

Electron Gas with Coulomb Interaction

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January 14, 2022

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

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

and the commutation relations are

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

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

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

We have

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

Easily, we find

$$\rho_{\mathbf{q}=0} = \int d^3\mathbf{r} \rho(\mathbf{r}) = N. \quad (5)$$

The Hamiltonian of electrons is

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

where

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

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

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

When $|\mathbf{q}| = 0$, $V(\mathbf{q})$ 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

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

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

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

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 $V(\mathbf{q} = 0)$.

Note that (7) differs with

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

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

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Li, Sec. 4.3

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

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

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

and from (9), we have

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

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

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

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 $\mathbf{q} \rightarrow 0$ case there is a finite ω solution, which is given by

$$\ddot{\rho}_{\mathbf{q}} + \omega_p^2 \rho_{\mathbf{q}} = 0, \quad \omega_p^2 = \frac{4\pi e^2 n}{m}. \quad (11)$$

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

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

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

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

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

and therefore we have

$$\begin{aligned} i\dot{\rho}_{\mathbf{k}\mathbf{q}}^\dagger &= [\rho_{\mathbf{k}\mathbf{q}}^\dagger, H_0] = \sum_{\mathbf{p},\alpha} \frac{\mathbf{p}^2}{2m} \sum_{\sigma} [c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k}\sigma}, c_{\mathbf{p}\alpha}^\dagger c_{\mathbf{p}\alpha}] \\ &= \sum_{\mathbf{p},\alpha,\sigma} \frac{\mathbf{p}^2}{2m} (c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{p}\alpha} \delta_{\mathbf{k}\mathbf{p}} \delta_{\sigma\alpha} - c_{\mathbf{p}\alpha}^\dagger c_{\mathbf{k}\sigma} \delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma\alpha}) \\ &= \sum_{\sigma} \left(\frac{\mathbf{k}^2}{2m} c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k}\sigma} - \frac{(\mathbf{q}+\mathbf{k})^2}{2m} c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k}\sigma} \right), \end{aligned}$$

so

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

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 $\rho_{\mathbf{k}} = \sum_{\mathbf{q}} \rho_{\mathbf{k}\mathbf{q}} \sim e^{-i\omega_{\mathbf{p}} t}$, and $\omega_{\mathbf{q}=0} \neq 0$, but here when $\mathbf{q} = 0$, $\omega_{\mathbf{k}\mathbf{q}}^{\text{pair}}$ 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

$$\begin{aligned} [\rho_{\mathbf{k}\mathbf{q}}^\dagger, H] &= [\rho_{\mathbf{k}\mathbf{q}}^\dagger, H_0 + H_{\text{Coulomb}}] = -\omega_{\mathbf{k}\mathbf{q}}^{\text{pair}} \rho_{\mathbf{k}\mathbf{q}}^\dagger + \frac{1}{2V} \sum_{\mathbf{q}' \neq 0} V(\mathbf{q}') [\rho_{\mathbf{k}\mathbf{q}}^\dagger, \rho_{-\mathbf{q}'} \rho_{\mathbf{q}'}] \\ &= -\omega_{\mathbf{k}\mathbf{q}}^{\text{pair}} \rho_{\mathbf{k}\mathbf{q}}^\dagger + \frac{1}{2V} \sum_{\mathbf{q}' \neq 0} V(\mathbf{q}') (\rho_{-\mathbf{q}'} [\rho_{\mathbf{k}\mathbf{q}}^\dagger, \rho_{\mathbf{q}'}] + [\rho_{\mathbf{k}\mathbf{q}}^\dagger, \rho_{-\mathbf{q}'}] \rho_{\mathbf{q}'}) \\ &= -\omega_{\mathbf{k}\mathbf{q}}^{\text{pair}} \rho_{\mathbf{k}\mathbf{q}}^\dagger + \frac{1}{2V} \sum_{\mathbf{q}' \neq 0} V(\mathbf{q}') (\rho_{-\mathbf{q}'} [\rho_{\mathbf{k}\mathbf{q}}^\dagger, \rho_{\mathbf{q}'}] + [\rho_{\mathbf{k}\mathbf{q}}^\dagger, \rho_{\mathbf{q}'}] \rho_{-\mathbf{q}'}), \end{aligned}$$

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 $\rho_{\mathbf{k}\mathbf{q}}^\dagger$ is finally

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$$i\dot{\rho}_{\mathbf{k}\mathbf{q}}^\dagger = -\omega_{\mathbf{k}\mathbf{q}}^{\text{pair}} \rho_{\mathbf{k}\mathbf{q}}^\dagger - \frac{1}{2V} \sum_{\mathbf{q}' \neq 0, \alpha} V(\mathbf{q}') \{ \rho_{-\mathbf{q}'} [c_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\alpha}^\dagger c_{\mathbf{k}\alpha} - c_{\mathbf{k}+\mathbf{q},\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}',\alpha}] \}. \quad (15)$$

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. A possible way to simplify (15) is to assume that $c_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\alpha}^\dagger c_{\mathbf{k}\alpha} - c_{\mathbf{k}+\mathbf{q},\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}',\alpha}$ 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

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

where

$$n_{\mathbf{k}} := \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle. \quad (\text{no summation over } \sigma) \quad (16)$$

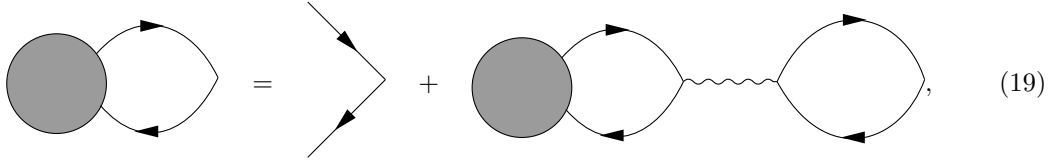
From the equation above we find

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

and summing over \mathbf{k} , we have

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

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



The diagram shows an equality between three terms. On the left is a bubble diagram consisting of a shaded circle on the left and a loop on the right. This is equal to the sum of two terms. The first term is a vertex diagram with two external lines meeting at a point. The second term is a bubble diagram where the shaded circle is connected to a loop, which is then connected via a wavy line to another loop.

where the $(n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}})/(\omega - \omega_{\mathbf{k}\mathbf{q}}^{\text{pair}})$ 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.

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

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Li, Sec. 4.6