

## Lindhard Dielectric Function - fixes Thomas-Fermi at large $\bar{k}$ .

Consider a potential  $U(\vec{r})$  applied to the electron gas. (for an electrostatic potential  $U = -eV^{tot}$ )

To compute the change in electron density  $\delta n(\vec{r})$  we could compute the effect of  $U$  on electron eigenstates, and then use these new eigenstates to compute  $\delta n$ , summing over all occupied eigenstates

Using ~~stationary~~ Rayleigh-Schrodinger stationary perturbation theory, to lowest order in  $U$  the eigenstates become

$$|\psi_k\rangle = |k\rangle + \sum_{k'} \frac{|k'\rangle \langle k'|U|k\rangle}{E_k - E_{k'}}$$

where  $|k\rangle$  is the unperturbed plane wave eigenstate with energy  $E_k = \hbar^2 k^2 / 2m$ , and  $|\psi_k\rangle$  is the new eigenstate resulting from the perturbation  $U$ .

The electron density as a function of position for the state  $|\psi_k\rangle$  is

$$|\langle r | \psi_k \rangle|^2$$

so the change in electron density due to the perturbation  $U$  is

$$|\langle r | \psi_k \rangle|^2 - |\langle r | k \rangle|^2$$

$$= \langle \psi_k | r \rangle \langle r | \psi_k \rangle - \langle k | r \rangle \langle r | k \rangle$$

$$= \left[ \langle r|k \rangle + \sum_{k'} \frac{\langle r|k' \rangle \langle k'|U|k \rangle}{\epsilon_k - \epsilon_{k'}} \right] \left[ \langle k|r \rangle + \sum_{k'} \frac{\langle k'|r \rangle \langle r|U|k' \rangle}{\epsilon_k - \epsilon_{k'}} \right] - \langle k|r \rangle \langle r|k \rangle$$

To linear order in  $U$  this gives

$$= \sum_{k'} \left\{ \frac{\langle r|k \rangle \langle k'|r \rangle \langle k'|U|k \rangle}{\epsilon_k - \epsilon_{k'}} + \frac{\langle k|r \rangle \langle r|k' \rangle \langle k'|U|k \rangle}{\epsilon_k - \epsilon_{k'}} \right\}$$

Now  $\langle r|k \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$   $V = \text{volume}$

$$\langle k|r \rangle = \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$$

$$\langle k'|U|k \rangle = \int \frac{d^3r}{V} e^{-i\vec{k}'\cdot\vec{r}} U(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

$$= \frac{1}{V} \int d^3r e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} U(\vec{r})$$

$$= \frac{1}{V} U_{\vec{k}'-\vec{k}} \quad \text{Fourier transf of } U(\vec{r})$$

So above is

$$= \frac{1}{V^2} \sum_{k'} \left\{ \frac{e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} U_{\vec{k}-\vec{k}'}}{\epsilon_k - \epsilon_{k'}} + \frac{e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} U_{\vec{k}'-\vec{k}}}{\epsilon_k - \epsilon_{k'}} \right\}$$

The total induced electron density  $\delta n$  is obtained by summing over all occupied states  
 spin degeneracy

$$\delta n(\vec{r}) = 2 \sum_{\vec{k}} f_{\vec{k}} \frac{1}{V} \sum_{\vec{k}'} \left\{ e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} \frac{U_{\vec{k} - \vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} + e^{-i(\vec{k} - \vec{k}') \cdot \vec{r}} \frac{U_{\vec{k}' - \vec{k}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} \right\}$$

where  $f_{\vec{k}}$  is the Fermi occupation function  $\frac{1}{e^{(\epsilon_{\vec{k}} - \mu)/k_B T} + 1}$

Fourier transform to get  $\delta n(\vec{q})$

$$\begin{aligned} \delta n(\vec{q}) &= \int d^3r e^{-i\vec{q} \cdot \vec{r}} \delta n(\vec{r}) \\ &= \frac{1}{V} \sum_{\vec{k}, \vec{k}'} f_{\vec{k}} \left\{ \frac{V \delta_{\vec{q}, \vec{k} - \vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} U_{\vec{k} - \vec{k}'} + \frac{V \delta_{\vec{q}, \vec{k}' - \vec{k}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}} U_{\vec{k}' - \vec{k}} \right\} \end{aligned}$$

where the integrals over the plane wave factors give the  $V \delta_{\vec{q}, \vec{k} - \vec{k}'}$  terms. Now use the  $\delta$ 's to do the sum on  $\vec{k}'$ .

$$\delta n(\vec{q}) = \frac{2}{V} \sum_{\vec{k}} f_{\vec{k}} \left\{ \frac{U_{\vec{q}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k} - \vec{q}}} + \frac{U_{\vec{q}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k} + \vec{q}}} \right\}$$

So

$$\frac{\delta n(\vec{q})}{U_{\vec{q}}} = \frac{2}{V} \sum_{\vec{k}} f_{\vec{k}} \left\{ \frac{1}{\epsilon_{\vec{k}} - \epsilon_{\vec{k} - \vec{q}}} + \frac{1}{\epsilon_{\vec{k}} - \epsilon_{\vec{k} + \vec{q}}} \right\}$$

