ii} = \frac{1}{2} N^2 V(0) \tag{5.14}$$

$$E_{ie} = - \sum_{k,k',s} f_{kk'} \langle \Omega | c_{k,s}^\dagger c_{k',s} | \Omega \rangle = - \sum_{k,k',s} f_{kk'} n_{k,s} \delta_{kk'} = -N^2 V(0) \tag{5.15}$$

$$E_{ee} = \frac{1}{2V} \sum_{k,k',q} \sum_{s,s'} V(q) \langle \Omega | c_{k+q,s}^\dagger c_{k'-q,s'}^\dagger c_{k',s'} c_{k,s} | \Omega \rangle \quad (5.16)$$

Since

$$\begin{aligned} c_{k+q,s}^\dagger c_{k'-q,s'}^\dagger c_{k',s'} c_{k,s} &= c_{k+q,s}^\dagger \left(\delta_{k'-q,k'} - c_{k',s'} c_{k'-q,s'}^\dagger \right) c_{k,s} \\ &= \delta_{q=0} c_{k+q,s}^\dagger c_{k,s} - c_{k+q,s}^\dagger c_{k',s'} c_{k'-q,s'}^\dagger c_{k,s} \\ &= \delta_{q=0} c_{k+q,s}^\dagger c_{k,s} - \delta_{k+q,k'} \delta_{ss'} c_{k'-q,s'}^\dagger c_{k,s} \\ &\quad + c_{k',s'} c_{k+q,s}^\dagger c_{k'-q,s'}^\dagger c_{k,s} \end{aligned} \quad (5.17)$$

From (16), we will have

$$E_{ee} = \frac{1}{2} N^2 V(0) - \frac{1}{2V} \sum_{q=k-k'} \sum_{k,k',s} V(q) n_{k,s} n_{k',s} \quad (5.18)$$

where the first part is direct Coulomb interaction energy, and the second part is the exchange interaction energy. Let us write

$$E_{ee} = \sum_k E_k \rightarrow E_k = \frac{\hbar^2 k^2}{2m} - \frac{2\pi e^2}{V} \sum_{k' \leq k_F} \frac{1}{|k-k'|^2} \quad (5.19)$$

$$\rightarrow E_k = \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} F(x), \quad x = \frac{k}{k_F} \quad (5.20)$$

where

$$\begin{aligned} \frac{1}{V} \sum_{k' \leq k_F} \frac{1}{|k-k'|^2} &= \frac{1}{(2\pi)^3} \int_{k' \leq k_F} d^3 k' \frac{1}{k^2 + k'^2 - 2kk' \cos \theta'} \\ &= \frac{1}{4\pi^2} \int_0^{k_F} dk' k'^2 \int_{-1}^{+1} d \cos \theta' \frac{1}{k^2 + k'^2 - 2kk' \cos \theta'} \\ &= \frac{1}{4\pi^2} \int_0^{k_F} dk' k'^2 \frac{1}{kk'} \ln \left| \frac{k+k'}{k-k'} \right| = \frac{1}{4\pi^2 k} \int_0^{k_F} dk' k' \ln \left| \frac{k+k'}{k-k'} \right| \\ &= \frac{1}{4\pi^2} \left(\frac{k_F^2 - k^2}{k} \ln \left| \frac{k_F+k}{k_F-k} \right| + 2k_F \right) \\ &= \frac{k_F}{\pi^2} \left(\frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right| + \frac{1}{2} \right) = \frac{k_F}{\pi^2} F(x) \end{aligned} \quad (5.21)$$

See figures (5.1) and (5.2).

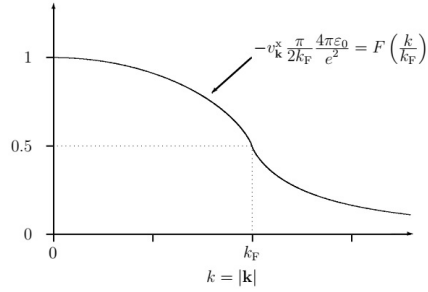


Figure 5.1: Graph of $F(x)$ function.

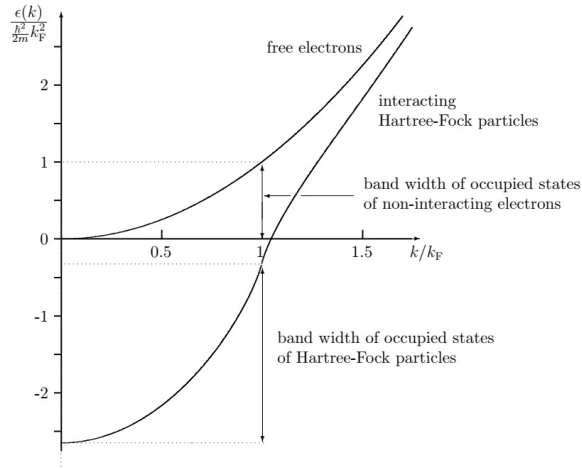


Figure 5.2: Electron spectrum in Jellium model.

