Chap 20 Phenomenological theory

- Dielectric function and EM wave propagation
- Drude model of the dielectric function
- Lorentz model of the dielectric function
- Kramers-Kronig relations
- Theory of linear response
 - Kubo-Greenwood formula





Dielectric function

$$(\mathbf{r}, t)$$
-space (\mathbf{k}, ω) -space $\nabla \cdot \vec{E}(\vec{r}, t) = 4\pi\rho(\vec{r}, t)$ $\mathbf{k} \cdot \vec{E}(\vec{k}, \omega) = 4\pi\rho(\vec{k}, \omega)$ $\nabla \cdot \vec{D}(\vec{r}, t) = 4\pi\rho_{ext}(\vec{r}, t)$ $\mathbf{k} \cdot \vec{D}(\vec{k}, \omega) = 4\pi\rho_{ext}(\vec{k}, \omega)$ $(\rho = \rho_{ext} + \rho_{ind})$

Take the Fourier "shuttle" between 2 spaces:

$$\vec{E}(\vec{r},t) = \int \frac{d^{3}\vec{k}}{(2\pi)^{3}} \frac{d\omega}{2\pi} \vec{E}(\vec{k},\omega) e^{i(\vec{k}\cdot\vec{r}-\omega t)}, \text{ same for } \vec{D}$$

$$\rho(\vec{r},t) = \int \frac{d^{3}\vec{k}}{(2\pi)^{3}} \frac{d\omega}{2\pi} \rho(\vec{k},\omega) e^{i(\vec{k}\cdot\vec{r}-\omega t)}, \text{ same for } \rho_{ext}$$

$$\vec{D}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\vec{E}(\vec{k},\omega) \quad \text{(by definition)}$$
or $\rho_{ext}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\rho(\vec{k},\omega) \quad \text{(easier to calculate)}$
or $\phi_{ext}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\phi(\vec{k},\omega) \quad \because \vec{E}(\vec{k},\omega) = -i\vec{k}\phi(\vec{k},\omega)... \text{ etc}$

Q: What is the relation between D(r,t) and E(r,t)?

EM wave propagation in solids

Maxwell equations

$$\nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} ; \nabla \cdot \vec{D} = 4\pi \rho_{ext} \qquad i\vec{k} \times \vec{E} = +\frac{i\omega}{c} \vec{B} ; \varepsilon_{ion} \vec{k} \cdot \vec{E} = 4\pi \rho_{ext}$$

$$\nabla \times \vec{B} = +\frac{1}{c} \frac{\partial \vec{D}}{\partial t} + \frac{4\pi}{c} \vec{J}_{ext} ; \nabla \cdot \vec{B} = 0 \qquad i\vec{k} \times \vec{B} = -\frac{i\omega}{c} \varepsilon_{ion} \vec{E} + \frac{4\pi}{c} \vec{J}_{ext} ; i\vec{k} \cdot \vec{B} = 0$$

$$\rightarrow \vec{k} \times (\vec{k} \times \vec{E}) = -\frac{\omega^2}{c^2} \varepsilon_{ion} \vec{E} - \frac{4\pi i\omega}{c^2} \sigma \vec{E} \qquad (\vec{J} = \sigma \vec{E})$$

$$\vec{k} (\vec{k} \cdot \vec{E}) - k^2 \vec{E}$$
• Transverse wave
$$k^2 = \frac{\omega^2}{c^2} \left(\varepsilon_{ion} + \frac{4\pi i\sigma}{\omega} \right)$$

$$\because \upsilon_p = \frac{\omega}{k} = \frac{c}{n}, \text{ refractive index } n = \sqrt{\varepsilon}$$

$$\therefore \varepsilon(\vec{k}, \omega) = \varepsilon_{ion} + \frac{4\pi i\sigma}{\omega} \qquad (\text{in the following,} \\ \text{let } \varepsilon_{ion} \sim 1)$$
• Longitudinal wave
$$\varepsilon(\vec{k}, \omega) = 0$$

On the contrary, if ε (**k**, ω) \neq 0, then the EM wave can only be transverse.



Lorentz model of the dielectric function

• Response of charged (independent) oscillators

For the ℓ -th oscillator (an atom or molecule with Z bound charges),

$$m_{\ell} \left(\frac{d^{2}}{dt^{2}} + \eta_{\ell} \frac{d}{dt} + \omega_{\ell}^{2} \right) \vec{r}_{\ell}(t) = -Z_{\ell} e \vec{E}_{\omega} e^{-i\omega t}$$

$$\vec{r}_{\ell}(t) = \vec{r}_{\ell\omega} e^{-i\omega t} \quad \text{(for steady state)}$$

$$\rightarrow \vec{r}_{\ell\omega} = \frac{-Z_{\ell} e}{m_{\ell} \left(\omega_{\ell}^{2} - \omega^{2} - i\eta_{\ell} \omega \right)} \vec{E}_{\omega}$$

$$\rightarrow \vec{j}_{\omega} = \frac{1}{V} \sum_{\ell} (-Z_{\ell} e) \vec{v}_{\ell\omega} = \sigma(\omega) \vec{E}_{\omega}$$

conductivity

$$\sigma(\omega) = \frac{1}{V} \sum_{\ell} \frac{-i\omega Z_{\ell}^2 e^2}{m_{\ell} \left(\omega_{\ell}^2 - \omega^2 - i\eta_{\ell}\omega\right)}$$
$$\varepsilon(\omega) = 1 + \frac{4\pi i\sigma}{\omega}$$
$$= 1 + \frac{1}{V} \sum_{\ell} \frac{4\pi Z_{\ell}^2 e^2 / m_{\ell}}{\omega_{\ell}^2 - \omega^2 - i\eta_{\ell}\omega}$$