Now make substitution  $\vec{k}' = \vec{k} - \vec{q}$  in first summation term to get

$$\frac{\delta m(q)}{U_q} = \frac{2}{V} \sum_{\vec{k}} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}}$$

$$\frac{\delta m(q)}{U_q} = \int \frac{d^3k}{4\pi^3} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}}$$

For electrostatic potential,  $U_q = -eV_{\vec{q}}^{\text{tot}}$ ,  
and  $\delta p = -e\delta m$ , so

~~$$\frac{\delta p}{V_{\text{tot}}}$$~~

$$\frac{\delta p(q)}{V_{\text{tot}}(q)} = \frac{-e\delta m_q}{U_q/(-e)} = e^2 \frac{\delta m_q}{U_q}$$

$$= e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}}$$

For small  $q$ ,  $f_{\vec{k}+\vec{q}} - f_{\vec{k}} \approx \frac{\partial f}{\partial \epsilon} \frac{\partial \epsilon}{\partial \vec{q}} \cdot \vec{q}$

$$\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} \approx \frac{\partial \epsilon}{\partial \vec{q}} \cdot \vec{q}$$

$$\frac{\delta p}{V_{\text{tot}}} = e^2 \int \frac{d^3k}{4\pi^3} \frac{\partial f}{\partial \epsilon} = e^2 \int d\epsilon g(\epsilon) \frac{\partial f}{\partial \epsilon}$$

as  $T \rightarrow 0$   $\frac{\partial f}{\partial \epsilon} \rightarrow -\delta(\epsilon - \epsilon_F)$

$$\frac{\delta p}{V_{\text{tot}}} = -e^2 g(\epsilon_F), \text{ so } \epsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \frac{\delta p}{V_{\text{tot}}} = 1 + \frac{4\pi e^2}{q^2} g(\epsilon_F)$$

Same as  
Thomas-Fermi  
result

Friedel oscillations + Kohn anomaly

Lindhard dielectric function at bigger q

$$\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} \sum_k \frac{f_k - f_{k+q}}{\epsilon_{k+q} - \epsilon_k}$$

$$\epsilon_{k+q} - \epsilon_k = \left( \frac{q^2 + 2\vec{k} \cdot \vec{q}}{2m} \right) \hbar^2$$

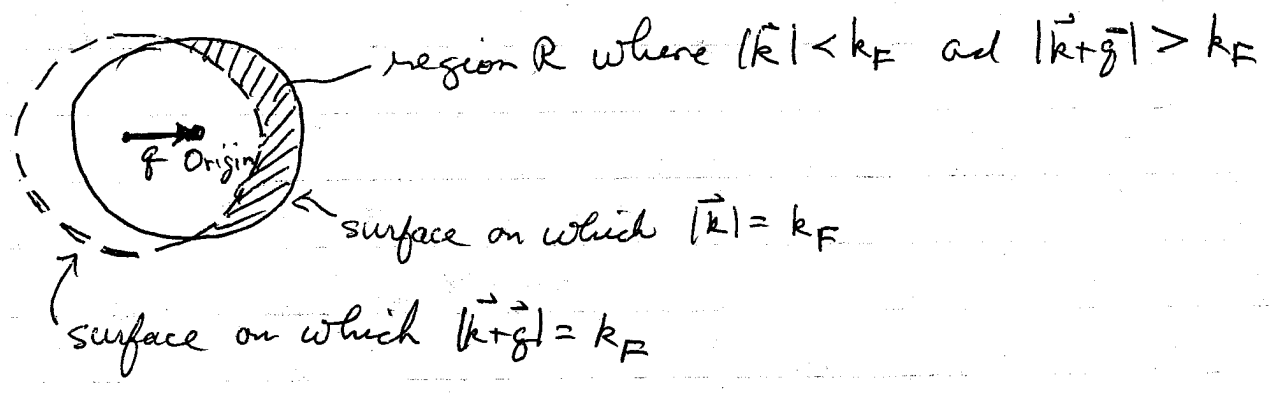
$$\epsilon_k = \frac{\hbar^2 k^2}{2m}$$

$$\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} \frac{2m}{\hbar^2} \int_R \frac{d^3k}{(2\pi)^3} \frac{1}{q^2 + 2\vec{k} \cdot \vec{q}}$$

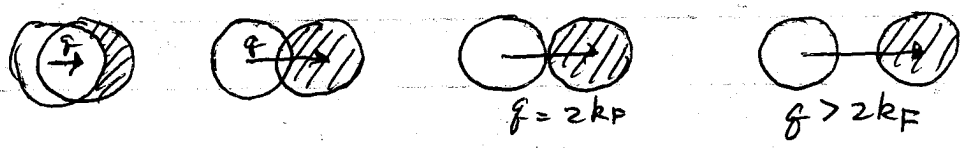
spin up  
or down  
x 2 x 2  
[k+q full  
k empty]

