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

Consider a potential $\mathcal{U}(\vec{r})$ applied to the electron gas. (for an electrostatic potential $\mathcal{U} = -eV^{tot}$)
To compute the change in electron density $\delta n(\vec{r})$ we could compute the effect of $\mathcal{U}$ on electron eigenstates, and then ~~use~~ these new eigenstates to compute δn, summing over all occupied eigenstates

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

$$|\psi_k\rangle = |k\rangle + \sum_{k'} \frac{|k'\rangle\langle k'|\mathcal{U}|k\rangle}{\varepsilon_k - \varepsilon_{k'}}$$

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

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 $\mathcal{U}$ is

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

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

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

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

To linear order in $\mathcal{U}$ this gives

$$= \sum_{k'} \left\{ \frac{\langle r|k\rangle\langle k'|r\rangle\langle k|\mathcal{U}|k'\rangle}{\varepsilon_k - \varepsilon_{k'}} + \frac{\langle k|r\rangle\langle r|k'\rangle\langle k'|\mathcal{U}|k\rangle}{\varepsilon_k - \varepsilon_{k'}} \right\}$$

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

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

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

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

$$= \frac{1}{V}\, \mathcal{U}_{k'-k}$$ Fourier transf of $\mathcal{U}(\vec{r})$

So above is

$$= \frac{1}{V^2} \sum_{k'} \left\{ \frac{e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}}\, \mathcal{U}_{k-k'}}{\varepsilon_k - \varepsilon_{k'}} + \frac{e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}\, \mathcal{U}_{k'-k}}{\varepsilon_k - \varepsilon_{k'}} \right\}$$

The total induced electron density δn is obtained by summing over all occupied states

spin degeneracy

$$\delta n(\vec{r}) = 2\sum_k f_k \frac{1}{V^2}\sum_{k'} \left\{ \frac{e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}}\, u_{k-k'}}{\varepsilon_k - \varepsilon_{k'}} + \frac{e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}\, u_{k'-k}}{\varepsilon_k - \varepsilon_{k'}} \right\}$$

where f_k is the Fermi occupation function $\frac{1}{e^{(\varepsilon_k-\mu)/k_BT}+1}$

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

$$\delta n(q) = \int d^3r\, e^{-i\vec{q}\cdot\vec{r}}\, \delta n(\vec{r})$$

$$= \frac{1}{V^2} 2 \sum_{k,k'} f_k \left\{ \frac{V\delta_{\vec{q},\vec{k}-\vec{k}'}\, u_{k-k'}}{\varepsilon_k - \varepsilon_{k'}} + \frac{V\delta_{\vec{q},\vec{k}'-\vec{k}}\, u_{k'-k}}{\varepsilon_k - \varepsilon_{k'}} \right\}$$

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

$$\delta n(q) = \frac{2}{V}\sum_k f_k \left\{ \frac{u_q}{\varepsilon_k - \varepsilon_{k-q}} + \frac{u_q}{\varepsilon_k - \varepsilon_{k+q}} \right\}$$

So

$$\frac{\delta n(q)}{u_q} = \frac{2}{V}\sum_k f_k \left\{ \frac{1}{\varepsilon_k - \varepsilon_{k-q}} + \frac{1}{\varepsilon_k - \varepsilon_{k+q}} \right\}$$

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

$$\frac{\delta n(q)}{U_q} = \frac{2}{V} \sum_k \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k}$$

$$\frac{\delta n(q)}{U_q} = \int \frac{d^3k}{4\pi^3} \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k}$$

For electrostatic potential, $U_q = -eV_q^{tot}$, and $\delta\rho = -e\,\delta n$, so

$$\frac{\delta\rho(q)}{V^{tot}(q)} = \frac{-e\,\delta n_q}{U_q/(-e)} = e^2 \frac{\delta n_q}{U_q}$$

$$= e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k}$$

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

$$\varepsilon_{k+q} - \varepsilon_q \simeq \frac{\partial \varepsilon}{\partial \vec{q}} \cdot \vec{q}$$

$$\frac{\delta\rho}{V^{tot}} = e^2 \int \frac{d^3k}{4\pi^3} \frac{\partial f}{\partial \varepsilon} = e^2 \int d\varepsilon\, g(\varepsilon) \frac{\partial f}{\partial \varepsilon}$$

as $T \to 0$ $\frac{\partial f}{\partial \varepsilon} \to -\delta(\varepsilon - \varepsilon_F)$