Or, electric polarization $\vec{P}_{\omega} = \frac{1}{V} \sum_{\ell} (-Z_{\ell} e) \vec{r}_{\ell \omega} = \chi_{e}(\omega) \vec{E}_{\omega}$ electric susceptibility $\chi_{e}(\omega) = \frac{1}{V} \sum_{\ell} \frac{Z_{\ell}^{2} e^{2}}{m_{\ell} \left(\omega_{\ell}^{2} - \omega^{2} - i\eta_{\ell} \omega\right)}$ $\varepsilon(\omega) = 1 + 4\pi\chi_{e}$ will get the same result

Conductivity of free electron gas

let $\omega_{\ell}=0$

$$\sigma(\omega) = \frac{1}{V} \sum_{\ell} \frac{i\omega e^2}{m(\omega^2 + i\eta\omega)} \qquad (\eta = 1/\tau)$$
$$= \frac{\sigma_0}{1 - i\omega\tau}, \quad \sigma_0 = \frac{ne^2\tau}{m}$$

Same as the Drude result

Q: what is the corresponding σ (*t*)?

• For a clean conductor at T=0 Plemelj formula (Landau QM p.156):

$$\lim_{\eta \to 0} \frac{1}{\omega \pm i\eta} = P \frac{1}{\omega} \mp i\pi \delta(\omega)$$
$$\therefore \sigma(\omega) = \frac{ne^2}{m} \left[\pi \delta(\omega) + \frac{i}{\omega} \right]$$

• Dielectric function

$$\varepsilon(\omega) = 1 + \frac{4\pi i\sigma}{\omega}$$



ω

D: Drude weight

Drude peak

From Peter Jung's thesis

ω

Reflectivity r and reflectance R

Response of a crystal to an EM field is characterized by ε (k, ω), ($k \sim 0$ compared to G/2)

- Experimentalists prefer to measure reflectivity r
- normal incidence



- It is easier to measure R than to measure θ
- \therefore measure R(ω) for every $\omega \rightarrow \theta(\omega)$ (with the help of KK relations)

$$\rightarrow \mathbf{n}(\omega)$$
$$\rightarrow \varepsilon(\omega)$$

Lorentz model again (for identical oscillators)

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\tau\omega \left(1 - \omega_0^2 / \omega^2\right)}$$

resonance at $\omega = \omega_0$
 $\varepsilon(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega / \tau}$
 $\varepsilon'(\omega) = 0$ at $\omega = \omega_L$
 $\omega_L \approx \sqrt{\omega_p^2 + \omega_0^2}$
 $\omega_p^2 \equiv \frac{4\pi ne^2}{m}$



Kramers-Kronig relations (1926)

KK relation connects real part of the response function with the imaginary part



Kramers-Kronig relations

$$\alpha'(\omega) = \frac{2}{\pi} \int_0^\infty \frac{s\alpha''(s)}{s^2 - \omega^2} ds$$
$$\alpha''(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\alpha'(s)}{s^2 - \omega^2} ds$$

- does not depend on any dynamic detail of the interaction
- the necessary and sufficient condition for its validity is causality

For conductivity, it's the Drude weight

(check, e.g., Lorentz model. Need exact form of ε for a general proof.) Ferrell and Glover (1958) (check Drude conductivity)

• A few sum rules:

$$\frac{2}{\pi}\int_0^\infty \frac{\alpha''(s)}{s}ds = \alpha'(0)$$

From α "($\omega >>1$) $\frac{2}{\pi} \int_0^\infty \alpha'(s) ds = \lim_{\omega \to \infty} \omega \alpha''(\omega)$





KK relation for reflection

$$E'_{\omega} = r(\omega)E_{\omega}$$
$$\ln r(\omega) = \ln R^{1/2}(\omega) + i\theta(\omega)$$
$$\mathsf{KK} \text{ related}$$

Why take log?

"That *In* r satisfies the conditions for the validity of this relation follows from a causality argument." (Jahoda 1957)

See Wooten, App G; Yu and Cardona p.252 for related discussion

Get the phase numerically

$$\theta(\omega) = -\frac{\omega}{\pi} \int_0^\infty \frac{\ln R(s)}{s^2 - \omega^2} ds$$
$$= -\frac{1}{2\pi} \int_0^\infty \ln \left| \frac{s + \omega}{s - \omega} \right| \frac{d \ln R}{ds} ds$$

- constant R(s) doesn't contribute
- s>>@, s<<@ don't contribute



This trick is first used by Jahoda, Phys. Rev. 1957.

