Kohn anomaly

Kohn anomaly is a singularity in the charge susceptibility at $q = 2K_F$. The textbook (AM) gives a full expression for the charge susceptibility valid for any q. I will focus here only in the vicinity of $2K_F$.

We start with a general expression for χ_c (Lindhard function)

$$\chi_c = 2e^2 \int \frac{d^3k}{(2\pi)^3} \frac{f_{\vec{k}} - f_{\vec{k}+\vec{q}}}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + \hbar\omega} .$$

At $\omega = 0$, the integrand has a pole determined by the condition $\varepsilon_{\vec{k}+\vec{q}} = \varepsilon_{\vec{k}}$. To regularize the singularity, we need to introduce infinitesimall weak damping, which amounts to replacing $\hbar\omega$ by $\hbar\omega + i\delta$. (the origin of this term can be understood using the semiclassical derivation of χ_c based on the Boltzmann eq-n. Suppose that we introduce very weak scattering modeled by the $-\frac{f-f_0}{\tau}$ term:

$$\frac{\partial f}{\partial t} + \vec{q}\cdot\vec{\nabla}_{\vec{r}} f + \vec{F}\cdot\vec{\nabla}_p f = -\frac{f-f_0}{\tau} .$$

this amounts to adding $\frac{i}{\tau}$ to ω.)

With such regularization, we can set $\omega = 0$

$$\chi_c(\vec{q},0) = 2e^2 \int \frac{d^3k}{(2\pi)^3} \frac{f_k - f_{\vec{k}+\vec{q}}}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + i\delta} .$$

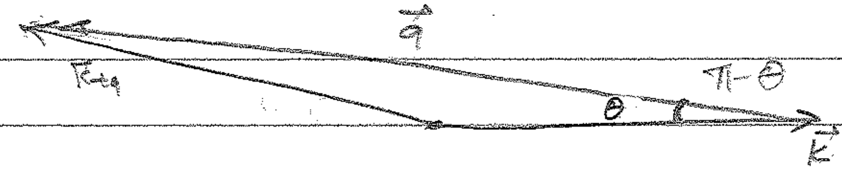
Shifting the variable in the 2^{nd} term as $\vec{k}+\vec{q} \to \vec{k}$ we obtain change of variable $\vec{k} \to -\vec{k}$

$$\chi_c(\vec{q},0) = 2e^2 \times \int \frac{d^3k}{(2\pi)^3} f_{\vec{k}} \left[\frac{1}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_k + i\delta} - \frac{1}{\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{q}} + i\delta} \right]$$

$$= 2e^2 \times \int \frac{d^3k}{(2\pi)^3} f_{\vec{k}} \left[\frac{1}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_k + i\delta} - \frac{1}{\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}} + i\delta} \right]$$

$$= 4e^2 \,\mathrm{Re} \int \frac{d^3k}{(2\pi)^3} f_{\vec{k}} \frac{1}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_k + i\delta} .$$

As we see, adding $i\delta$ makes χ_c manifestly real. For the inital state near the FS ($k \approx k_F$) and $q \approx 2k_F$, the final state $\vec{k}+\vec{q}$ is almost at the diametrically point of the FS.



For $k \approx k_F$, the energy $\varepsilon_{\vec{k}}$ can be written as

$$\varepsilon_k = \frac{\hbar k^2}{2m} = \hbar\left[\frac{k^2 - k_F^2}{2m} + \frac{k_F^2}{2m} = \frac{(k-k_F)(k+k_F)}{2m}\right] + \varepsilon_F$$

$$\approx \hbar v_F (k - k_F) + \varepsilon_F = \xi_k + \varepsilon_F$$

where $\xi_k \equiv \hbar v_F(k-k_F)$ is the excitation energy. We also introduce $q' = q - 2k_F$, $|q'| \ll k_F$ and angle φ with magnitude $|\varphi| \ll 1$, as shown in the figure. In terms of these variables, $\varepsilon_{\vec{k}+\vec{q}}$ can be written as

$$\varepsilon_{\vec{k}+\vec{q}} = \hbar^2\left[\frac{k^2}{2m} - \frac{k \cdot q}{m}\cos\theta + \frac{q^2}{2m}\right] =$$

$$= \xi_k + \varepsilon_F - \hbar^2\left(k_F + \frac{\xi_k}{v_F}\right)(q' + 2k_F)\left(1 - \frac{\theta^2}{2}\right) +$$
$$+ 2\varepsilon_F + 2\hbar q' v_F + O(q'^2)$$