Same as Thomas-Fermi result

$$\frac{\delta\rho}{V^{tot}} = -e^2 g(\varepsilon_F), \text{ so } \epsilon(q) = 1 - \frac{4\pi}{q^2}\frac{\delta\rho}{V^{tot}} = 1 + \frac{4\pi e^2}{q^2} g(\varepsilon_F)$$

Friedel oscillations + Kohn anomaly

Lindhart dielectric function at bigger q

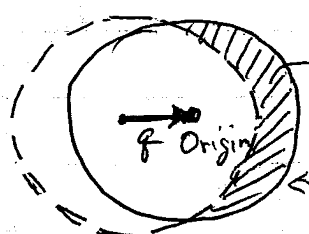
$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2} \sum_k \frac{f_k - f_{k+q}}{\varepsilon_{k+q} - \varepsilon_k}$$

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

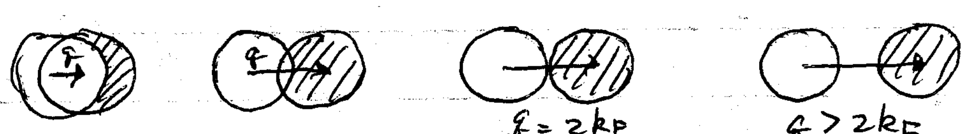
$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2}\,\frac{2m}{\hbar^2} \int_R \frac{d^3k}{(2\pi)^3}\,\frac{1}{q^2 + 2\vec{k}\cdot\vec{q}} \times \underset{\text{spin up or down}}{2} \times \underset{\left[\begin{smallmatrix}k+q \text{ full} \\ k \text{ empty}\end{smallmatrix}\right]}{2}$$

R: Region of k-space such that $\left[\begin{matrix}k \text{ full} \\ k+q \text{ empty}\end{matrix}\right]$

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 $\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2} \frac{8m}{\hbar^2} \int_R \frac{d^3k}{(2\pi)^3} \frac{1}{q^2 + 2\vec{k}\cdot\vec{q}}$

can be done explicitly and one gets

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

where $x = q/2k_F$

as $x \to 0$, $[\cdots] = 1$ and we get back Thomas-Fermi result

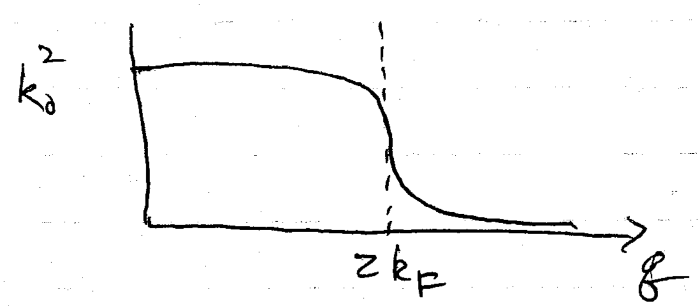
at $x = 1$, ie $q = 2k_F$, $\varepsilon(q)$ has a logarithmic singularity

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

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

Then

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



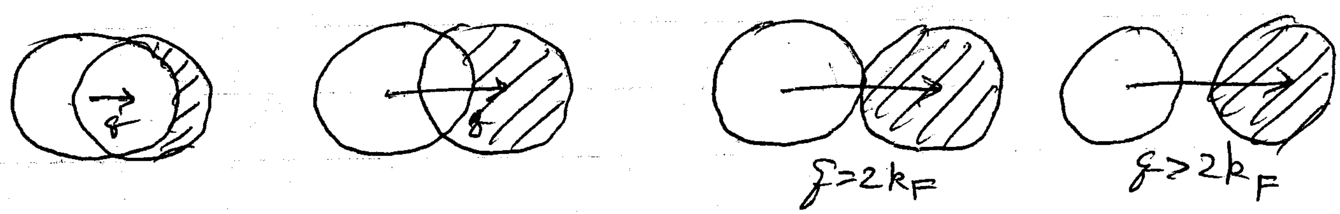
as q increases the effective screening length $1/k_0$ increases. Screening is less effective at small length scales than in Thomas Fermi approx