An application of the sum rule

Figs from Ibach and Luth

Boltzmann approach to AC conductivity

$$\begin{aligned} \frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} - e\vec{E} \cdot \frac{\partial f}{\hbar \partial \vec{k}} &= -\frac{f - f^{0}}{\tau_{\varepsilon}} \\ \frac{\partial f_{0}}{\partial t} = \frac{\partial f_{0}}{\partial \vec{r}} = 0 \\ \rightarrow \frac{\partial \delta f}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial \delta f}{\partial \vec{r}} - e\vec{E} \cdot \frac{\partial f_{0}}{\hbar \partial \vec{k}} &= -\frac{\delta f}{\tau_{\varepsilon}} \\ \text{assume } \vec{E}(\vec{r}, t) &= \vec{E}_{0}e^{i(\vec{q}\cdot\vec{r}-\omega t)} \\ \delta f &= \Phi(\vec{k})e^{i(\vec{q}\cdot\vec{r}-\omega t)} \\ \rightarrow -i\omega \Phi + i\vec{q} \cdot \vec{v} \Phi - e\vec{E}_{0} \cdot \vec{v} \frac{\partial f_{0}}{\partial \varepsilon} &= -\frac{\Phi}{\tau_{\varepsilon}} \\ \rightarrow \Phi &= \frac{e\tau \vec{E}_{0} \cdot \vec{v}}{1 - i\tau \left(\omega - \vec{q} \cdot \vec{v}\right)} \frac{\partial f_{0}}{\partial \varepsilon} \\ \vec{j} &= -e\int [dk]\vec{v} \delta f \\ \rightarrow \sigma(\vec{q}, \omega) &= e^{2}\int [dk] \frac{\tau \vec{v} \vec{v}}{1 - i\tau \left(\omega - \vec{q} \cdot \vec{v}\right)} \left(-\frac{\partial f_{0}}{\partial \varepsilon}\right) \end{aligned}$$

An improvement over the classical expression Note: $\boldsymbol{\sigma}(0,0) = e^2 \int [dk] \tau \vec{v} \vec{v} \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \equiv \boldsymbol{\sigma}_{dc}$ (see chap 17) $\boldsymbol{\sigma}(0,\omega) = \frac{\boldsymbol{\sigma}_{dc}}{1-i\omega\tau}$

Time-dependent perturbation theory, a review

 $H=H_0+H'(t)$ • Without H', $|\ell(t)\rangle = e^{-i\varepsilon_{\ell}^0 t/\hbar} |\ell\rangle$, where $H_0 |\ell\rangle = \varepsilon_{\ell}^0 |\ell\rangle$ $\left|\ell(t)\right\rangle \rightarrow \left|\tilde{\ell}(t)\right\rangle = \sum c_m(t)e^{-i\varepsilon_m t/\hbar} \left|m\right\rangle, \quad c_m(0) = \delta_{\ell m}$ • With H', $i\hbar \left| \frac{d\tilde{\ell}(t)}{dt} \right\rangle = \left(H_0 + H'(t) \right) \left| \tilde{\ell}(t) \right\rangle$ $\rightarrow i\hbar\dot{c}_n = \sum \langle n | H'(t) | m \rangle e^{i\omega_{nm}t} c_m(t), \quad \omega_{nm} \equiv (\varepsilon_n^0 - \varepsilon_m^0) / \hbar$ To 1st order, $\cong \sum \langle n | H'(t) | m \rangle e^{i\omega_{nm}t} c_m^0(t), \quad c_m^0(t) = \delta_{\ell m}$ $c_n^{1}(t) = \delta_{\ell n} + \frac{1}{i\hbar} \int^t dt \, \langle n | H'(t') | \ell \rangle e^{i\omega_{n\ell}t'}$ $\rightarrow \left| \tilde{\ell}(t) \right\rangle = \sum_{n} c_n^1(t) e^{-i\omega_n t} \left| n \right\rangle$ $=e^{-i\omega_{\ell}t}\left|\ell\right\rangle+\frac{1}{i\hbar}\sum_{\ell}\int^{t}dt'e^{-i\omega_{n}(t-t')}\left\langle n\right|H'(t')\left|\ell\right\rangle e^{-i\omega_{\ell}t'}\left|n\right\rangle$ or $\left|\tilde{\ell}(t)\right\rangle = e^{-i\omega_{\ell}t} \left|\ell\right\rangle + \frac{1}{i\hbar} \sum_{i} \int^{t} dt' \left\langle n \left| H'_{I}(t') \right| \ell\right\rangle e^{-i\omega_{n}t} \left|n\right\rangle$ Interaction representation $H'_{t}(t) \equiv e^{iH_{0}t/\hbar}H'(t)e^{-iH_{0}t/\hbar}$

