Poor man's linear response theory by Prof. Kun Din

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In the previous lecture we discussed the K-K relation and its generalization in metals, the analytic structure of electrodynamic response functions, and sum rules. We also introduced a poor man's linear response theory.

1 Poor man's linear response theory

The ground state is determined by

$$\left.\frac{\delta G}{\delta n}\right|_0 + e\phi_0 = \mu, \quad \nabla^2 \phi_0 = \frac{e}{\epsilon_0}(n_{\text{lattice}} - n_0). \tag{1}$$

The excitation is determined by

$$\frac{\partial \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{j}_1 = 0, \quad \frac{\partial \boldsymbol{j}_1}{\partial t} = -\frac{e n_0}{m} \boldsymbol{\nabla} \left(\frac{\delta G}{\delta n}\right)_1 + \frac{e^2 n_0}{m} \boldsymbol{E}_1. \tag{2}$$

Note that since the system can be charged (for example in the case of capacitors), maybe

$$\int \mathrm{d}^3 \boldsymbol{r}\, (n_{\text{lattice}} - n_0) \neq 0. \tag{3}$$

By the Fourier transformation of t we have

$$(-\mathrm{i}\omega + \gamma)\boldsymbol{j}_1 = -\frac{e n_0}{m} \boldsymbol{\nabla} \left(\frac{\delta G}{\delta n}\right)_1 + \frac{e^2 n_0}{m} \boldsymbol{E}(\omega), \quad \boldsymbol{\nabla} \cdot \boldsymbol{j}_1 - \mathrm{i}\omega\rho_1 = 0. \tag{4}$$

Adding the wave function

$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{E}_1(\omega)) - \left(\frac{\omega}{c}\right)^2 \boldsymbol{E}_1(\omega) = \mathrm{i}\omega\mu_0 \boldsymbol{j}_1(\omega), \tag{5}$$

the electrodynamic behavior can be found.

A specific case can be immediately seen from these equations. If the $G[n]$ term is not important, we already find that

$$\epsilon_{\mathrm{r}}(\infty) = 1 - \frac{\omega_0^2}{\omega^2}, \tag{6}$$

which is the prediction of Drude model. Let

$$G[n] = \int \mathrm{d}^3 \boldsymbol{r}\, g(n, \boldsymbol{\nabla} n, \ldots). \tag{7}$$

The leading term of g is the famous **Thomas-Fermi energy**

$$g(n, \boldsymbol{\nabla} n, \ldots) = \frac{3\hbar^2}{10 m_{\mathrm{e}}} (3\pi)^{2/3} n^{5/3} + \cdots, \tag{8}$$

and we can add the **von-Weizsäcker energy** and **exchange-correlation terms** (the exact meaning of which can be found in Section 7.1.3 in the solid state physics note), for example

$$g(n, \boldsymbol{\nabla} n, \ldots) = \frac{3\hbar^2}{10 m_{\mathrm{e}}} (3\pi)^{2/3} n^{5/3} + \underbrace{\frac{\lambda\hbar^2}{8 m_{\mathrm{e}}} \frac{|\boldsymbol{\nabla} n|^2}{n}}_{E_{\mathrm{vW}}} + E_{\mathrm{XC}}. \tag{9}$$

The exact expression of g does not matter, since if the wave function does not appear explicitly, phenomena that are purely quantum mechanical are hard to repeat in our model. For example, if somehow the *phase* of the electron wave function influences the electric field, then the prediction of our fluid dynamic approach is *qualitatively wrong*.

2 Thomas-Fermi screening

We consider a static example. The problem is

$$\boldsymbol{\nabla}\cdot\boldsymbol{D}=\rho_{\text{ext}},\quad \nabla^2\phi_1=-\frac{\rho_{\text{ext}}+\rho_1}{\epsilon_0},\quad \epsilon_0\boldsymbol{\nabla}\cdot\boldsymbol{E}=\underbrace{\rho_{\text{ext}}+\rho_1}_{\rho_{\text{total}}}. \tag{10}$$