5.2 Screening effect

Let us define a local electron density in the bulk as

$$n(r_{bulk}) \simeq \int_0^{\epsilon_F} N(\epsilon) d\epsilon \quad (5.22)$$

and assume one electron is an extra from the bulk, so it perturbs the system with extra potential $+e\delta V(r)$ and produces the variation of local density

$$\delta n(r) \simeq \int_0^{\epsilon_F + e\delta V(r)} N(\epsilon) d\epsilon - \int_0^{\epsilon_F} N(\epsilon) d\epsilon \simeq eN_0\delta V(r) \quad (5.23)$$

$$\rightarrow \nabla^2 \delta V(r) = 4\pi e \delta n(r) = 4\pi e^2 N_0 \delta V \quad (5.24)$$

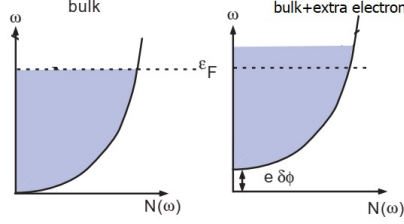


Figure 5.3: Electron density variation.

See figure (5.3). In spherical system $\nabla\delta V = r^{-2}d_r(r^2d_rV(r))$, so that

$$d_r^2\delta V(r) + \frac{2}{r}d_r\delta V(r) = \underbrace{4\pi e^2 N_0}_{\kappa^2}\delta V(r) = \kappa^2\delta V(r) \quad (5.25)$$

$$\rightarrow \delta V(r) = -2e\frac{e^{-\kappa r}}{r} \quad (5.26)$$

So that the extra electron feels screening Coulomb potential from the surround electrons, with screening length

$$l = \frac{1}{\kappa} \quad (5.27)$$

Since $k_F = (3\pi^2n)^{1/3}$, $a_0 = \hbar^2/me^2$, and $N_0 = mk_F/\hbar^2\pi^2$, then we have

$$\kappa^2 = \frac{a_0\pi}{4(3\pi^2n)^{1/3}} \simeq \frac{a_0}{4n^{1/3}} \rightarrow l \simeq \frac{1}{2}(a_0^3/n)^{1/6} \quad (5.28)$$

5.3 Dielectric function

From electrostatic, the external potential $V_{ext}(r, t)$ will be related to potential in the bulk $V(r, t)$ by the dielectric function ϵ , in Fourier space, as

$$V_{ext}(k, \omega) = \epsilon(k, \omega)V(k, \omega) \quad (5.29)$$

On the other hand, the potential in the bulk may be determined from the combination of the external potential and the induced potential as

$$V = V_{ind} + V_{ext} \quad (5.30)$$

where the induced potential arise from the electron density fluctuation in the bulk as

$$\nabla^2 V_{ind} = -4\pi\delta\rho_{ind} \rightarrow k^2 V_{ind} = 4\pi\delta\rho_{ind} \quad (5.31)$$

$$\text{where } \delta\rho_{ind} = e^2\chi V_{ext} \rightarrow V_{ind} = \frac{4\pi e^2}{k^2}\chi V_{ext} \quad (5.32)$$

From above we will have

$$\epsilon(k, \omega) = \frac{1}{1 + \frac{4\pi e^2}{k^2} \chi(k, \omega)} \quad (5.33)$$

where χ is known as density-density correlation function.

5.4 Plasma oscillation

5.5 Friedel oscillation

5.6 Fermi liquid theory

Appendix: Correlation function

There are at least two kinds of quantum operators in quantum mechanics. Schrodinger operator O_S is time-independent, its quantum expectation value is derived from time-dependent state function $|\psi(t)\rangle$ from Schrodinger equation

$$i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle, \quad H \neq H(t) \quad (5.34)$$

$$\langle O \rangle(t) = \langle \psi(t) | O_s | \psi(t) \rangle \quad (5.35)$$

Heisenberg operator $O_H(t)$ is time dependent and is related to Schrodinger operator through similarity transformation and satisfy Heisenberg equation

$$O_H(t) = U^\dagger(t) O_s U(t), \quad U(t) = e^{-iHt/\hbar} \quad (5.36)$$

$$i\hbar\partial_t O_H(t) = [O_H(t), H] \quad (5.37)$$

Its quantum expectation value is derived from time-independent Heisenberg state $|\psi(0)\rangle$ as

$$\begin{aligned} |\psi(t)\rangle = U(t)|\psi(0)\rangle \rightarrow \langle O \rangle(t) &= \langle \psi(0) | U^\dagger(t) O_s | U(t) | \psi(0) \rangle \\ &= \langle \psi(0) | O_H(t) | \psi(0) \rangle \end{aligned} \quad (5.38)$$

Let $n(r)$ be local number density operator, its Heisenberg operator is $n(r, t) = e^{iHt/\hbar} n(r) e^{-iHt/\hbar}$. The density correlation function is defined to be

$$\chi(t, t') = -i\langle [n(t), n(t')] \rangle \theta(t - t') \quad (5.39)$$