Theory of linear response

Assume $H'(t) = \int d^{3}r'\hat{B}(\vec{r}') \cdot h(\vec{r}',t)$ then $\langle \tilde{\ell}(t) | \hat{A} | \tilde{\ell}(t) \rangle = \langle \ell | \hat{A} | \ell \rangle + \frac{1}{n!} \int^{t} dt' \langle \ell \rangle + \frac{1}{n!} \int^{t} dt' \langle$

$$\begin{aligned} (t) \left| \hat{A} \right| \tilde{\ell}(t) \right\rangle &= \left\langle \ell \left| \hat{A} \right| \ell \right\rangle + \frac{1}{i\hbar} \int^{t} dt' \left\langle \ell \right| \left[\hat{A}_{I}(t), \hat{H}'_{I}(t') \right] \left| \ell \right\rangle \\ &= \left\langle \ell \left| \hat{A} \right| \ell \right\rangle + \frac{1}{i\hbar} \int^{t} dt' d^{3}r' \left\langle \ell \right| \left[\hat{A}_{I}(t), \hat{B}_{I}(\vec{r}', t') \right] \left| \ell \right\rangle h(\vec{r}', t') \end{aligned}$$

In general, need to take thermal average

$$\left\langle \ell \left| \hat{O} \right| \ell \right\rangle \rightarrow \left\langle \hat{O} \right\rangle \equiv \sum_{\ell} f_{\ell} \left\langle \ell \left| \hat{O} \right| \ell \right\rangle, \quad f_{\ell} = \frac{e^{-\varepsilon_{\ell}^{0}/kT}}{Z}$$

• Kubo formula (1957)

$$\delta \langle A(\vec{r},t) \rangle = \frac{1}{i\hbar} \int^t dt' d^3 r' \langle \left[A_I(\vec{r},t), B_I(\vec{r}',t') \right] \rangle h(\vec{r}',t')$$

Response function

• Harmonic perturbation (1-particle):

$$H'(t) = U(\vec{r})e^{+\eta t}e^{-i\omega t}$$

$$= U(\vec{r})e^{-i\Omega t}, \quad \Omega \equiv \omega + i\eta!$$

(adiabatically turning on the perturbation)

then

$$\delta \langle A(t) \rangle = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' \langle [A_{I}(t), U_{I}(t')] \rangle e^{-i\Omega t'}$$

$$= \sum_{\ell m} \frac{f_{\ell} - f_{m}}{\hbar(\omega_{\ell m} + \Omega)} \langle \ell | A | m \rangle \langle m | U | \ell \rangle e^{-i\Omega t}$$

$$\omega_{\ell m} \equiv \omega_{\ell} - \omega_{m}$$

Density response: susceptibility

$$H'(t) = -e\phi_{ext}(q,\omega)e^{i\vec{q}\cdot\vec{r}-i\Omega t} \leftrightarrow U(\vec{r}) = -e\phi_{ext}(q,\omega)e^{i\vec{q}\cdot\vec{r}}$$

Charge density

$$\begin{split} \left\langle \hat{\rho}(\vec{r},t) \right\rangle &= -e \sum_{\ell} f_{\ell} \left| \left\langle \vec{r} \, \big| \, \tilde{\ell}(t) \right\rangle \right|^{2} \\ &= \sum_{\ell} f_{\ell} \left\langle \tilde{\ell}(t) \big| - e \delta(\hat{\vec{r}} - \vec{r}) \big| \, \tilde{\ell}(t) \right\rangle \\ &\to \hat{\rho}(\vec{r}) = -e \delta(\hat{\vec{r}} - \vec{r}) \end{split}$$

• Change of charge density (Prob. 5)

$$\delta \left\langle \hat{\rho}(\vec{r},t) \right\rangle = \sum_{\ell m} \frac{f_{\ell} - f_{m}}{\hbar(\omega_{\ell m} + \Omega)} \left\langle \ell \left| \hat{\rho}(\vec{r}) \right| m \right\rangle \left\langle m \left| \hat{U}(\vec{r}) \right| \ell \right\rangle e^{-i\Omega t}$$

• Take plane waves as the unperturbed states

$$\langle \vec{r} | \boldsymbol{\ell} \rangle \rightarrow \langle \vec{r} | \vec{k} \sigma \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \chi_{\sigma}$$

$$\rightarrow \delta\rho(\vec{q}, \omega) = \chi(\vec{q}, \omega)\phi_{ext}(q, \omega)$$

$$\chi(\vec{q}, \omega) = \frac{e^2}{V} \sum_{k\sigma} \frac{f_k - f_{k+q}}{\hbar(\omega_k - \omega_{k+q} + \omega + i\eta)}$$

$$\rho = \rho_{ext} + \delta\rho$$

$$q^{2}\phi_{ext} = 4\pi\rho_{ext}$$

$$\therefore \rho = \left(1 + 4\pi\frac{\chi}{q^{2}}\right)\rho_{ext}$$

• Random Phase Approx. (RPA)

$$\rho = \left[1 + \alpha + \alpha^{2} + \cdots\right] \rho_{ext}$$
$$= \frac{1}{1 - 4\pi \frac{\chi}{q^{2}}} \rho_{ext} = \frac{\rho_{ext}}{\varepsilon}$$

