3.3 Screening of Coulomb interactions in a metal

Ref: [AM] Chapter 17.

As we saw in the previous sections, the Hartree–Fock approximation does not include any screening of long-range Coulomb interactions. As a particular consequence of this neglect, the spectrum of excitations near the Fermi surface gets, within the Hartree–Fock approximation, an unphysical logarithmic singularity. This problem can be repaired by including screening.

In this section, we discuss screening at the linear-response level in the static situation (no time dependence). Namely, we assume a small probe charge Q at the position $x = 0$ and calculate the resulting electrostatic potential $\phi(r)$ around this charge.

In the absence of screening, the potential is

$$\phi^{\text{ext}}(R) = \frac{Q}{R} \tag{3.3.1}$$

The screening results from a redistribution of the electronic density due to the potential, which, in turn, itself changes the potential. In other words, the potential and the density distribution need to be calculated self-consistently.

The response of the density to the potential can be written in the momentum representation as

$$\delta n(q) = \chi(q)\, e\phi(q)\,. \tag{3.3.2}$$

On the other hand, the feedback of the density modulation on the potential is given by the Gauss equation

$$-\frac{1}{4\pi}\nabla^2\phi(x) = Q\,\delta(x) + e\,\delta n(x)\,, \tag{3.3.3}$$

which, in the momentum representation takes the form

$$\frac{q^2}{4\pi}\phi(q) = Q + e\,\delta n(q) \tag{3.3.4}$$

Putting the two equations together, we find

$$\phi(q) = \frac{Q}{\frac{q^2}{4\pi} - e^2\,\chi(q)}\,. \tag{3.3.5}$$

The Fourier transform of this function gives the screened interaction potential $\phi(r)$.

3.3.1 Thomas–Fermi theory of screening

The simplest approximation we can make is to assume that all the coordinate dependences are slow and calculate the response (3.3.2) in the static approximation (which amounts to putting $q = 0$). Then we immediately find

$$\chi(q{=}0) = -\nu_0\,, \tag{3.3.6}$$

the density of states at the Fermi level (including spin degeneracy),and

$$\phi(q) = \frac{4\pi Q}{q^2 + \kappa^2}\,, \tag{3.3.7}$$

Figure 14: RPA series for screening.

where

$$\kappa = (4\pi e^2 \nu_0)^{1/2} \,. \tag{3.3.8}$$

The Fourier transform of this potential gives

$$\phi(R) = \frac{Q}{R} e^{-\kappa R} \,, \tag{3.3.9}$$

i.e., κ^{-1} has the meaning of the screening length.

3.3.2 Lindhard theory of screening

A more accurate approximation is to calculate the response (3.3.2) within the free-fermion gas model. This was, in fact, done in the problem 7.2, and the answer reads

$$\chi(R) = -i \int \frac{d\omega}{2\pi} [G^c_\omega(R)]^2 \,. \tag{3.3.10}$$

To convert this result into the screened potential, we need to Fourier transform $\chi(r) \mapsto \chi(q)$, substitute into eq. (3.3.5) and Fourier transform back to the real space.

An exact calculation for the free 3D gas (without spin) gives

$$G^c_\omega(R) = -\frac{m}{2\pi R} e^{i(\operatorname{sign}\omega) k_\omega r} \,, \tag{3.3.11}$$

where $k_\omega = [2m(\mu + \omega)]^{1/2}$,

$$\chi(R) = -\frac{m}{16\pi^3 R^4} \left[\sin(2k_F R) - (2k_F R)\cos(2k_F R)\right] \,, \tag{3.3.12}$$

and

$$\chi(q) = -\frac{m k_F}{2\pi^2} F\left(\frac{q}{2k_F}\right) \,, \tag{3.3.13}$$

where

$$F(\alpha) = \frac{1}{2} + \frac{1-\alpha^2}{4\alpha} \ln\left|\frac{1+\alpha}{1-\alpha}\right| \,. \tag{3.3.14}$$

For the spinful case, the results for $\chi(R)$ and $\chi(q)$ must be multiplied by 2 (for the two spin components).

We see that at $q = 0$ it reproduces the Thomas–Fermi approximation. Thus the long-range $1/r$ part is screened in exactly the same way as described above (at the scale κ^{-1}). At the same time, the logarithmic singularity in (3.3.13) may be shown to give rise to the oscillating contribution

$$\phi(R) \propto \frac{1}{R^3} \cos(2k_F R) \,. \tag{3.3.15}$$

3.3.3 Diagrammatic interpretation of the Lindhard theory

We can also obtain the Lindhard theory by simply summing the diagrammatic series in Fig. 14. Each loop corresponds to $\chi(R)$ as given by (3.3.10) while each wavy line corresponds to the bare potential

$$V_0(R) = \frac{e^2}{R} \qquad \Rightarrow \qquad V_0(q) = \frac{4\pi e^2}{q^2} \, . \tag{3.3.16}$$

Summing up the geometric series gives

$$\begin{aligned} V(q) &= V_0(q) + V_0(q)\,\chi(q)\,V_0(q) + V_0(q)\,\chi(q)\,V_0(q)\,\chi(q)\,V_0(q) + \ldots \\ &= \frac{V_0(q)}{1 - \chi(q)\,V_0(q)} \, , \end{aligned} \tag{3.3.17}$$

which exactly reproduces the result of the Lindhard theory.

This type of approximation (corresponding to the summation of the series shown in Fig. 14) is also frequently called *random phase approximation* (RPA). It can also be extended to include dynamic screening (and plasmon excitations) by considering this series at a finite frequency (our calculation only considered the zero-frequency limit).

Problem Set 8

Problem 8.1

Estimate the screening length in a typical metal.

Problem 8.2

Starting from Eq. (3.3.12), derive the results (3.3.13)–(3.3.14) and (3.3.15).

Hint: in calculating the integrals leading to (3.3.14), first integrate over the angular coordinates. When integrating over R, it may be helpful to integrate by parts to reduce the power of R in the denominator and use the following formula:

$$\int_{\epsilon}^{\infty} \frac{e^{ikx}}{x}\, dx = C_0 - \ln(\epsilon|k|) + o(\epsilon)\,,$$

where C_0 is some constant (which will drop out from the result) and ϵ is a small cut-off (which will be set to zero at the end of the calculation).