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

$$\rho(\mathbf{r}) = \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}, \mathbf{k}', \sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma} e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} = \frac{1}{V} \sum_{\mathbf{q}} \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k} + \mathbf{q}, \sigma} e^{i\mathbf{q} \cdot \mathbf{r}},$$
(1)

and the commutation relations are

$$[c_{\mathbf{k}}, c_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'}. \tag{2}$$

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

$$\rho(\mathbf{r}) = \sum_{i} \delta(\mathbf{r} - \mathbf{r}_{i}) = \sum_{i} \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_{i})} = \frac{1}{V} \sum_{\mathbf{q}} \sum_{i} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_{i})}.$$
 (3)

We have

$$\rho_{\mathbf{q}} := \sum_{i} e^{-i\mathbf{q}\cdot\mathbf{r}_{i}} = \sum_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q},\sigma}, \quad \rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} \rho_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}.$$
(4)

Easily, we find

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

The Hamiltonian of electrons is

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

where

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

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

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

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

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

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

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{q} \neq 0} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}'-\mathbf{q},\sigma'}^{\dagger} V(q) c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$

$$= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}}^{\dagger} V(q) \rho_{\mathbf{q}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{q} \neq 0} \rho_{-\mathbf{q}} V(q) \rho_{\mathbf{q}}.$$

$$(7)$$

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(q = 0).

Note that (7) differs with

$$H = \sum_{i} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$
 (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

$$\dot{\rho}_{\boldsymbol{q}} = \sum_{j} (-\mathrm{i}\boldsymbol{q}) \cdot \boldsymbol{v}_{j} \mathrm{e}^{-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}_{j}},$$

$$\ddot{\rho}_{\boldsymbol{q}} = \sum_{j} (-\mathrm{i}\boldsymbol{q} \cdot \dot{\boldsymbol{v}}_{j} - (\boldsymbol{q} \cdot \boldsymbol{v}_{j})^{2}) \mathrm{e}^{-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}_{j}}.$$
(9)

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

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

and from (9), we have

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

Now we make the random phase approximation (RPA) in its original form: We assume that only the q=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 $q \neq 0$, both $\rho_{q'}$ and $\rho_{q-q'}$ are sums of almost random phase factors $e^{-iq \cdot r_j}$, and therefore are both small enough. So we get the EOM after RPA:

$$\ddot{\rho}_{\mathbf{q}} = -\frac{4\pi e^2}{mV} \rho_{\mathbf{q}} \rho_0 - \sum_j (\mathbf{q} \cdot \mathbf{v}_j)^2 e^{-i\mathbf{q} \cdot \mathbf{r}_j}$$

$$= -\frac{4\pi e^2 n}{m} \rho_{\mathbf{q}} - \sum_j (\mathbf{q} \cdot \mathbf{v}_j)^2 e^{-i\mathbf{q} \cdot \mathbf{r}_j},$$
(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 $q \to 0$ case there is a finite ω solution, which is given by

$$\ddot{\rho}_{\mathbf{q}} + \omega_{\mathbf{p}}^2 \rho_{\mathbf{q}} = 0, \quad \omega_{\mathbf{p}}^2 = \frac{4\pi e^2 n}{m}.$$
 (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**. We know it is plasmon, or quantized plasma oscillation, because our derivation above also works for the oscillation of negative charges around positive charges in a plasma.

3 Second quantized EOM of density modes

Now we try to derive plasmon in the second quantization EOM framework. Generally speaking, a generalized hydrodynamic mode in an electron gas is made of a linear combination of

Zhengzhong Li, Sec. 4.4

$$\rho_{\mathbf{k}\mathbf{q}}^{\dagger} =: \sum_{\sigma} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma}. \tag{12}$$

By evaluating the EOM, we may be able to identify stable density modes.

