Electron Gas with Coulomb Interaction

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It is said that for a simple demonstration of what happens in a metal, we can only work with the jellium model, ignoring the details of the lattice, which means we can just work with a non-relativistic electron gas with Coulomb interaction. This article is an extension of Section 6.2 in this solid state physics note. We will discuss some early development of RPA. Zhengzhong Li, Sec. 4.2

1 Notations and basic facts about the jellium model

We define

$$\rho(\boldsymbol{r}) = \sum_\sigma \psi^\dagger_\sigma(\boldsymbol{r})\psi_\sigma(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \frac{1}{V}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}+\boldsymbol{q},\sigma}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}, \tag{1}$$

and the commutation relations are

$$[c_{\boldsymbol{k}}, c^\dagger_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k}\boldsymbol{k}'}. \tag{2}$$

We can also write down $\rho(\boldsymbol{r})$ in the first quantization formulation, i.e.

$$\rho(\boldsymbol{r}) = \sum_i \delta(\boldsymbol{r}-\boldsymbol{r}_i) = \sum_i \frac{1}{V}\sum_{\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)} = \frac{1}{V}\sum_{\boldsymbol{q}}\sum_i \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)}. \tag{3}$$

We have

$$\rho_{\boldsymbol{q}} := \sum_i \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i} = \sum_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}+\boldsymbol{q},\sigma}, \quad \rho(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{q}}\rho_{\boldsymbol{q}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}. \tag{4}$$

Easily, we find

$$\rho_{\boldsymbol{q}=0} = \int \mathrm{d}^3\boldsymbol{r}\,\rho(\boldsymbol{r}) = N. \tag{5}$$

The Hamiltonian of electrons is

$$H_{\text{electron}} = \sum_{\boldsymbol{k},\sigma}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + \frac{1}{2V}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma'} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}V(q)c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma},$$

where

$$V(q) = \int \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\frac{e^2}{r} = \frac{4\pi e^2}{\boldsymbol{q}^2}. \tag{6}$$

The Hamiltonian of the lattice and the electron-lattice coupling is

$$H_{\text{lattice}} = \frac{1}{2V}\sum_{\boldsymbol{q}}\rho_{\text{ion},-\boldsymbol{q}}V(q)\rho_{\text{ion},\boldsymbol{q}} - \frac{1}{V}\sum_{\boldsymbol{q}}\rho_{\text{ion},\boldsymbol{q}}V(q)\rho_{\boldsymbol{q}}.$$

When $|\boldsymbol{q}| = 0$, $V(q)$ is divergent, but this does not matter. In the jellium model, the only non-zero Fourier component of $\rho_{\text{ion}}(\boldsymbol{r})$ is $\rho_{\text{ion},\boldsymbol{q}=0} = N$ (the solid is neutral so the number of positive charges must be equal to the number of negative charges), and we soon find

$$H_{\text{lattice}} + \frac{1}{2V}\sum_{\boldsymbol{q}=0,\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}V(q)c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma} = 0.$$

So all divergences cancel with each other, and in the end, the total Hamiltonian is

$$\begin{aligned} H &= \sum_{\boldsymbol{k},\sigma}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + \frac{1}{2V}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}V(q)c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma} \\ &= \sum_{\boldsymbol{k},\sigma}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + \frac{1}{2V}\sum_{\boldsymbol{q}\neq 0}\rho^\dagger(\boldsymbol{q})V(q)\rho(\boldsymbol{q}). \end{aligned} \tag{7}$$

The contribution of the positive ion "jell" both constrains the electrons in the solid (or in other words, give a chemical potential) and regularize the singularity of $V(\boldsymbol{q}=0)$.

Note that (7) differs with

$$H=\sum_i \frac{\boldsymbol{p}_i^2}{2m}+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\boldsymbol{r}_i-\boldsymbol{r}_j|} \tag{8}$$

with the $i=j$ term. This is an infinite constant and does not matter.

