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8.512 Theory of Solids II
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Lecture 4

3.1 Thomas-Reiche-Kuhn or f-sum rule

Motivation :- One can derive following equation for one particle energy levels

$$\sum_n 2m(\omega_n - \omega_0) |\langle n | \hat{x} | 0 \rangle|^2 = 1 \quad (3.1)$$

Proof :-

$$\begin{aligned} 1 &= -i \langle 0 | [\hat{x}, \hat{p}] | 0 \rangle \\ 1 &= \sum_n \langle 0 | \hat{x} | n \rangle \langle n | \hat{p} | 0 \rangle - \langle 0 | \hat{p} | n \rangle \langle n | \hat{x} | 0 \rangle \\ \hat{p} &= im[\hat{H}, \hat{x}] \\ \Rightarrow \langle n | \hat{p} | 0 \rangle &= im(\omega_n - \omega_0) \langle 0 | \hat{x} | n \rangle \\ \Rightarrow 1 &= \sum_n 2m(\omega_n - \omega_0) |\langle n | \hat{x} | 0 \rangle|^2 \end{aligned}$$

One can extend the above formalism to condensed matter systems. As wave functions are extended, position operator becomes unbounded for an infinite system. Thus we use density operator instead of position operator. Final equation that can be obtained would be

$$\sum_n (\varepsilon_n - \varepsilon_0) |\langle n | \hat{\rho}_{\vec{q}}^\dagger | 0 \rangle|^2 = Nq^2/2m \quad (3.2)$$

One can see that for localised states, $\exp(i\vec{q} \cdot \vec{r}) \rightarrow 1 + i\vec{q} \cdot \vec{r}$ And two sides of above equation look reasonable. Consider,

$$\langle 0 | [[\hat{\rho}_{\vec{q}}, \hat{H}], \hat{\rho}_{\vec{q}}^\dagger] | 0 \rangle = \sum_n (E_n - E_0) |\langle n | \hat{\rho}_{\vec{q}}^\dagger | 0 \rangle|^2 + \sum_m (E_m - E_0) |\langle m | \hat{\rho}_{\vec{q}} | 0 \rangle|^2 \quad (3.3)$$

By time reversal symmetry, eigenfunctions of hamiltonian ϕ_n , are real. Thus,

$$\begin{aligned} \langle n | \hat{\rho}_{\vec{q}}^\dagger | 0 \rangle &= \int d^3r \phi_n^* \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \phi_0 \\ \langle n | \hat{\rho}_{\vec{q}}^\dagger | 0 \rangle^* &= \int d^3r \phi_n \sum_i \exp(-i\vec{q} \cdot \vec{r}_i) \phi_0 \\ &= \langle n | \hat{\rho}_{\vec{q}} | 0 \rangle \\ \Rightarrow nq^2 &= 2m \sum_n (E_n - E_0) |\langle n | \hat{\rho}_{\vec{q}}^\dagger | 0 \rangle|^2 \end{aligned}$$

By using the expression for the fluctuation function one can rewrite the above expression

$$\int_0^\infty d\omega \omega S(\bar{q}, \omega) = Nq^2/2m \quad (3.4)$$

In case of neutron scattering from phonons, \mathbf{r}_i represents the lattice position and m should be replaced by the ion mass M .

3.2 Longitudinal f sum rule

Recall :-

$$\begin{aligned} \mathbf{D}(\mathbf{q}, \omega) &= \epsilon(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega) \\ \nabla \cdot \mathbf{D}(\mathbf{q}, \omega) &= 4\pi\rho_{ext} \\ \nabla \cdot \mathbf{E}(\mathbf{q}, \omega) &= 4\pi\rho_{tot} \end{aligned}$$

Define,

$$\begin{aligned} e\mathbf{D} &= \nabla U_{ext} \\ e\mathbf{E} &= \nabla U \end{aligned}$$

Thus,

$$U(\mathbf{q}, \omega) = \frac{U_{ext}(\mathbf{q}, \omega)}{\epsilon(\mathbf{q}, \omega)}$$

From linear response

$$\begin{aligned} n(\mathbf{q}, \omega) &= \chi(\mathbf{q}, \omega)U_{ext}(\mathbf{q}, \omega) \\ \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} &= \frac{E_{||}(\mathbf{q}, \omega)}{D_{||}(\mathbf{q}, \omega)} = \frac{U}{U_{ext}} \\ &= 1 + \frac{4\pi e^2 \langle n \rangle}{q^2 U_{ext}} \end{aligned}$$

$$\frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = 1 + \frac{4\pi e^2}{q^2} \chi(\mathbf{q}, \omega) \quad (3.5)$$

