Lindhard Dielectric Function - Fixas Thomas-Ferr

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

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

Using stationary Rayleigh-Schrödinger stationary perturbation theory, to lowest order in \( U \) the eigenstates become

\[
|\psi_{k}'\rangle = |\psi_{k}\rangle + \sum_{k'} \frac{|\psi_{k'}\rangle \langle k'|U|k\rangle}{E_{k} - E_{k'}}
\]

where \( |\psi_{k}\rangle \) is the unperturbed plane wave eigenstate with energy \( E_{k} = \frac{1}{2}m^{*}k^{2}/\hbar^{2} \), 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

\[
|\langle r|\psi_{k}'\rangle|^{2} - |\langle r|\psi_{k}\rangle|^{2} = \langle \psi_{k}'|\psi_{k}' \rangle - \langle \psi_{k}|\psi_{k} \rangle
\]

\[
= \langle \psi_{k}'|\psi_{k}' \rangle - \langle \psi_{k}|\psi_{k} \rangle
\]
\[
\begin{align*}
&= \left[ \langle \eta | k \rangle + \sum_{k'} \frac{\langle r | k' \times k' | w k \rangle}{\varepsilon_k - \varepsilon_{k'}} \right] \left[ \langle k l r | + \sum_{k'} \frac{\langle k | l r \rangle \langle k | w k \rangle}{\varepsilon_k - \varepsilon_{k'}} \right] \\
&\quad - \langle k l r | \langle r | k \rangle \\
\end{align*}
\]

To linear order in \( U \), this gives

\[
\begin{align*}
&= \sum_{k'} \left\{ \frac{\langle r | k \times k' | l r \rangle \langle k | w k' \rangle}{\varepsilon_k - \varepsilon_{k'}} + \frac{\langle k | l r \rangle \langle r | k' \times k' | w k \rangle}{\varepsilon_k - \varepsilon_{k'}} \right\} \\
\end{align*}
\]

Now \( \langle r | k \rangle = \frac{e^{i \mathbf{k} \cdot \mathbf{r}}}{\sqrt{V}} \), \( V = \text{volume} \)

\[
\begin{align*}
\langle k l r | = \frac{e^{-i \mathbf{k} \cdot \mathbf{r}}}{\sqrt{V}} \\
\langle k' l w k \rangle = \frac{\int d^3r}{V} e^{-i \mathbf{k} \cdot \mathbf{r}} U(\mathbf{r}) e^{i \mathbf{k} \cdot \mathbf{r}} \\
\end{align*}
\]

\[
\begin{align*}
= \frac{1}{V} \int d^3r e^{-i (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} U(\mathbf{r}) \\
= \frac{1}{V} U_{k'k} \quad \text{Fourier transform of } U(\mathbf{r}) \\
\end{align*}
\]

So above is

\[
\begin{align*}
&= \frac{1}{V^2} \sum_{k' k} \left\{ \frac{e^{-i (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}}}{\varepsilon_k - \varepsilon_{k'}} U_{k-k'} + \frac{e^{-i (\mathbf{k} - \mathbf{k}) \cdot \mathbf{r}}}{\varepsilon_k - \varepsilon_{k'}} U_{k'k} \right\} \\
\end{align*}
\]
The total induced electron density $\delta m$ is obtained by summing over all occupied states.

Spin degeneracy

$$\delta m(r) = \sum_{k} \left( \frac{1}{V} \sum_{k'} \left\{ e^{-\frac{i\langle k', k \rangle \cdot \mathbf{r}}} \left( \frac{U_{k+k'}}{\varepsilon_k - \varepsilon_{k'}} + \frac{U_{k-k'}}{\varepsilon_k - \varepsilon_{k'}} \right) + \frac{1}{2} \delta_{k, k'} \right\} \right)$$

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

Fourier transform to get $\delta m(q)$

$$\delta m(q) = \int d^3r \ e^{i\mathbf{q} \cdot \mathbf{r}} \delta m(r)$$

$$= \frac{1}{V} \sum_{k} f_k \left\{ \frac{V \delta_{k, k'}}{\varepsilon_k - \varepsilon_{k'}} U_{k+k'} + \frac{V \delta_{k, -k'}}{\varepsilon_k - \varepsilon_{k'}} U_{k-k'} \right\}$$

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

$$\delta m(q) = \frac{2}{V} \sum_{k} f_k \left\{ \frac{U_{k}}{\varepsilon_k - \varepsilon_{k-q}} + \frac{U_{k}}{\varepsilon_k - \varepsilon_{k+q}} \right\}$$

So

$$\frac{\delta m(q)}{U_q} = \frac{2}{V} \sum_{k} f_k \left\{ \frac{1}{\varepsilon_k - \varepsilon_{k-q}} + \frac{1}{\varepsilon_k - \varepsilon_{k+q}} \right\}$$
Now make substitution \( h' = \frac{h}{\epsilon_0} \) in last summation term to get

\[
\frac{S_{m}(g)}{U_g} = \frac{2}{V} \sum_{k} \frac{f_{k+g} - f_k}{\epsilon_{k+g} - \epsilon_k}
\]

\[
\frac{S_{m}(g)}{U_g} = \int \frac{d^3k}{4\pi^3} \frac{f_{k+g} - f_k}{\epsilon_{k+g} - \epsilon_k}
\]

