Static screening in a degenerate electron plasma

Suppose we switch on an appropriately screened test charge potential δV (actually the so colled Hartree potential) in a free Fermi gas. The Hartree potential $\delta V(\mathbf{r})$ created at a distance r from a static point charge of magnitude e should be evaluated self-consistently from the Poisson equation,

$$\nabla^2 \delta V(\mathbf{r}) = -4\pi e^2 [\delta(\mathbf{r}) + \delta n(\mathbf{r})] \quad , \tag{1}$$

where $\delta n(\mathbf{r})$ is the change in electronic density induced by the foreign charge. The electron density $n(\mathbf{r})$ may be written as

$$n(\mathbf{r}) = 2 \sum_{\mathbf{k}} |\psi_{\mathbf{k}}(\mathbf{r})|^2 \quad , \tag{2}$$

where $\psi_{\mathbf{k}}(\mathbf{r})$ are single-electron orbitals, the sum over $\mathbf{k}$ is restricted to occupied orbitals ($|\mathbf{k}| \leq k_F$, k_F Fermi wave vector) and the factor 2 comes from the sum over spin orientations. We must now calculate how the orbitals in the presence of the foreign charge, differ from plane waves $\exp(i\mathbf{k} \cdot \mathbf{r})$. We use for this purpose the Schrödinger equation,

$$\nabla^2 \psi_{\mathbf{k}}(\mathbf{r}) + [k^2 - \frac{2m}{\hbar^2} \delta V(r)] \psi_{\mathbf{k}}(\mathbf{r}) = 0 \quad , \tag{3}$$

having imposed that the orbitals reduce to plane waves with energy $\hbar^2 k^2/(2m)$ at large distance [1].

With the aforementioned boundary condition the Schrödinger equation may be converted into an integral equation,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2} \int G_{\mathbf{k}}(\mathbf{r} - \mathbf{r}') \delta V(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}') d\mathbf{r}' \quad , \tag{4}$$

with $G_{\mathbf{k}}(\mathbf{r}) = -\exp(i\mathbf{k} \cdot \mathbf{r})/(4\pi r)$ and Ω the volume of the system.

[1] This approach (which lead to the Random Phase Approximation, RPA) is approximate insofar as the potential entering the Schrödinger equation has been taken as the Hartree potential, thus neglecting exchange and correlation between an incoming electron and the electronic screening cloud.

Within linear response theory we can replace $\psi_{\mathbf{k}}(\mathbf{r})$ by $\Omega^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r})$ inside the integral. This yields

$$\delta n(\mathbf{r}) = -\frac{mk_F^2}{2\pi^3\hbar^2}\int j_1(2k_F|\mathbf{r}-\mathbf{r}'|)\frac{\delta V(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}' \quad , \tag{5}$$

with $j_1(x)$ being the first-order spherical Bessel function $[\sin(x)-x\cos(x)]/x^2$. Using this result in the Poisson equation we get

$$\nabla^2\delta V(r) = -4\pi e^2\delta(\mathbf{r}) + \frac{2mk_F^2e^2}{\pi^2\hbar^2}\int j_1(2k_F|\mathbf{r}-\mathbf{r}'|)\frac{\delta V(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}' \quad , \tag{6}$$

which is easily soluble in Fourier transform. Writing $\delta V(k) = 4\pi e^2/[k^2\varepsilon(k)]$ we find,

$$\varepsilon(k) = 1 + \frac{2mk_Fe^2}{\pi k^2\hbar^2}\left[1 + \frac{k_F}{k}\left(\frac{k^2}{4k_F^2}-1\right)\ln\left|\frac{k-2k_F}{k+2k_F}\right|\right] \quad , \tag{7}$$

which is the static dielectric function in RPA.

For $k\to 0$ this expression gives $\varepsilon(k)\to 1+k_{TF}^2/k^2$ with $k_{TF}=3\omega_p^2/v_F^2$ (ω_p being the plasma frequency and v_F the fermi velocity.) i.e. the result of the Thomas-Fermi theory. However $\varepsilon(k)$ has a singularity at $k=\pm 2k_F$, where its derivative diverges logarithmically [2]. This singularity in $\delta V(k)$ determines after Fourier transform the behaviour of $\delta V(r)$ at large r. $\delta V(r)$ turns out to be an oscillating function [3] rather than a monotonically decreasing function as in the Thomas-Fermi theory. Indeed,

$$\delta V(r) = \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{4\pi e^2}{k^2\varepsilon(k)}e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{e^2}{i\pi r}\int_{-\infty}^{\infty}dk\frac{e^{ikr}}{k\varepsilon(k)} \quad , \tag{8}$$

and the integrand has non-analytic behaviour at $q=\pm 2k_F$,

$$\left[\frac{1}{k\varepsilon(k)}\right]_{k\to\pm 2k_F} = -A(k-(\pm)2k_f)\ln|k-(\pm)2k_F| + \text{regular terms} \quad , \tag{9}$$

[2]The discontinuity in the momentum distribution across the Fermi surface introduces a singularity in elastic scattering processes with momentum transfer equal to $2k_F$.

[3]J. Friedel, *N. Cimento Suppl.* **7**, 287 (1958).

with $A = (k_{TF}^2/4k_F^2)/(k_{TF}^2 + 8k_F^2)$. Hence,

$$\delta V(r)|_{r\to\infty} = -\frac{Ae^2}{i\pi r}\int_{-\infty}^{\infty} dk\, e^{ikr}[(k-2k_F)\ln|k-2k_F| + (k+2k_F)\ln|k+2k_F|] = -2Ae^2\frac{\cos(2k_F r)}{r^3} \quad . \tag{10}$$

This result is based on a theorem on Fourier transforms [4], stating that the asymptotic behaviour of $\delta V(r)$ is determined by the low-k behaviour as well as the singularities of $\delta V(k)$. Obviously, in the present case the asymptotic contribution from the singularities is dominant over the exponential decay of Thomas-Fermi type. The result implies that the screened ion-ion interaction in a metal has oscillatory character and ranges over several shells of neighbours.

[4] M. Lighthill, "Introduction to Fourier Analysis and Generalized Functions" (University Press, Cambridge 1958)