Switching to the momentum space, we have

$$\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{D}(\boldsymbol{k})=\epsilon_0|\boldsymbol{k}|^2\phi_{\text{ext}}(\boldsymbol{k})=\rho_{\text{ext}}(\boldsymbol{k}),$$

and by definition we have

$$\epsilon_{\text{r}}(\boldsymbol{k},\omega=0)=\frac{\phi_{\text{ext}}(\boldsymbol{k})}{\phi_1(\boldsymbol{k})}=\frac{\rho_{\text{ext}}}{\rho_{\text{total}}}=1-\frac{\rho_1(\boldsymbol{k})}{\rho_{\text{total}}(\boldsymbol{k})}. \tag{11}$$

If we just consider the Thomas-Fermi term, we have

$$\frac{\delta G}{\delta n}=\frac{\partial g}{\partial n}-\boldsymbol{\nabla}\cdot\frac{\partial g}{\partial\boldsymbol{\nabla}n}=\frac{\hbar^2}{2m_{\text{e}}}(3\pi^2n)^{2/3},$$

and therefore

$$\left(\frac{\delta G}{\delta n}\right)_1=\frac{\hbar^2}{2m_{\text{e}}}(3\pi^2)^{2/3}((n_1+n_0)^{3/2}-n_0^{3/2})\approx\frac{\hbar^2}{m_{\text{e}}}(3\pi^2)^{2/3}\frac{n_1}{n_0}n_0^{2/3}=\frac{2\epsilon_{\text{F}}^0}{3n_0}n_1,$$

where we define

$$\epsilon_{\text{F}}^1:=\frac{\hbar^2}{2m_{\text{e}}}(3\pi^2n_0)^{2/3}. \tag{12}$$

So finally we have

$$\epsilon(\boldsymbol{k},\omega=0)=1+\frac{k_{\text{s}}^2}{|\boldsymbol{k}|^2}, \tag{13}$$

where

$$k_{\text{s}}=\frac{3e^2n_0}{2\epsilon_{\text{F}}^0\epsilon_0} \tag{14}$$

is called the **Thomas-Fermi wave number**.

Here is the magnitude of k_{s}: We have

$$\frac{k_{\text{s}}}{k_{\text{F}}}=\sqrt{r_{\text{s}}\left(\frac{16}{3\pi^2}\right)^{2/3}}=0.814\sqrt{r_{\text{s}}}, \tag{15}$$

where r_{s} is usually between 2 and 6. Therefore k_{S} is of the same magnitude of k_{F}, and is quite a large momentum compared to ordinary electromagnetic waves.

Switching back to the real space, we have

$$\begin{aligned}\phi_1(\boldsymbol{r})&=\frac{q}{\epsilon_0(2\pi)^3}\int\mathrm{d}^3\boldsymbol{k}\,\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{|\boldsymbol{k}|^2+k_{\text{S}}^2}\\&=\frac{q}{\epsilon_0(2\pi)^2}\frac{1}{2\mathrm{i}r}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{k(\mathrm{e}^{\mathrm{i}kr}-\mathrm{e}^{-\mathrm{i}kr})}{(k+\mathrm{i}k_{\text{s}})(k-\mathrm{i}k_{\text{s}})},\end{aligned}$$

Note that there is no causality in the spacial dimensions, so there may be poles on the upper plane. Competing the contour integrals we have

$$\phi_1(\boldsymbol{r})=\frac{q}{4\pi\epsilon_0r}\mathrm{e}^{-k_{\text{s}}r}, \tag{16}$$

which is called the **Yukawa potential**. Usually the screening length is $1/k_{\text{s}}\sim 1\,\text{Å}$, so the electric field in a metal is screened almost perfectly.

3 Dynamic screening

Now we consider a scenario where both the charge and the current are perturbed. We have

$$(-\mathrm{i}\omega + \gamma)\boldsymbol{j}_1 + \frac{v_\mathrm{p}^2}{3}\boldsymbol{\nabla}\rho_1 = \epsilon_0 \omega_\mathrm{p}^2 \boldsymbol{E}_1(\omega), \tag{17}$$

or to eliminate the dependence on ρ_1, we take the time derivative and obtain

$$\omega(\omega + \mathrm{i}\gamma)\boldsymbol{j}_1 + \beta^2 \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{j}_1) = \mathrm{i}\omega\epsilon_0\omega_\mathrm{p}^2 \boldsymbol{E}_1(\omega). \tag{18}$$