If you take the Fourier transf of $\frac{4\pi Q}{q^2 \varepsilon(q)}$ 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 $\frac{\pi}{k_F}$

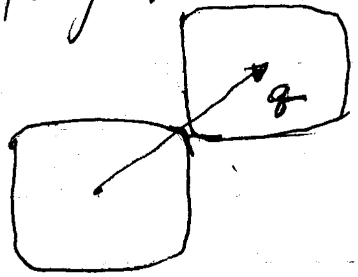
These are known as "Friedel" or "Rudderman-Kittel" oscillations; these are important for giving the "RKKY" interaction between magnetic impurities, that is the origin of "spin glasses". — see homework problem for details.

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 $\mathcal{E}(q)$ at $q = 2k_F$

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



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

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

RKKY Interaction and Spin Glasses

In our discussion of the Lindhard dielectric function we saw that:

If there is a potential energy $U(\vec{r})$ that couples to the electron density, ie the perturbation in the Hamiltonian is

$$\sum_i U(\vec{r}_i) = \int d^3r \, U(\vec{r}) \, n(\vec{r})$$

with $n(\vec{r}) \equiv \sum_i \delta(\vec{r}-\vec{r}_i)$ is the electron density
then U induces a change in electron density $\delta n(\vec{r})$ given, in Fourier transform space, by

$$\delta n(\vec{q}) = \chi(\vec{q}) \, U(\vec{q})$$

with $$\chi(\vec{q}) \equiv \frac{2}{V} \sum_k \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k}$$

where f_k is the Fermi occupation function for the free electron state with wave vector $\vec{k}$ and energy ε_k.

Consider a magnetic impurity with spin $\vec{S}_0$ located at position $\vec{R}_0$. We will assume the interaction of $\vec{S}_0$ with the conduction electrons is via a <u>local</u> spin-spin interaction.

$$\delta H = -J\mu_B \vec{S}_0 \cdot \sum_i \vec{s}_i \, |\psi_i(\vec{R}_0)|^2$$

spin of electron i — probability for electron i to be at position $\vec{R}_0$

$$= J\, \vec{S}_0 \cdot \vec{m}(R_0)$$

magnetization density of electrons

Let us take the direction of $\vec{S}_0$ to be $\hat{z}$. Then

$$\delta H = -J\mu_B S_0 \left[n_\uparrow(\vec{R}_0) - n_\downarrow(\vec{R}_0) \right]$$

density of $\uparrow$ electrons — density of $\downarrow$ electrons

$$= \delta H_\uparrow + \delta H_\downarrow$$

$$\delta H_\uparrow \equiv -J\mu_B S_0 \, n_\uparrow(\vec{R}_0) = \int d^3r \; U_\uparrow(\vec{r})\, n_\uparrow(\vec{r})$$

$$\delta H_\downarrow = +J\mu_B S_0 \, n_\downarrow(\vec{R}_0) = \int d^3r \; U_\downarrow(\vec{r})\, n_\downarrow(\vec{r})$$

$$\text{where} \begin{cases} U_\uparrow(\vec{r}) = -J\mu_B S_0 \, \delta(\vec{r}-\vec{R}_0) \\ U_\downarrow(\vec{r}) = J\mu_B S_0 \, \delta(\vec{r}-\vec{R}_0) \end{cases}$$

We then have that $U_\uparrow$ and $U_\downarrow$ induce perturbations $\delta n_\uparrow$ and $\delta n_\downarrow$ in the spin ↑ and spin ↓ electron densities.