 \rightarrow dielectric function

$$\varepsilon(\vec{q}, \omega) = 1 - \frac{4\pi\chi}{q^2}$$

This χ is not the electric susceptibility mentioned earlier

Long wavelength limit (H.W.)

$$\varepsilon(\vec{q},\omega) = 1 - \frac{4\pi e^2}{q^2 V} \sum_{k\sigma} \frac{f_k - f_{k+q}}{\hbar \left(\omega_k - \omega_{k+q} + \Omega\right)}$$
$$= 1 - \frac{4\pi e^2}{\hbar q^2 V} \sum_{k\sigma} f_k \frac{2(\omega_k - \omega_{k+q})}{\left(\omega_k - \omega_{k+q}\right)^2 - \Omega^2}$$

• For $\omega \gg v_F q$

$$\varepsilon(\vec{q},\omega) \approx 1 - \frac{4\pi e^2}{V} \sum_{k\sigma} \frac{f_k}{m\Omega^2} \left[1 + 3\frac{\hbar^2(\vec{q}\cdot\vec{k})^2}{m^2\Omega^2} \right]$$
$$= 1 - \frac{4\pi e^2}{m\Omega^2} \frac{1}{V} \sum_{k\sigma} f_k \left(1 + \frac{\hbar^2 q^2}{m^2\Omega^2} k^2 \right)$$
$$\frac{1}{V} \sum_{k\sigma} f_k k^2 = \frac{3}{5} n k_F^2 \quad \text{(at T=0)}$$
$$\therefore \ \varepsilon(\vec{q} \to 0, \omega) = 1 - \frac{\omega_p^2}{\omega^2} \left[1 + \frac{3}{5} \left(\frac{\hbar k_F}{m\omega} \right)^2 q^2 \right] \quad \omega_p^2 \equiv \frac{4\pi n e^2}{m}$$

Static limit $(\omega \ll v_F q)$ $\chi(\vec{q}, \mathbf{0}) = \frac{e^2}{V} \sum_{k\sigma} \frac{f_k - f_{k+q}}{\hbar(\omega_k - \omega_{k+q})}$

• For long wavelength

$$\chi(\vec{q}) \approx -\frac{2e^2}{V} \sum_{\vec{k}} \left(-\frac{\partial f_k}{\partial \varepsilon} \right)$$
$$= -e^2 g(\varepsilon_F), \quad \text{or } e^2 \frac{\partial n}{\partial \varepsilon} \quad (=\chi_{TF})$$

• For general wave length, we have

$$\chi(\vec{q}) = -e^2 g(\varepsilon_F) \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln\left(\frac{1+x}{1-x}\right) \right]$$
$$= \chi_{TF} F(x), \ x = q/2k_F$$

1

1.5

2

0

0.5

• It can be shown (not easy) that for $k_{\rm F}r >>1$

$$\phi_{ind}(\vec{r}) = \int \frac{d^3 \vec{q}}{(2\pi)^3} \left[\frac{\phi_{ext}(\vec{q})}{\varepsilon(\vec{q})} - \phi_{ext}(\vec{q}) \right] e^{i\vec{q}\cdot\vec{r}}$$
$$\approx \frac{c}{r^3} \cos 2k_F r$$

Friedel oscillation

Current response: conductivity

Note: $\sigma_{\alpha\beta}(\vec{q},\omega): p_{\alpha}, p_{\beta} \to p_{\alpha}e^{-i\vec{q}\cdot\vec{r}}, p_{\beta}e^{i\vec{q}\cdot\vec{r}}$

A brief summary:

• Classical (Drude, Lorentz)

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

• Semiclasical (Boltzmann)

$$\sigma_{\alpha\beta}(\vec{q},\omega) = e^{2} \int [dk] \left(-\frac{\partial f_{0}}{\partial \varepsilon} \right) \frac{\tau v_{\alpha} v_{\beta}}{1 - i\tau \left(\omega - \vec{q} \cdot \vec{v} \right)}$$

• Quantum (Kubo-Greenwood)

$$\sigma_{\alpha\beta}(\vec{q},\omega) = -\frac{e^{2}}{i\Omega} \left[\frac{n}{m_{0}} \delta_{\alpha\beta} + \frac{1}{V} \sum_{\ell m} \frac{f_{\ell} - f_{m}}{\hbar(\omega_{\ell m} + \Omega)} v_{\ell m}^{\alpha} v_{m\ell}^{\beta} \right]$$

• interband transitions

$$v_{m\ell}^{\beta} = \frac{1}{m_{0}} \langle m | p_{\beta} e^{i\vec{q}\cdot\vec{r}} | \ell \rangle$$

• Quantum manybody (Kubo-Greenwood, in 2nd quantized form)