Now we perform the Helmholtz decomposition. Let

$$\boldsymbol{E}_1 = \boldsymbol{E}_\mathrm{l} + \boldsymbol{E}_\mathrm{t}, \quad \boldsymbol{j}_1 = \boldsymbol{j}_\mathrm{l} + \boldsymbol{j}_\mathrm{t}, \tag{19}$$

where the subscript l means "longitude" and t means "transverse". The equations for the longitude modes are

$$\omega(\omega + \mathrm{i}\gamma)\boldsymbol{j}_\mathrm{l} - \beta^2 \boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{j}_\mathrm{l}) = \mathrm{i}\omega\epsilon_0\omega_\mathrm{p}^2 \boldsymbol{E}_\mathrm{l}, \tag{20}$$

while the equations for the transverse modes are

$$\omega(\omega + \mathrm{i}\gamma)\boldsymbol{j}_\mathrm{t} = \mathrm{i}\omega\epsilon_0\omega_\mathrm{p}^2 \boldsymbol{E}_\mathrm{t}, \quad \boldsymbol{k}\times(\boldsymbol{k}\times\boldsymbol{E}_\mathrm{t}) + \left(\frac{\omega}{c}\right)^2 \boldsymbol{E}_\mathrm{t} = -\mathrm{i}\omega\epsilon_0\omega_\mathrm{p}^2 \boldsymbol{E}_\mathrm{t}(\omega). \tag{21}$$

By the routine mentioned in the last section we have

$$\epsilon_\mathrm{l}(\boldsymbol{k},\omega) = 1 - \frac{\omega_\mathrm{p}^2}{\omega(\omega + \mathrm{i}\gamma) - \beta^2 |\boldsymbol{k}|^2}, \tag{22}$$

and

$$\epsilon_\mathrm{t}(\boldsymbol{k},\omega) = 1 - \frac{\omega_\mathrm{p}^2}{\omega(\omega + \mathrm{i}\gamma)}. \tag{23}$$

The pole in ϵ_l is given by

$$|\boldsymbol{k}|^2 = \left(\frac{\omega}{c}\right)^2 \left(1 - \frac{\omega_\mathrm{p}^2}{\omega(\omega + \mathrm{i}\gamma)}\right), \tag{24}$$

and when there is no dissipation we get

$$\omega^2 = \omega_\mathrm{p}^2 + \boldsymbol{k}^2 c^2, \tag{25}$$

again the prediction of Drude model.

When k/k_s is small, there is almost no propagating modes in metals: the longitude mode is gapped, and the frequency of the transverse mode is just too low to be noticed. Therefore, in the $k/k_\mathrm{s} \ll 1$ limit, a metal essentially blocks any propagating modes, and screens any external sources. When $k/k_\mathrm{s} \gg 1$, the frequency of the longitude mode is just too high to be relevant, and now we have propagating transverse modes in the metal. In this limit the metal looks "transparent".

4 Boundaries and other inhomogeneous systems

The Thomas-Fermi term is definitely not enough for inhomogeneous systems. An extreme case is a boundary, where on one side we have no electrons at all and therefore the electron density has a sharp decay with a big $\boldsymbol{\nabla} n$, which must be included into the energy functional $G[n]$. Actually in the 10 nm to 1 nm region, violations of continuum electromagnetism most frequently come from boundaries. Violations of the continuum theory appear usually in the < 1 nm region in bulks.

With an energy functional $G[n]$ that is accurate enough, it can be found that the electron density has a peak near the boundary, and the electric field changes sharply. In the macroscopic electrodynamics, we do a coarse-graining of all fields around the boundary and approximate all high wave number components of the fields with δ-functions. *Boundary conditions* are introduced to characterize the boundary, which is not necessary in the microscopic theory.

5 A summary of continuum electromagnetism

- Microscopic and macroscopic Maxwell equations; continuum of approximation.
  - Spacial averaging; test functions.
  - Long wave length condition.
- Constitutive relations.
  - Macroscopic description of materials.
  - Weak field approximation: only linear susceptibility.
  - Low speed movement.
  - Multipole expansion.
- Response functions in the frequency domain.
  - The K-K relations.
  - Causality.
- Poor man's linear response theory.