Now, imaginary part of dielectric constant corresponds to imaginary part of response function which is density correlation function. Thus from above equation we see that

$$\int_0^\infty d\omega \omega \text{Im} \frac{1}{\epsilon_{||}(\mathbf{q}, \omega)} = \frac{-\pi}{2} \omega_{pl}^2 \quad (3.6)$$

This is the longitudinal f-sum rule.
Define Π that can be used for approximations,

$$n(\mathbf{q}, \omega) = \Pi(\mathbf{q}, \omega)U(\mathbf{q}, \omega) \quad (3.7)$$

$$\begin{aligned} \epsilon_{\parallel}(\mathbf{q}, \omega) &= \frac{D_{\parallel}(\mathbf{q}, \omega)}{E_{\parallel}(\mathbf{q}, \omega)} = \frac{U_{ext}}{U} \\ &= 1 - \frac{4\pi e^2 \langle n \rangle}{q^2 U} \\ &= 1 - \frac{4\pi e^2}{q^2} \Pi(\mathbf{q}, \omega) \end{aligned}$$

If we approximate Π by Π_0 for free fermions, we recover the RPA for $\epsilon(\mathbf{q}, \omega)$.

3.3 Conductivity sum rule

Ohm's law and continuity equation can be written as,

$$\mathbf{j}_{\parallel}(\mathbf{q}, \omega) = \sigma_{\parallel}(\mathbf{q}, \omega)\mathbf{E}_{\parallel}(\mathbf{q}, \omega) \quad (3.8)$$

$$\begin{aligned} \nabla \cdot \mathbf{j} - e \frac{\partial n}{\partial t} &= 0 \\ \mathbf{q} \cdot \mathbf{j}(\mathbf{q}, \omega) + e\omega n(\mathbf{q}, \omega) &= 0 \\ qj_{\parallel}(\mathbf{q}, \omega) + e\omega n(\mathbf{q}, \omega) &= 0 \end{aligned}$$

Where $\mathbf{E}_{\parallel}(\mathbf{q}, \omega)$ is internal electric field.

$$\begin{aligned} \epsilon_{\parallel}(\mathbf{q}, \omega) &= 1 - \frac{4\pi e^2 \langle n \rangle}{q^2 U} \\ &= 1 - i \frac{4\pi e^2 \langle n \rangle}{q E_{\parallel}} \\ &= 1 + i \frac{4\pi e}{\omega} \frac{j_{\parallel}}{E_{\parallel}} \end{aligned}$$

Hence we obtain the important relation :

$$\epsilon_{\parallel}(\mathbf{q}, \omega) = 1 + \frac{4\pi i}{\omega} \sigma_{\parallel}(\mathbf{q}, \omega) \quad (3.9)$$

Thus imaginary part of conductivity is related to real part of dielectric constant which is in turn related to real part of response function. For large frequency limit one can approximate the response function as ($\omega \rightarrow \omega + i\eta$),

$$\begin{aligned}
\chi &= \sum_n |\langle 0 | \hat{\rho}_{\bar{q}} | n \rangle|^2 \left(\frac{1}{\omega - E_n + E_0} + \frac{1}{\omega + E_n - E_0} \right) \\
&\rightarrow \sum_n |\langle 0 | \hat{\rho}_{\bar{q}} | n \rangle|^2 \frac{2(E_n - E_0)}{\omega^2 - (E_n - E_0)^2} \\
&\rightarrow \sum_n |\langle 0 | \hat{\rho}_{\bar{q}} | n \rangle|^2 \frac{2(E_n - E_0)}{\omega^2}
\end{aligned}$$

Where we have taken the limit of large frequency in the third step. Using the sum rule 3.2 we get

$$\chi \rightarrow \frac{\omega_{pl}^2}{\omega^2} \quad (3.10)$$

Using equations 3.5 and 3.10 we conclude,

$$\frac{1}{\epsilon(\mathbf{q}, \omega)} \rightarrow 1 + \frac{\omega_{pl}^2}{\omega^2} \quad (3.11)$$

$$\lim_{\omega \rightarrow \infty} \epsilon(\mathbf{q}, \omega) = 1 - \frac{\omega_{pl}^2}{\omega^2} \quad (3.12)$$

On the other hand from equation 3.9 we see that :

$$\sigma''(\omega) = \frac{-\omega}{4\pi} (\epsilon' - 1) \quad (3.13)$$

In large frequency limit Kramers-Kronig relation can be written as

$$\sigma''(\omega) = - \int \frac{d\omega'}{2\pi} \frac{\sigma'(\omega')}{\omega} \quad (3.14)$$

Combining the last three equations one gets the desired conductivity sum rule,

$$\int_0^\infty d\omega \sigma'_{||}(\omega, \mathbf{q}) = \omega_{pl}^2/8 \quad (3.15)$$