1 Screening and Plasmons

When a positive charge Q is introduced into an electron gas, to restore charge neutrality at the site of the positive charge, the electrons will screen the charge, thereby decreasing its net electric field. In fact, screening occurs regardless of the sign of the test charge. This state of affairs arises because as an electron moves through the electron gas, it does not have to push all the other electrons out of the way. The mutual repulsions among all the electrons in the electron gas help to clear a path for an electron to move. As a result, the effective interaction between the electrons is diminished from the long-range Coulomb $\frac{1}{r}$ to a much more short-ranged interaction. At the level of Thomas-Fermi, the new interaction falls off exponentially. While this interaction overestimates the effect of screening, it does illustrate how efficiently repulsive interactions screen electrons in an electron gas.

1.1 Thomas Fermi Screening

Let us assume a charge Q is at the origin. In the absence of the electron gas, an electron a distance r away from the origin feels a potential $\phi = Q/r$, such that the potential energy is given by

$$U = -e\phi = -e\frac{Q}{r} \tag{1}$$

In the presence of the electron gas, the potential around the charge Q will be screened. Physically, the screening charge is determined by the difference between the charge density of the electron gas in the presence of the charge, Q, and the charge density in the absence of the external charge. Let $-e\delta n(r)$ represent this difference. Poisson's equation for the total charge distribution,

$$-\nabla^2\phi_{eff}(r) = 4\pi[Q\delta(r) - e\delta n(r)], \tag{2}$$

depends on both Q and the screening charge, $-e\delta n(r)$, with ϕ_{eff}, the true potential of the charge Q in the electron gas. The easiest way to solve eqution (2) is by Fourier transform. We define

$$f(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}r} f(\mathbf{r}) \tag{3}$$

As a consequence,

$$k^2 U_{eff}(\mathbf{k}) = -4\pi eQ + 4\pi e^2 \delta n(\mathbf{k}) \tag{4}$$

The simplest approximation to solve this equaton is that of Thomas and Fermi in which the electron gas is assumed to respond to the charge Q as if it were locally a free-electron gas. Physically, this assumption implies that the potential is a slowly varying function on a distance scale set by the

Fermi wavelength. The net effect, then, is a shift in the chemical potential of the form $\mu \to \mu + U_{eff}(r)$. Let us define a new single-particle energy level,

$$\epsilon_{\mathbf{k}}(\mathbf{r}) = \frac{\hbar^2 k^2}{2m} + U_{eff}(\mathbf{r}) \tag{5}$$

The effective Fermi-Dirac distribution function is

$$n_{\mathbf{k}}(\mathbf{r}) = \frac{1}{1 + e^{\beta(\epsilon_{\mathbf{k}}(\mathbf{r}) - \mu)}}, \tag{6}$$

so that the effective density at r is

$$\begin{aligned} \langle n(r) \rangle &= 2 \int \frac{dk}{(2\pi)^3} n_k(r) \\ &= n_e - 2\beta \int \frac{dk}{(2\pi)^3} U_{eff}(\mathbf{r}) \frac{e^{\beta(\epsilon_{\mathbf{k}} - \mu)}}{(1 + e^{\beta(\epsilon_{\mathbf{k}} - \mu)})^2} + \cdots \\ &\simeq n_e - \frac{\partial n(e)}{\partial \mu} U_{eff}(\mathbf{r}) + \cdots , \end{aligned} \tag{7}$$

where we expanded the distribution function and retained only the linear term in U_{eff}. This expansion is valid only if $\epsilon_F \gg U_{eff}(\mathbf{r})$.We can now calculate $\delta n(\mathbf{r})$ because

$$\delta n(\mathbf{r}) = \langle n(\mathbf{r}) \rangle - n_e = -\frac{\partial n_e}{\partial \mu} U_{eff}(\mathbf{r}), \tag{8}$$

which implies that

$$k^2 U_{eff}(\mathbf{k}) = -4\pi e \left(Q + e \frac{\partial n_e}{\partial \mu} U_{eff}(\mathbf{k}) \right), \tag{9}$$

or, equivalently,

$$U_{eff}(\mathbf{k}) = \frac{-4\pi e Q}{k^2 + 4\pi e^2 \, \partial n_e / \partial \mu}. \tag{10}$$

The inverse Fourier transform of $U_{eff}(\mathbf{k})$,

$$\begin{aligned} U_{eff}(\mathbf{r}) &= -\frac{4\pi e Q}{(2\pi)^3} \int \frac{e^{i\mathbf{kr}} d\mathbf{k}}{k^2 + 4\pi e^2 \, \partial n_e / \partial \mu} \\ &= -\frac{eQ}{\pi r} \int_{-\infty}^{\infty} dk \frac{k \sin(kr)}{k^2 + 4\pi e^2 \, \partial n_e / \partial \mu} \\ &= -eQ \frac{e^{-\kappa_{TF} r}}{r}, \end{aligned} \tag{11}$$

demonstrates that the electrostatic potential arising from the electrons around the charge Q,

$$\phi_{eff}(\mathbf{r}) = -e\frac{e^{-\kappa_{TF} r}}{r}, \tag{12}$$

decays exponentially. The electron gas attenuates the bare Coulomb field by screening the charge on a length scale determined by

$$\kappa_{TF}^2 = 4\pi e^2 \frac{\partial n_e}{\partial \mu} \tag{13}$$

To reiterate, this result is valid in the limit of a slowly varying field induced by the electron gas. We estimate κ_{TF} by recalling that

$$n_e = \Big(\frac{2m\mu_0}{\hbar^2}\Big)^{\frac{3}{2}} \frac{1}{3\pi^2} \tag{14}$$

As a consequence,

$$\frac{\partial n_e}{\partial \mu_0} = \frac{3}{2}\frac{n_e}{\mu_0} = \frac{3n_e}{mv_F^2} \tag{15}$$

and

$$\kappa_{TF}^2 = \frac{12\pi e^2 n_e}{mv_F^2} = \frac{4}{\pi}\Big(\frac{9\pi}{4}\Big)^{\frac{1}{3}} \frac{1}{a_0 r_e} = \frac{2.434}{a_0^2}\frac{1}{r_s} \tag{16}$$

Recall that $r_s \sim 2-6$. Hence, $\kappa_{TF}^{-1} = 0.34\sqrt{r_s}$Å $\simeq 0.45$Å $- 0.9$Å.While Thomas-Fermi theory predicts a screening length of electrons in metals generally shorter than the interparticle spacing, the result only describes the long-distance fall-off of the potential surrounding a given charge, as in Eq. (11). The theory does not correctly account for screening at distances comparable to the interparticle spacing.

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