Descendant of the Kubo-Greenwood formula (I)

$$\sigma_{\alpha\beta}(0,\omega) = -\frac{e^2}{i\Omega m_0} \left[n\delta_{\alpha\beta} + \frac{1}{m_0 V} \sum_{\ell m} \frac{f_\ell - f_m}{\hbar(\omega_{\ell m} + \Omega)} p^{\alpha}_{\ell m} p^{\beta}_{m\ell} \right]$$

•
$$\frac{1}{\omega_{\ell m} \pm \Omega} = \frac{1}{\omega_{\ell m}} \left(1 \mp \frac{\Omega}{\omega_{\ell m} \pm \Omega} \right)$$

• f-sum rule (note: many sum rules are called f-sum rules)

$$n\delta_{\alpha\beta} + \frac{1}{m_0 V} \sum_{\ell m} \frac{f_{\ell} - f_m}{\hbar \omega_{\ell m}} p^{\alpha}_{\ell m} p^{\beta}_{m\ell} = 0$$
$$\rightarrow \sigma_{\alpha\beta}(\omega) = \frac{e^2}{iV} \sum_{\ell m} \frac{f_{\ell} - f_m}{\hbar \omega_{\ell m}} \frac{v^{\alpha}_{\ell m} v^{\beta}_{m\ell}}{\omega_{\ell m} + \Omega}$$

• real and imaginary parts

H.W.: Verify this. Hint: $p_{\alpha} = (im/\hbar)[H, r_{\alpha}]$ $[r_{\alpha}, p_{\beta}] = i\hbar \delta_{\alpha\beta}$

A result of gauge invariance. See Tremblay A.M.- N-corps, p.102 Akkermans and Montambaux, p.299 P.Allen's article, p.174

Grosso and Parravicini, p.430 $q \neq 0$ allowed

P.Allen's article, p.173

$$\begin{cases} \sigma'_{\alpha\alpha}(\omega) = -\frac{\pi e^2}{V} \sum_{\ell m} \frac{f_{\ell} - f_m}{\hbar \omega_{\ell m}} |v_{\ell m}^{\alpha}|^2 \,\delta\big(\omega + \omega_{\ell m}\big) \\ \sigma''_{\alpha\alpha}(\omega) = -\frac{e^2}{V} \sum_{\ell m} \frac{f_{\ell} - f_m}{\hbar \omega_{\ell m}} \frac{|v_{\ell m}^{\alpha}|^2}{\omega_{\ell m} + \omega} \end{cases}$$

$$\alpha \neq \beta$$
 is allowed
Check
 $\int_{-\infty}^{\infty} \sigma_{\alpha\alpha} '(s) ds = \frac{1}{4} \omega_p^2$

Consider a perfect crystal. The current matrix elements are k-diagonal. For a semiconductor or insulator, this is the usual optical inter-band conductivity. For a metal, we have additional diagonal elements within a band.

• Intraband conductivity

$$\begin{split} \left\langle \vec{k} \cdot \left| e^{i\vec{q}\cdot\vec{r}} p_{\beta} \right| \vec{k} \right\rangle &\cong m_{0} v_{\beta} \delta_{k',k+q} \\ \sigma_{\alpha\beta}(\vec{q},\omega) &\cong \frac{2e^{2}}{iV} \sum_{k} \frac{f_{k} - f_{k+q}}{\hbar(\omega_{k} - \omega_{k+q})} \frac{v_{\alpha} v_{\beta}}{\omega_{k} - \omega_{k+q} + \omega + i\eta} \\ \text{for } q \ll k, \quad \frac{\partial f}{\partial \varepsilon} &\cong \frac{f_{k+q} - f_{k}}{\varepsilon_{k+q} - \varepsilon_{k}} \\ \therefore \sigma_{\alpha\beta}(\vec{q},\omega) &\cong ie^{2} \int [dk] \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{v_{\alpha} v_{\beta}}{\omega_{k} - \omega_{k+q} + \omega + i\eta}, \end{split}$$
Note:

$$\sigma_{\alpha\beta}^{DC} &= \lim_{\omega \to 0} \lim_{q \to 0} \sigma_{\alpha\alpha}(\vec{q},\omega) \\ \omega_{k} - \omega_{k+q} &\cong -\vec{q} \cdot \vec{v}; \quad \eta = \tau^{-1} \\ \rightarrow \sigma_{\alpha\beta}(\vec{q},\omega) &\cong e^{2} \int [dk] \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{v_{\alpha} v_{\beta} \tau}{1 - i\tau(\omega - \vec{q} \cdot \vec{v})} \end{aligned}$$
redue to
Boltzmann result

$$\sigma_{\alpha\beta}(0,\omega) &\cong \frac{ie^{2}}{\omega + i\tau^{-1}} \int [dk] \left(-\frac{\partial f}{\partial \varepsilon} \right) v_{\alpha} v_{\beta} = \frac{ie^{2}}{\omega + i\tau^{-1}} \frac{n}{m_{\alpha}^{op}} \delta_{\alpha\beta} \end{aligned}$$
See P.Allen's article, p.167, 174