We start from the free theory. It can be verified that

$$[c_1^{\dagger}c_2, c_3^{\dagger}c_4] = \delta_{23}c_1^{\dagger}c_4 - \delta_{14}c_3^{\dagger}c_2, \tag{13}$$

and therefore we have

$$i\dot{\rho}_{\mathbf{k}\mathbf{q}}^{\dagger} = [\rho_{\mathbf{k}\mathbf{q}}^{\dagger}, H_{0}] = \sum_{\mathbf{p},\alpha} \frac{\mathbf{p}^{2}}{2m} \sum_{\sigma} [c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma}, c_{\mathbf{p}\alpha}^{\dagger} c_{\mathbf{p}\alpha}]$$

$$= \sum_{\mathbf{p},\alpha,\sigma} \frac{\mathbf{p}^{2}}{2m} (c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{p}\alpha} \delta_{\mathbf{k}\mathbf{p}} \delta_{\sigma\alpha} - c_{\mathbf{p}\alpha}^{\dagger} c_{\mathbf{k}\sigma} \delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma\alpha})$$

$$= \sum_{\sigma} \left(\frac{\mathbf{k}^{2}}{2m} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma} - \frac{(\mathbf{q}+\mathbf{k})^{2}}{2m} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}\sigma} \right),$$

SO

$$i\dot{\rho}_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} = [\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger}, H_0] = -\omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}} \rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger}, \quad \omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}} = \frac{(\boldsymbol{q} + \boldsymbol{k})^2}{2m} - \frac{\boldsymbol{k}^2}{2m}.$$
(14)

Therefore, we find there are electron-hole pairs in the free theory. In the last section we find that in a plasmon mode, we have $\rho_{\mathbf{k}} = \sum_{\mathbf{q}} \rho_{\mathbf{k}\mathbf{q}} \sim \mathrm{e}^{-\mathrm{i}\omega_{\mathbf{p}}t}$, and $\omega_{\mathbf{q}=0} \neq 0$, but here when $\mathbf{q}=0$, $\omega_{\mathbf{k}\mathbf{q}}^{\mathrm{pair}}$ vanishes, so there is no plasmon. This is expected, since in the last section we find the plasmon comes from the Coulomb interaction.

Now we move on to discuss the jellium model. We have

$$\begin{split} [\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},H] &= [\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},H_{0} + H_{\text{Coulomb}}] = -\omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}}\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} + \frac{1}{2V}\sum_{\boldsymbol{q}'\neq 0}V(q')[\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},\rho_{-\boldsymbol{q}'}\rho_{\boldsymbol{q}'}] \\ &= -\omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}}\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} + \frac{1}{2V}\sum_{\boldsymbol{q}'\neq 0}V(q')(\rho_{-\boldsymbol{q}'}[\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},\rho_{\boldsymbol{q}'}] + [\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},\rho_{-\boldsymbol{q}'}]\rho_{\boldsymbol{q}'}) \\ &= -\omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}}\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} + \frac{1}{2V}\sum_{\boldsymbol{q}'\neq 0}V(q')(\rho_{-\boldsymbol{q}'}[\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},\rho_{\boldsymbol{q}'}] + [\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger},\rho_{\boldsymbol{q}'}]\rho_{-\boldsymbol{q}'}), \end{split}$$

where

$$\begin{aligned} [\rho_{\mathbf{k}\mathbf{q}}^{\dagger}, \rho_{\mathbf{q}'}] &= \sum_{\alpha} \sum_{\mathbf{k}', \beta} [c_{\mathbf{k}+\mathbf{q}, \alpha}^{\dagger} c_{\mathbf{k}\alpha}, c_{\mathbf{k}'\beta}^{\dagger} c_{\mathbf{k}'+\mathbf{q}', \beta}] \\ &= \sum_{\alpha} (c_{\mathbf{k}+\mathbf{q}, \alpha}^{\dagger} c_{\mathbf{k}+\mathbf{q}', \alpha} - c_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \alpha}^{\dagger} c_{\mathbf{k}\alpha}). \end{aligned}$$

So the EOM of $\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger}$ is finally

Zhengzhong Li (4.4.9)

$$i\dot{\rho}_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} = -\omega_{\boldsymbol{k}\boldsymbol{q}}^{\text{pair}}\rho_{\boldsymbol{k}\boldsymbol{q}}^{\dagger} - \frac{1}{2V}\sum_{\boldsymbol{q}'\neq0,\alpha}V(q')\{\rho_{-\boldsymbol{q}'},c_{\boldsymbol{k}+\boldsymbol{q}-\boldsymbol{q}',\alpha}^{\dagger}c_{\boldsymbol{k}\alpha} - c_{\boldsymbol{k}+\boldsymbol{q},\alpha}^{\dagger}c_{\boldsymbol{k}+\boldsymbol{q}',\alpha}\}.$$
 (15)