Expanding the product of the factors to linear order in ξ_k, q' and φ^2 we obtain

$$\varepsilon_{\vec{k}+\vec{q}} = \varepsilon_F - \xi_k + \hbar q' v_F + 2\varepsilon_F \theta^2 .$$

Therefore,

$$\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_k = -2\xi_k + \hbar q' v_F + 2\varepsilon_F \varphi^2 .$$

The integral over $\vec{k}$ is contained by the Fermi function to run from $k=0$ to $k=k_F$. This means that $\xi_k < 0$. The integration measure is transformed as

$$2\int_{0<k<k_F} \frac{d^3k}{(2\pi)^3} = \frac{g(\varepsilon_F)}{2} \int_{-\Lambda}^{0} d\xi_k \int_{-\theta_0}^{\theta_0} d\theta \underbrace{\sin\theta}_{\approx\theta} = \frac{g(\varepsilon_F)}{2} \int_{-\Lambda}^{0} d\xi_k \int_{-\theta_0}^{\theta_0} d\theta\, \theta ,$$

where Λ is an arbitrary cut off in energy and θ_0 in angle.

Thus

$$\chi_c(\vec{q},0) = \frac{g(\varepsilon_F)}{2} \,\mathrm{Re} \int_{-\Lambda}^{0} d\xi_k \int_{-\theta_0}^{\theta_0} d\theta\, \theta \, \frac{1}{-2\xi_k + \hbar q' v_F + 2\varepsilon_F\theta^2 - i\delta}$$

To eliminate the dependence on Λ, we subtract χ_c exactly at $q = 2k_F$ (or $q' = 0$)

$$\delta\chi_c(\vec{q},0) \equiv \chi_c(q,0) - \chi_c(2k_F,0)$$

$$= \frac{g(\varepsilon_F)}{2}\,\mathrm{Re} \int_{-\infty}^{0} d\xi_k \int d\theta\, \theta \left\{ \frac{1}{-2\xi_k + \hbar q' v_F + 2\varepsilon_F\theta^2 - i\delta} - \frac{1}{-2\xi_k + 2\varepsilon_F\theta^2 - i\delta} \right\}.$$

The integral over ξ_k is now convergent and yields

$$\delta\chi_c(q,0) = \frac{g(\varepsilon_F)}{2}\mathrm{Re}\int_{-\theta_0}^{\theta_0} d\theta\,\theta \quad \ln \frac{2\varepsilon_F\theta^2 \ldots}{q' v_F + 2\varepsilon_F\theta^2 - i\delta}$$

$$= \frac{1}{2} g(\varepsilon_F) \int_0^{\theta_0^2} dx \quad \ln \frac{x}{\left|\frac{q'}{k_F} + x\right|}$$

with $x \equiv \theta^2$.

For $q' > 0$, $\left|\frac{q'}{k_F} + x\right| = \frac{q'}{k_F} + x$.

Making use of $\int dy \ln y = y(\ln y - 1)$, we obtain

$$\delta\chi_c(q > 2k_F, 0) = \frac{1}{2} g(\varepsilon_F) \left\{ \theta_0^2 \left[\ln\theta_0^2 - 1\right] - \left[\theta_0^2 + \frac{q'}{k_F}\right] \times \right.$$
$$\left. \times \left[\ln\left[\theta_0^2 + \frac{q'}{k_F}\right] - 1\right] + \frac{q'}{k_F}\left[\ln\frac{q'}{k_F} - 1\right] \right\}$$

at $q' \to 0$ and θ_0 fixed, the most singular term in $\delta\chi_c$ is the last one:

$$\delta\chi_c(q > 2k_F, 0) = \frac{1}{2} g(\varepsilon_F) \frac{q'}{k_F} \ln \frac{q'}{k_F}.$$