2 Classical (or first quantized) theory of the collective oscillation of electrons

From (4), we have

Zhengzhong Li, Sec. 4.3

$$\begin{aligned}\dot{\rho}_{\boldsymbol{q}}&=\sum_j(-\mathrm{i}\boldsymbol{q})\cdot\boldsymbol{v}_j\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j},\\ \ddot{\rho}_{\boldsymbol{q}}&=\sum_j(-\mathrm{i}\boldsymbol{q}\cdot\dot{\boldsymbol{v}}_j-(\boldsymbol{q}\cdot\boldsymbol{v}_j)^2)\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}.\end{aligned} \tag{9}$$

Now $\dot{\boldsymbol{v}}_j$ can be derived from (7):

$$\begin{aligned}m\dot{\boldsymbol{v}}_j&=-\boldsymbol{\nabla}_j\frac{1}{2V}\sum_{\boldsymbol{q}\neq 0}V(q)\rho_{\boldsymbol{q}}^\dagger\rho_{\boldsymbol{q}}\\ &=-\frac{1}{2V}\boldsymbol{\nabla}_j\sum_{\boldsymbol{q}\neq 0}V(q)\sum_{i,k}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_k)}\\ &=-\frac{1}{2V}\sum_{\boldsymbol{q}\neq 0}V(q)\sum_k(\mathrm{i}\boldsymbol{q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_k)}+\sum_i(-\mathrm{i}\boldsymbol{q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_i)}\\ &=-\frac{1}{V}\sum_{\boldsymbol{q}\neq 0}\mathrm{i}\boldsymbol{q}V(q)\sum_i\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_i)}\\ &=-\frac{4\pi e^2}{V}\sum_{\boldsymbol{q}\neq 0}\frac{\mathrm{i}\boldsymbol{q}}{q^2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}\rho_{\boldsymbol{q}},\end{aligned}$$

and from (9), we have

$$\begin{aligned}\ddot{\rho}_{\boldsymbol{q}}&=-\sum_j\frac{4\pi e^2}{mV}\sum_{\boldsymbol{q}'\neq 0}\frac{\boldsymbol{q}\cdot\boldsymbol{q}'}{q'^2}\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}_j}\rho_{\boldsymbol{q}'}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}-\sum_j(\boldsymbol{q}\cdot\boldsymbol{v}_j)^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}\\ &=-\frac{4\pi e^2}{mV}\sum_{\boldsymbol{q}'\neq 0}\rho_{\boldsymbol{q}'}\rho_{\boldsymbol{q}-\boldsymbol{q}'}-\sum_j(\boldsymbol{q}\cdot\boldsymbol{v}_j)^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}.\end{aligned}$$

Now we make the **random phase approximation (RPA)** in its original form: We assume that only the $\boldsymbol{q}=\boldsymbol{q}'$ term in the first term is important, because in the high density limit, there are no position preference of electrons (when the density is low, there might be a Wigner crystal, and RPA fails), and when $\boldsymbol{q}\neq 0$, both $\rho_{\boldsymbol{q}'}$ and $\rho_{\boldsymbol{q}-\boldsymbol{q}'}$ are sums of almost random phase factors $\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}$, and therefore are both small enough. So we get the EOM after RPA:

$$\begin{aligned}\ddot{\rho}_{\boldsymbol{q}}&=-\frac{4\pi e^2}{mV}\rho_{\boldsymbol{q}}\rho_0-\sum_j(\boldsymbol{q}\cdot\boldsymbol{v}_j)^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j}\\ &=-\frac{4\pi e^2 n}{m}\rho_{\boldsymbol{q}}-\sum_j(\boldsymbol{q}\cdot\boldsymbol{v}_j)^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j},\end{aligned} \tag{10}$$

where $n=N/V$ is the jellium density. Section (5.4.2) in this solid state physics note tells us that the electron-hole pair excitations are gapless, but from the EOM above we soon find that in the $\boldsymbol{q}\to 0$ case there is a finite ω solution, which is given by

$$\ddot{\rho}_{\boldsymbol{q}}+\omega_{\mathrm{p}}^2\rho_{\boldsymbol{q}}=0,\quad \omega_{\mathrm{p}}^2=\frac{4\pi e^2 n}{m}. \tag{11}$$

We see that this term arises from the Coulomb interaction. In other words, long range interaction induces a collective modes in the metal, which is now known as **plasmon**.

3 Second quantized EOM of density modes

Zhengzhong Li, Sec. 4.4

4 The Green function theory

5 The electric susceptibility and bosonic modes

Now it is time to evaluate

Zhengzhong Li, Sec. 4.6