For electrostatic potential, \( U_g = -eV_{tot} \)
and \( \delta p = -eS_m \), so

\[
\frac{\delta p}{\delta V_{tot}} \bigg|_{g} = -eS_m \frac{e^2}{U_g/(-e)} \frac{S_{m}}{U_g}
\]

\[
= e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{k+g} - f_k}{\epsilon_{k+g} - \epsilon_k}
\]

For small \( g \), \( f_{k+g} - f_k \approx \frac{\partial f}{\partial \epsilon} \frac{2\epsilon}{\delta g} \cdot \frac{\epsilon_{k+g} - \epsilon_k}{2}\)

\[
\epsilon_{k+g} - \epsilon_k \approx \frac{2\epsilon}{\delta g} \cdot \frac{\epsilon_{k+g} - \epsilon_k}{2}
\]

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

as \( T \to 0 \) \( \frac{\partial f}{\partial \epsilon} \to -8(\epsilon - \epsilon_F) \)

\[
\frac{\delta p}{\delta V_{tot}} = -e^2 g(\epsilon_F), \quad \text{so} \quad \epsilon(\epsilon) = -\frac{4\pi}{\beta^2} \frac{\delta p}{\delta V_{tot}} + 1 + \frac{4\pi e^2}{\beta^2} \]
Friedel oscillations and Kohn anomaly

Lindhard dielectric function at higher $g$

$$\varepsilon(g) = 1 + \frac{4\pi e^2}{\varepsilon_0 k} \sum_k \frac{\varepsilon_k f_k - f_{k+g}}{\varepsilon_{k+g} - \varepsilon_k}$$

$$\varepsilon_{k+g} - \varepsilon_k = \left( \frac{\varepsilon_0}{2m} \right)^2 g^2$$

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

$$\varepsilon(g) = 1 + \frac{4\pi e^2}{\varepsilon_0 k} \frac{2m}{\hbar^2} \int R \frac{d^3k}{(2\pi)^3} \frac{1}{\varepsilon_0^2 + 2k \cdot f}$$

Region of $k$-space such that

- $k$ full
- $k+g$ empty

The region $R$ is such that $|k| < k_F$ and $|k+g| > k_F$

We can depict it graphically as

The region $R$ where $|k| < k_F$ and $|k+g| > k_F$

Surface on which $|k| = k_F$

Surface on which $|k+g| = k_F$

As $g$ increases, region $R$ also increases until $g > 2k_F$
The integral 
\[ \varepsilon(q) = 1 + \frac{4\pi e^2}{g^2} \frac{g_m}{m} \int \frac{d^3k}{(2\pi)^3} \frac{1}{g^2 + 2k \cdot q - \Delta} \]
can be done explicitly and one gets
\[ \varepsilon(q) = 1 + \frac{4\pi e^2}{g^2} g(\varepsilon_F) \left[ \frac{1}{2} + \frac{1 - x^2}{4x} \ln \left( \frac{1 + x}{1 - x} \right) \right] \]
where \( x = \frac{g}{2k_F} \)
as \( x \to 0 \), \( [\cdots] = 1 \) and we get back Thomas-Fermi result at \( x = 0 \), i.e. \( g = 2k_F \), \( \varepsilon(q) \) has a logarithmic singularity.

If we formally write \( \varepsilon(q) = 1 + \frac{\Delta(q)}{g^2} \)
to define a \( g \)-dependent screening length \( k_0(q) \)
Then
\[ \frac{k_0^2(q)}{k_0^2(0)} = [\cdots] \]
as \( g \) increases the effective screening length \( k_0 \) increases. Screening is less effective at small length scales than a Thomas-Fermi approximation.

If you take the Fourier transform of \( \frac{4\pi G}{g^2 \varepsilon(q)} \)
to get real space potential of a front charge,
The singularity at \( g = 2k_F \) gives rise to a term
\[
- \frac{1}{r^3} \cos(2k_F r)
\]
decays more slowly than \( T \) and oscillates in sign.

This 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. They 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 \( g = 2k_F \) is understood more physically in terms of the behavior of the region of integration \( \mathbf{R} \).

As \( g \) increases, the region \( \mathbf{R} \) increases, until \( g = 2k_F \). When \( g > 2k_F \), \( \mathbf{R} \) is the entire Fermi sphere and no longer changes as \( g \) increases further. This singularity in the volume \( V \) gives rise to the singularity in \( \Sigma(g) \) at \( g = 2k_F \).
This is true also for more generally shaped Fermi surfaces - \( E(\mathbf{q}) \) will be singular for any \( \mathbf{q} \) that displaces the Fermi surfaces so they touch at a tangential point.

**Kohn effect**: a phonon (ion-lattice vibration) at a wavevector \( \mathbf{q} \) sets up an electrostatic potential with wavevector \( \mathbf{q}' \).

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