$$\delta n_\uparrow(\vec{q}) = \tfrac{1}{2}\chi(\vec{q})\, U_\uparrow(\vec{q})$$

$$\delta n_\downarrow(\vec{q}) = \tfrac{1}{2}\chi(\vec{q})\, U_\downarrow(\vec{q}) = -\tfrac{1}{2}\chi(\vec{q})\, U_\uparrow(\vec{q})$$

factor of $\frac{1}{2}$ since $n_\uparrow$ and $n_\downarrow$ are both $\frac{1}{2}$ of total density $n = n_\uparrow + n_\downarrow$

induced electron magnetization is then

$$m_z(\vec{q}) = -\mu_B\left[\delta n_\uparrow(\vec{r}) - \delta n_\downarrow(\vec{r})\right]$$
$$= -\mu_B\, \chi(\vec{q})\, U_\uparrow(\vec{q})$$

Now $U_\uparrow(\vec{r}) = -J\mu_B S_0\, \delta(\vec{r}-\vec{R}_0)$

so $U_\uparrow(\vec{q}) = \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}}\, U_\uparrow(\vec{r})$

$$= -J\mu_B S_0\, e^{-i\vec{q}\cdot\vec{R}_0}$$

$$\Rightarrow\ m_z(\vec{r}) = -\int \frac{d^3q}{(2\pi)^3}\, J\mu_B^2 S_0\, \chi_q\, e^{-i\vec{q}\cdot\vec{R}_0}\, e^{i\vec{q}\cdot\vec{r}}$$

$$= -J\mu_B^2 S_0 \int \frac{d^3q}{(2\pi)^3}\, \chi(\vec{q})\, e^{i\vec{q}\cdot(\vec{r}-\vec{R}_0)}$$

$$m_z(\vec{r}) = -J\mu_B^2 S_0\, \chi(\vec{r}-\vec{R}_0)$$

Fourier transform of $\chi(\vec{q})$ evaluated at position $\vec{r}-\vec{R}_0$

induced magnetization is in the same direction as $\vec{S}_0$, so

$$\vec{m}(\vec{r}) = -J\mu_B^2 \vec{S}_0 \, \chi(\vec{r}-\vec{R}_0)$$

For many impurities $\vec{S}_i$ at positions $\vec{R}_i$, the total induced electron magnetization is obtained from the above by superposition

$$\vec{m}(\vec{r}) = -J\mu_B^2 \sum_i \vec{S}_i \, \chi(\vec{r}-\vec{R}_i)$$

The interaction Hamiltonian is then

$$\delta H = J \sum_j \vec{S}_j \cdot \vec{m}(\vec{R}_j)$$

$$\boxed{\delta H = -J^2\mu_B^2 \sum_{i,j} \vec{S}_j \cdot \vec{S}_i \, \chi(\vec{R}_j-\vec{R}_i)}$$

Above result shows how the magnetization of the conduction electrons mediates an interaction between the two magnetic impurities $\vec{S}_i$ and $\vec{S}_j$. If $\chi(\vec{R}_j-\vec{R}_i) > 0$ then the interaction is <u>ferromagnetic</u>. If $\chi(\vec{R}_j-\vec{R}_i) < 0$ then the interaction is anti<u>ferromagnetic</u>.

Now $\chi(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} e^{-i\vec{q}\cdot\vec{r}} \chi(\vec{q})$

with $\chi(\vec{q}) = 2\int \frac{d^3k}{(2\pi)^3} \left[\frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k} \right]$

$$= g(\varepsilon_F) \left[1 + \frac{1-x^2}{2x} \ln\left| \frac{1+x}{1-x} \right| \right]$$

where $x = q/2k_F$

As discussed in connection with the Lindhard dielectric function, $\chi(\vec{q})$ has a singularity at $x=0$ or $|\vec{q}| = 2k_F$. This results in $\chi(\vec{r})$ having a piece that goes as

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

which oscillates in sign depending on the value of the distance r. Since the magnetic impurities $\vec{S}_i$ are randomly positioned in the metal, with an average spacing several times the atomic lattice constant, then $k_F |\vec{R}_i - \vec{R}_j|$ in general is large and hence $\chi(\vec{R}_i - \vec{R}_j)$ will be randomly positive or negative, according to the particular random separation between the spins. Thus the interaction between spins $\vec{S}_i$ and $\vec{S}_j$ is randomly ferro or anti-ferro magnetic. This is the the model interaction for a "spin glass" where the spins freeze into random orientations as T decreases