Region of k-space  
such that [k full  
k+q empty]

The region R is such that  $|\vec{k}| < k_F$  and  $|\vec{k} + \vec{q}| > k_F$   
We can depict it graphically as



as q increases, region R also increases until  $q \geq 2k_F$



The integral  $\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} \frac{g m}{\hbar^2} \int_R \frac{d^3 k}{(2\pi)^3} \frac{1}{q^2 + 2\vec{k} \cdot \vec{q}}$   
 can be done explicitly and one gets

$$\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} g(\epsilon_F) \left[ \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right| \right]$$

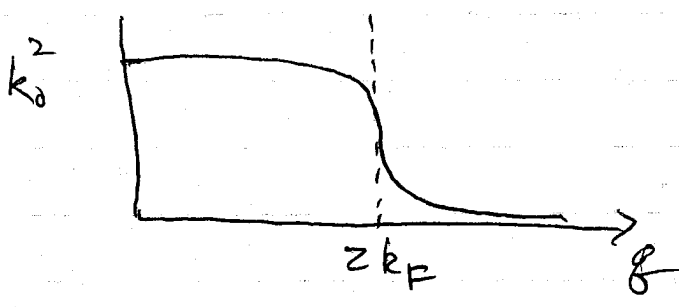
where  $x = q/2k_F$

as  $x \rightarrow 0$ ,  $[\dots] = 1$  and we get back Thomas-Fermi result  
 at  $x=1$ , i.e.  $q=2k_F$ ,  $\epsilon(q)$  has a logarithmic singularity

If we formally write  $\epsilon(q) = 1 + \frac{k_0^2(q)}{q^2}$

to define a  $q$  dependent screening length  $k_0(q)$   
 then

$$\frac{k_0^2(q)}{k_0^2(0)} = [\dots]$$



as  $q$  increases the effective screening length  $1/k_0$  increases.  
 Screening is less effective at small length scales than in Thomas Fermi approx

If you take the Fourier transf of  $\frac{4\pi Q}{q^2 \epsilon(q)}$   
 to get real space potential of a point charge,

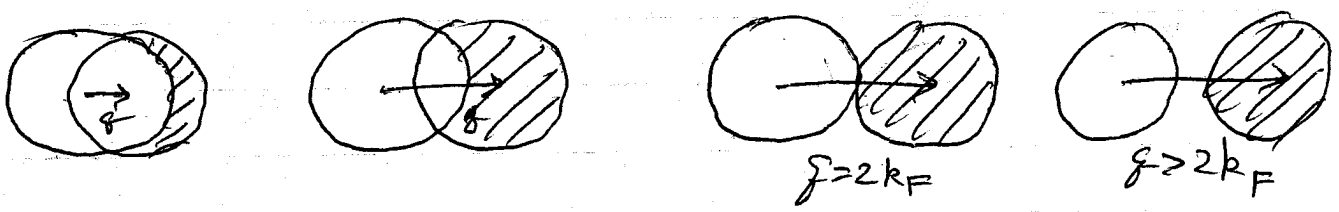
the singularity at  $q = 2k_F$  gives rise to a piece

$$\sim \frac{1}{r^3} \cos(2k_F r)$$

decays more slowly than T-F and oscillates in sign, electron is alternatively attracted and repelled by the charge Q with a period  $\frac{\pi}{k_F}$

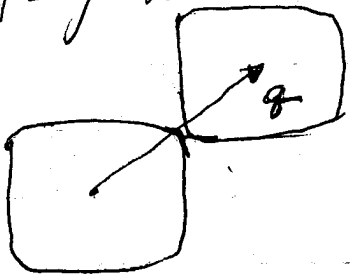
These are known as "Friedel" or "Ruderman-Kittel" oscillations. These are important for giving the "RKKY" interaction between magnetic impurities, that is the origin of "spin glasses". - see homework problem for details.

The origin of the singularity at  $q = 2k_F$  is understood more physically in terms of the behavior of the region of integration R.



As  $q$  increases, the region R increases, until  $q = 2k_F$ . When  $q > 2k_F$ , R is the entire Fermi sphere and no longer changes as  $q$  increases further. This singularity in the volume R gives rise to the singularity in  $\epsilon(q)$  at  $q = 2k_F$

This is true also for more generally shaped Fermi surfaces -  $\epsilon(\vec{q})$  will be singular for any  $\vec{q}$  that displaces the Fermi surfaces so they touch at a tangential point.



Kohn effect: a phonon (ion lattice vibration) at ~~such~~ a wavevector  $\vec{q}$  sets up an electrostatic potential with wavevector  $\vec{q}$ .

If  $\vec{q}$  is just such a critical  $\vec{q}$  as above, where  $\epsilon(\vec{q})$  has a singularity, the screened ion-ion interaction will be proportional to  $1/\epsilon(\vec{q})$ , and also have a singularity. Since the phonon frequency  $\omega(\vec{q})$  is determined by the ion-ion interaction, we expect to see  $\omega(\vec{q})$  have a weak singularity at the above critical  $\vec{q}$ 's.