By taking all possible momenta in (15), we get a closed group of equations about density modes. In principle, this gives the (generalized) hydrodynamic modes in the jellium model

completely, though we all know it is highly difficult to solve EOM of operators. This can also be seen as a successful bosonization the theory, though unlike the case in a Luttinger liquid, this does not help us understand the behavior of the jellium model. A possible way to simplify (15) is to assume that $c^{\dagger}_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\alpha}c_{\mathbf{k}\alpha}-c^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha}c_{\mathbf{k}+\mathbf{q}',\alpha}$ does not fluctuate much, and we can replace it by the expectation value. if under this approximation we find a stable mode, then we have

$$\begin{split} (\omega - \omega_{\mathbf{k}\mathbf{q}}^{\mathrm{pair}}) \rho_{\mathbf{k}\mathbf{q}}^{\dagger} &= \frac{1}{2V} \sum_{\mathbf{q}' \neq 0, \alpha} V(q') \{ \rho_{-\mathbf{q}'}, \langle c_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \alpha}^{\dagger} c_{\mathbf{k}\alpha} - c_{\mathbf{k}+\mathbf{q}, \alpha}^{\dagger} c_{\mathbf{k}+\mathbf{q}', \alpha} \rangle \} \\ &= \frac{1}{2V} \sum_{\mathbf{q}' \neq 0, \alpha} 2V(q') \rho_{\mathbf{q}'}^{\dagger} (n_{\mathbf{k}} \delta_{\mathbf{q}\mathbf{q}'} - n_{\mathbf{k}+\mathbf{q}} \delta_{\mathbf{q}\mathbf{q}'}) \\ &= \frac{2}{V} \rho_{\mathbf{q}}^{\dagger} (n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}) V(q), \end{split}$$

where

$$n_{\mathbf{k}} \coloneqq \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle$$
. (no summation over σ) (16)

From the equation above we find

$$\rho_{\mathbf{k}\mathbf{q}}^{\dagger} = \frac{2V(q)}{V} \rho_{\mathbf{q}}^{\dagger} \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\omega - \omega_{\mathbf{k}\mathbf{q}}^{\text{pair}}},\tag{17}$$

and summing over k, we have

$$1 = \frac{2V(q)}{V} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}} - n_{\mathbf{k} + \mathbf{q}}}{\omega - \omega_{\mathbf{k}\mathbf{q}}^{\text{pair}}}.$$
 (18)

What we are doing here is actually a mean field approximation. It is natural to guess that the approximation corresponds to one Green function resummation strategy, which we will discuss in detail in Section 4. An intuitive way to see what is going on is to note that (17) is actually

$$= + (19)$$

where the $(n_{\mathbf{k}}-n_{\mathbf{k}+\mathbf{q}})/(\omega-\omega_{\mathbf{k}\mathbf{q}}^{\mathrm{pair}})$ factor is "the propagator of an electron-hole pair". The approximation we have made is also a random phase approximation, because after the approximation, all $\mathbf{q}' \neq \mathbf{q}$ terms in (15) disappear.

Now we can easily find the frequencies and the states of all density modes. This also shows a benefit of our operator EOM based approach: in a Green function based approach, we can only easily find the spectrum of the density modes by checking the singularities of $\langle nn \rangle$, but it is not that easy to identify their actual "shape". We, however, will postpone the solution of (18) to Section 5, since TODO: can we find the lifetime of the excitons purely by this section's approach?

4 The Green function theory

We have already discussed the density-density Green function in the free theory in (5.58) in this solid state physics note.

5 The electric susceptibility and bosonic modes

Now it is time to evaluate the analytic properties of the susceptibility. The dispersion relations are given by $\epsilon=0$ (not $\epsilon\to\infty$ - see Section 2.2.1 in this optics note). Note that the imaginary part of ϵ indicates damping (see Section 8.1.1 in this optics note), and therefore if $\operatorname{Im} \epsilon \neq 0$, even if on an (ω, \mathbf{k}) point we have $\operatorname{Re} \epsilon = 0$, this is not an eigenmode. However, if $\operatorname{Im} \epsilon$ is not large, we can still say that "there is a mode at (ω, \mathbf{k}) with a finite lifetime". So what we are going to do is to solve the equation $\operatorname{Re} \epsilon(\omega, \mathbf{k}) = 0$ and check the lifetime of each mode.

Zhengzhong Li, Sec. 4.6