Grosso and Parravicini, p.414

Recall ch 17 (also see Marder p.694)

$$v_{\alpha} v_{\beta} \left(-\frac{\partial f_{0}}{\partial \varepsilon} \right) = v_{\alpha} \frac{\partial \varepsilon}{\hbar \partial k_{\beta}} \left(-\frac{\partial f_{0}}{\partial \varepsilon} \right) = v_{\alpha} \left(-\frac{\partial f_{0}}{\hbar \partial k_{\beta}} \right)$$
$$\therefore \int [dk] v_{\alpha} v_{\beta} \left(-\frac{\partial f_{0}}{\partial \varepsilon} \right)$$
$$= \int [dk] \left[-\frac{\partial (f_{0} v_{\alpha})}{\hbar \partial k_{\beta}} + f_{0} \frac{\partial v_{\alpha}}{\hbar \partial k_{\beta}} \right]$$
$$= \int [dk] f_{0} \cdot m_{\alpha\beta}^{*} (\vec{k})^{-1}$$
$$\equiv \frac{n}{m_{\alpha\beta}^{op}} \delta_{\alpha\beta} \quad \text{aka: optical effective mass}$$

• $m^{op} = m^*$ if the carriers are near band bottom

• $1/m^{op} = 0$ for a filled band

• This seems to be an effect related to the exclusion principle. Less carriers are able to transit in a fuller band. Again see F. Wooten p.78.

Descendant of the Kubo-Greenwood formula (II)

$$\begin{aligned} \sigma_{\alpha\beta}(\omega) &= -\frac{e^2}{i\Omega m_0} \left[n\delta_{\alpha\beta} + \frac{1}{m_0 V} \sum_{\ell m} \frac{f_\ell - f_m}{\hbar(\omega_{\ell m} + \Omega)} p_{\ell m}^{\alpha} p_{m\ell}^{\beta} \right] \\ \cdot \frac{1}{\Omega} \frac{1}{\omega_{\ell m} \pm \Omega} &= \frac{1}{\Omega} \frac{1}{\omega_{\ell m}} \mp \frac{1}{\omega_{\ell m}} \frac{1}{\omega_{\ell m} \pm \Omega} \\ \rightarrow \sigma_{\alpha\beta}(\omega) &= \frac{ine^2}{\Omega} \left(\frac{1}{m^{op}} \right)_{\alpha\beta} \delta_{\alpha\beta} + \frac{e^2}{im_0^2} \frac{1}{V} \sum_{\ell m} \frac{f_\ell - f_m}{\hbar \omega_{\ell m} (\omega_{\ell m} + \Omega)} p_{\ell m}^{\alpha} p_{m\ell}^{\beta} \\ \cdot \frac{1}{\omega_{\ell m} (\omega_{\ell m} + \Omega)} &= \frac{1}{\omega_{\ell m}^2 - \Omega^2} + \frac{\Omega}{\omega_{\ell m}} \frac{1}{\omega_{\ell m}^2 - \Omega^2} \\ \therefore \text{ 2nd term in } \sigma_{\alpha\beta}(\omega) &= \frac{e^2}{im_0^2} \frac{1}{\hbar V} \left[\sum_{\ell m} (f_\ell - f_m) \frac{p_{\ell m}^{\alpha} p_{m\ell}^{\beta}}{\omega_{\ell m}^2 - \Omega^2} + \sum_{\ell m} (f_\ell - f_m) \frac{\Omega}{\omega_{\ell m}} \frac{p_{\ell m}^{\alpha} p_{m\ell}^{\beta}}{\omega_{\ell m}^2 - \Omega^2} \right] \\ \begin{cases} \sigma_{\alpha\beta}^2(\omega) &= \frac{e^2}{m_0^2} \frac{1}{\hbar V} \sum_{\ell m} (f_\ell - f_m) \frac{\operatorname{Im}(p_{\ell m}^{\alpha} p_{m\ell}^{\beta})}{\omega_{\ell m}^2 - \Omega^2} & \text{AC (optical) Hall conductivity} \\ e.g., see Rashba PRB 2004 \end{cases} \\ \begin{cases} \sigma_{\alpha\beta}^3(\omega) &= \frac{e^2}{im_0^2} \frac{1}{\hbar V} \sum_{\ell m} (f_\ell - f_m) \frac{\operatorname{Re}(p_{\ell m}^{\alpha} p_{m\ell}^{\beta})}{\omega_{\ell m}^2 - \Omega^2} \frac{\Omega}{\omega_{\ell m}} \end{cases} \end{cases}$$

DC Hall conductivity for a filled Landau subband (Thouless et al, 1982)

$$\sigma_{\alpha\neq\beta}^{DC} = 0 + \frac{e^2}{im_0^2} \frac{1}{\hbar V} \sum_{\ell m} f_{\ell} \frac{p_{\ell m}^{\alpha} p_{m\ell}^{\beta} - p_{\ell m}^{\beta} p_{m\ell}^{\alpha}}{\omega_{\ell m}^2} + 0$$

