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

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 δn, summing over all occupied eigenstates.

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

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

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

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

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

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

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

To linear order in U this gives

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

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

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

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

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

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

So above is

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

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 $\dfrac{1}{e^{(\varepsilon_k-\mu)/k_BT}+1}$

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

$$\varepsilon_{k+q} - E_q \approx \frac{\partial \varepsilon}{\partial \vec{q}} \cdot \vec{q}$$

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

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

Same as Thomas-Fermi result

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

Friedel oscillations + Kohn anomaly

Lindhart dielectric function at bigger q

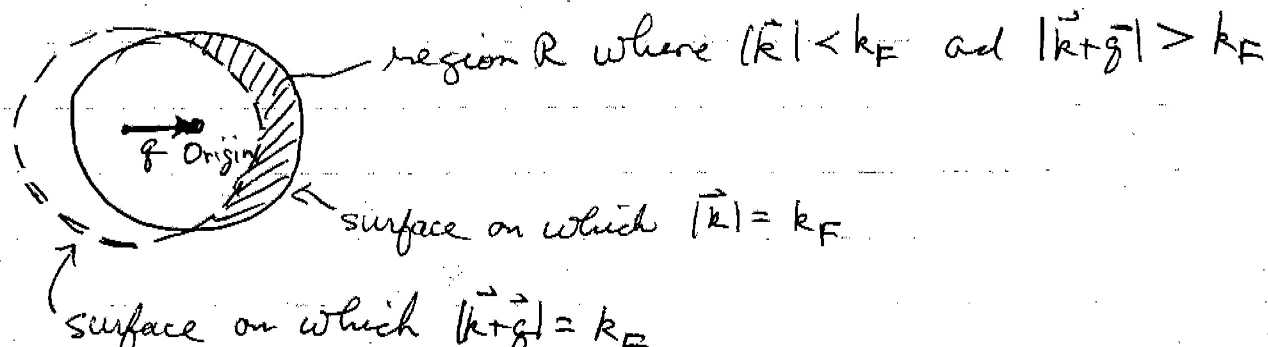
$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2}\sum_k \frac{f_k - f_{k+q}}{\varepsilon_{k+q} - \varepsilon_k}$$

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

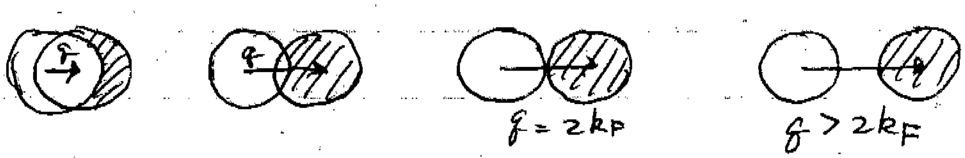
$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2}\frac{2m}{\hbar^2}\int_R \frac{d^3k}{(2\pi)^3}\frac{1}{q^2 + 2\vec{k}\cdot\vec{q}} \times \underbrace{2}_{\text{spin up or down}} \times \underbrace{2}_{\left[\begin{smallmatrix}k+q \text{ full} \\ k \text{ empty}\end{smallmatrix}\right]}$$

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

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

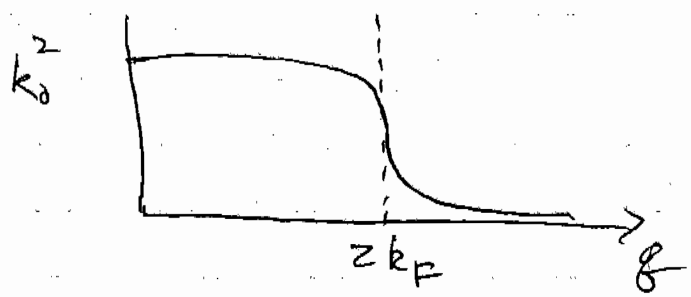
where $x = q/2k_F$

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

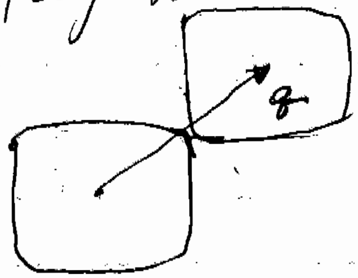
$\sim \frac{1}{r^3} \cos(2k_F r)$ decays more slowly than T-F and oscillates in sign. electron is alternatively attracted and repelled by the charge Q with a period $\frac{\pi}{k_F}$

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 $\epsilon(q)$ at $q = 2k_F$

This is true also for more generally shapped Fermi surfaces — $\varepsilon(\vec{q})$ 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 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 $1/\varepsilon(\vec{q})$, 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.