561 Fall 2005 Lecture 5b

Dielectric Response Function

References: Phillips Ch. 8; Pines, 121 ff. See also Mahan, Sec. 5.5; Fetter, p 151 ff; Doniach Sec. 6.4; P. C. Martin

1. The most important response function in condensed matter

- Directly related to electron-electron interactions, correlations, total energy in solids
- Determines response to charged particles, electrical conductivity, optical properties
- Directly measurable

2. Definition

- If $\mathbf{D}$ is the external applied field and $\mathbf{E}$ is the internal field, then the standard notation of electrodynamics is

$$\mathbf{D} = \epsilon\mathbf{E}, \ \ or \ \ \mathbf{E} = \epsilon^{-1}\mathbf{D} = \mathbf{D} + 4\pi\mathbf{P} = \mathbf{D} + (\epsilon^{-1} - 1)\mathbf{D}), \tag{1}$$

  where $4\pi\mathbf{P}$ is the response of the medium.

- Therefore $\mathbf{P} = (1/4\pi)(\epsilon^{-1} - 1)\mathbf{D}$ and $(1/4\pi)(\epsilon^{-1} - 1)$ is the response function for the charge due to an external electric field. (Note: ϵ is also a response function (to internal fields) – more latter.)

- For longitudinal fields in an isotropic medium, this can also be written in terms of scalar potentials

$$V_{int} = \epsilon^{-1}V_{ext}; \ V_{ext} = \epsilon V_{int}. \tag{2}$$

- In terms of charge densities,

$$\delta\rho = \delta\rho_{ext} + \delta\rho_{int}. \tag{3}$$

- Combining above, we find

$$\delta\rho_{int} = (\epsilon^{-1} - 1)\frac{k^2}{4\pi e^2}V_{ext}. \tag{4}$$

3. Density-Density Response Function

- Define $(\epsilon^{-1}(\mathbf{k},\omega) - 1) = \frac{4\pi e^2}{k^2}\Pi^R(\mathbf{k},\omega)$, where $\Pi^R = \frac{\delta\rho_{int}}{\delta(V_{ext})}$
- Thus $\Pi^R(\mathbf{k},\omega) = \frac{1}{\hbar}D^R(\mathbf{k},\omega)$, where D^R is the retarded density-density response function defined before in notes number 5.

- Explicitly at $T = 0$, and using the density operator $\rho_k = \sum_i e^{-ikr_i}$,

$$\Pi^R(\mathbf{k},\omega) = \sum_m |\langle 0|\rho_k|m\rangle|^2 \left[\frac{1}{E_0 - E_m + \omega + i\eta} - \frac{1}{E_m - E_0 + \omega + i\eta}\right], \tag{5}$$

and

$$Im\Pi^R(\mathbf{k},\omega) = -\pi \sum_m |\langle 0|\rho_k|m\rangle|^2 \left[\delta(E_0 - E_m + \omega) - \delta(E_m - E_0 + \omega)\right], \tag{6}$$

which is the same as Pines (3-110).

4. Dynamic Structure Factor

- At $T = 0$:

$$S(\mathbf{q},\omega) = -\frac{\hbar}{\pi} Im\Pi^R(\mathbf{q},\omega),\ \omega > 0$$
$$S(\mathbf{q},\omega) = 0,\ \omega < 0 \tag{7}$$

- It is then easy to show that: $S(\mathbf{q},\omega) = \sum_m |\langle 0|\rho_k|m\rangle|^2 \delta(\omega - (E_m - E_0))$
- Static Structure factor:

$$S(\mathbf{q}) = \int_0^\infty d\omega S(\mathbf{q},\omega) = \sum_m |\langle 0|\rho_k|m\rangle|^2 = \langle 0|\rho_{-q}\rho_q|0\rangle, \tag{8}$$

from which it follows that

$$S(\mathbf{q}) = -\frac{\hbar}{\pi}\frac{k^2}{4\pi e^2}\int_0^\infty d\omega Im\epsilon^{-1}(\mathbf{q},\omega) \tag{9}$$

- Directly measured by scattering of fast charged particles:

$$\frac{d^2\sigma}{d\Omega d\omega)} \propto S(\mathbf{q},\omega) \propto -2Im\epsilon^{-1}(\mathbf{q},\omega) \tag{10}$$

- $S(\mathbf{q},\omega)$ directly related to total elect.-elect. interaction energy (Previous lecture notes and Homework Problem)

5. Response to internal fields E

- Since $\mathbf{D} = \epsilon\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}$, it follows that the response to internal fields is given by

$$\delta\rho_{int} = \delta\rho - \delta\rho_{ext} = (1-\epsilon)\delta\rho = (1-\epsilon)\frac{k^2}{4\pi e^2}V_{int} \tag{11}$$

- We can define the response function to internal fields as

$$(\epsilon(\mathbf{k},\omega) - 1) = -\frac{4\pi e^2}{k^2} P^R(\mathbf{k},\omega) \text{ } or \text{ } \epsilon(\mathbf{k},\omega) = 1 - V_C(k) P^R(\mathbf{k},\omega) \tag{12}$$

(Compare with $\epsilon^{-1} = 1 + V_C(k)\Pi^R$. Note + vs. - sign.)

- The conductivity is defined for $\mathbf{k} \approx 0$: $\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega)$
- It follows that:

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega) \tag{13}$$

- Note: *Both* ϵ and ϵ^{-1} are response functions.

6. Kramers-Kronig transform and Sum Rules

- Kramers-Kronig Relations for *both* $\epsilon^{-1}(\mathbf{k},\omega)$ and $\epsilon(\mathbf{k},\omega)$
- Plasma Sum rules for *both* $\epsilon^{-1}(\mathbf{k},\omega)$ and $\epsilon(\mathbf{k},\omega)$ derived from the high frequency limits

$$\epsilon^{-1} \to 1 + \frac{\omega_P^2}{\omega^2} \tag{14}$$

and

$$\epsilon \to 1 - \frac{\omega_P^2}{\omega^2} \tag{15}$$

- Other sum rules given by Mahan, sec. 5.7.
- The above is ready translated in to sum rule on $S(\mathbf{k},\omega)$; see, e.g., Pines (Eq. 3-137).

7. ϵ and transverse waves

- The dispersion relation of transverse photons in materials are determined by $\epsilon(\mathbf{k} \approx 0,\omega)$
- Defined by response of current $\mathbf{j}$ to vector potential $\mathbf{A}$. (Not carried out here. More later. See also P. C. Martin)

8. General form of relation of ϵ^{-1} and ϵ

- From our definitions

$$\epsilon^{-1} = 1 + V_k\Pi = \frac{1}{\epsilon} = \frac{1}{1 - V_k P} \tag{16}$$

- It follows that the response functions are related by

$$\Pi = \frac{P}{1 - V_k P} \tag{17}$$

- This is a general form that will appear again. It is a very useful relation giving the response to external fields in terms of the response to internal fields, and is the general form of the Random Phase Approximation (RPA).