For $q' < 0$, we have

$$\delta\chi_c(q,0) = \frac{1}{2} g(\varepsilon_F) \left\{ \int_0^{\frac{|q'|}{k_F}} dx \ln \frac{x}{\frac{|q'|}{k_F} - x} + \int_{\frac{|q'|}{k_F}}^{\theta_0^2} dx \ln \frac{x}{x - \frac{|q'|}{k_F}} \right\}$$

$$= \frac{1}{2} g(\varepsilon_F) \left\{ \underbrace{\int_0^{|q'|/k_F} dx \ln x - \int_0^{|q'|/2k_F} dx \ln x}_{=0} + \int_{\frac{|q'|}{k_F}}^{\theta_0^2} dx \ln x - \right.$$

$$\left. - \int_0^{\theta_0^2 - |q'|/k_F} \ln x \, dx \right\} = \frac{1}{2} g(\varepsilon_F)(-)\frac{|q'|}{k_F} \ln\frac{|q'|}{k_F} =$$

$$= \frac{1}{2} g(\varepsilon_F) \frac{q'}{k_F} \ln \frac{|q'|}{k_F}$$

Restoring $q = q' + 2k_F$, we write the singular part of χ_c as

$$\delta\chi_c = \frac{1}{2}\, g(\varepsilon_F)\, \frac{q-2k_F}{k_F} \ln \frac{|q-2k_F|}{k_F}.$$

χ_c by itself is continuous but its derivative has a log singularity: $\frac{\partial}{\partial q}\delta\chi_c \propto \ln\frac{|q-k_F|}{k_F}$.

Friedel oscillations

Even such a weak singularity does lead to a new effect: Friedel oscillations in the induced electron density. Recall that

$$\varphi(r) = \int \frac{d^3q}{(2\pi)^3}\, \tilde{\varphi}(q)\, e^{iq\cdot r\cos\theta} =$$

$$= \frac{2}{\pi}\frac{1}{r}\int dq\, q \cdot \tilde{\varphi}(q)\, \sin qr$$

Suppose the $\tilde{\varphi}(q)$ results from introducing point charge Q, then

$$\tilde{\varphi}(q) = \frac{4\pi Q}{q^2}\, \frac{1}{\epsilon(q,0)} = \frac{4\pi Q}{q^2}\, \frac{1}{1 - \frac{4\pi}{q^2}\chi_c(q,0)}$$

The singular part of $\tilde{\varphi}(q)$ result from that of χ_c. Expanding in $\delta\chi_c$, we obtain for the singular part of $\tilde{\varphi}(q)$

$$\delta\tilde{\varphi}(q) = \frac{16\pi^2 Q}{q^4}\, \delta\chi_c(q,0).$$

Everywhere but in the singular part one can set $q = 2k_F \Rightarrow$

$$\delta\tilde{\varphi}(q') = \frac{16\pi^2 Q}{(2k_F)^4} \frac{1}{2} g(\varepsilon_F) \frac{q'}{k_F} \ln \frac{|q'|}{k_F} =$$

$$= A \; q' \ln (|q'|/k_F) \text{, where } A = \text{const.}$$

Oscillatory part of $\varphi(r)$

$$\varphi_{osc}(r) = \frac{2}{\pi} \frac{1}{r} \int^{2k_F} dq \, q \; \delta\tilde{\varphi}(q') \sin(q'+2k_F)r$$

$$= A' \frac{1}{r} \int dq' \; q' \ln \frac{|q'|}{k_F} \Big(\sin(q'r) \cos 2k_F r +$$

$$+ \cos(q'r) \sin 2k_F r \Big).$$

In the integral $q'r$ forms a dimensionless variable. Rescaling q' by $\frac{1}{r}$, we obtain

$$\varphi_{osc}(r) \propto \frac{1}{r^3} \cos(2k_F r + \delta_0)$$

where δ_0 is a phase shift.