(one-band)
$$= \frac{2e^2}{i\hbar V} \sum_{k} f_{k} \left(\left\langle \frac{\partial u_{nk}}{\partial k_{\alpha}} \middle| \frac{\partial u_{nk}}{\partial k_{\beta}} \right\rangle - \left\langle \frac{\partial u_{nk}}{\partial k_{\beta}} \middle| \frac{\partial u_{nk}}{\partial k_{\alpha}} \right\rangle \right)$$
$$= \frac{e^2}{\hbar} \int_{filled} [dk] \Omega_{n\gamma}(\vec{k}) \quad (\alpha, \beta, \gamma \text{ are cyclic})$$

- This integral has a close connection with topology (1st Chern number)
- \rightarrow quantization of the quantum Hall conductance
- Recall an alternative, semiclassical approach

$$\begin{aligned} \frac{d\vec{r}}{dt} &= \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \vec{k}} - \dot{\vec{k}} \times \vec{\Omega}(\vec{k}) \\ \vec{j} &= -e \int [dk] \vec{v}_k f_0 \\ &= -\frac{e}{\hbar} \int [dk] \frac{\partial \varepsilon}{\partial \vec{k}} f_0 + \frac{e^2}{\hbar} \int [dk] \vec{\Omega}(\vec{k}) f_0 \times \vec{E} \\ &\to \sigma_{xy} = \frac{e^2}{\hbar} \int_{filled} [dk] \Omega_z(\vec{k}) \end{aligned}$$

Onsager relation for the response function

Kubo formula
$$\delta \langle A(\vec{r},t) \rangle = \int_{-\infty}^{\infty} dt' d^3 r' \chi^R_{AB}(\vec{r}-\vec{r}',t-t')h(\vec{r}',t')$$

• Retarded response function

• Time reversal

$$\chi_{AB}^{R}(\vec{k},t-t') \equiv \frac{1}{i\hbar} \theta(t-t') \left\langle \left[A(-\vec{k},t), B(\vec{k},t') \right] \right\rangle$$
• Time reversal

$$\langle \ell | A | m \rangle \rightarrow \langle m | A(-t) | \ell \rangle$$

$$= \eta_{A} \left\langle m | A(t) | \ell \rangle, \quad \eta_{A} = \pm \left\langle A(-\vec{k},t)B(\vec{k},0) \right\rangle \rightarrow \eta_{A} \left\langle B(-\vec{k},0)A(\vec{k},t) \right\rangle = \eta_{A} \eta_{B} \left\langle B(-\vec{k},t)A(\vec{k},0) \right\rangle$$

$$\therefore \chi_{AB}^{R}(\vec{k},t) \rightarrow \eta_{A} \eta_{B} \frac{1}{i\hbar} \theta(t) \left\langle \left[B(-\vec{k},t), A(\vec{k},0) \right] \right\rangle = \eta_{A} \eta_{B} \chi_{BA}^{R}(\vec{k},t)$$

$$\chi_{AB}^{R}(\vec{k},\omega) \rightarrow \eta_{A} \eta_{B} \chi_{BA}^{R}(\vec{k},\omega) \quad \text{Onsager relation}$$

• By the way, another response function

$$\chi_{AB}(\vec{k},t-t') \equiv \frac{1}{i\hbar} \left\langle \left[A(-\vec{k},t), B(\vec{k},t') \right] \right\rangle$$

aka: generalized susceptibility

$$\chi_{AB}(\vec{k},\omega) = \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \left\langle \left[A(-\vec{k},t), B(\vec{k},0) \right] \right\rangle e^{i\omega t}$$
$$= \begin{cases} 2i\chi \, \|_{AB}^{R}(\vec{k},\omega) & \text{if } \eta_{A} = - \\ 2\chi \, \|_{AB}^{R}(\vec{k},\omega) & \text{if } \eta_{A} = + \end{cases} \leftarrow \chi_{AB}^{R}(-\omega) = \chi_{AB}^{R}(\omega)$$

See L.P. Levy, p.154, 164

Fluctuation-dissipation theorem (Callen and Welton 1951, Takahashi, Kubo 1952 ...)

Thus random impacts of surrounding molecules generally cause two kinds of effect: firstly, they act as a random driving force on the Brownian particle or the mirror to maintain its incessant irregular motion, and, secondly, they give rise to the frictional force for a forced motion. The first is the systematic part of the effect and the second is the random part. This in turn means that the frictional force and the random force must be related, because both come from the same origin. This internal relationship between the systematic and the random parts of microscopic forces is, in fact, a very general matter, which is manifested in the so-called fluctuation-dissipation theorem.

As we shall see in the following, this theorem states a general relationship between the response of a given system to an external disturbance and the internal fluctuation of the system in the absence of the disturbance. Such a response is characterized by a response function or equivalently by an admittance, or an impedance. The internal fluctuation is characterized by a correlation function of relevant physical quantities of the system fluctuating in thermal equilibrium, or equivalently by their fluctuation spectra. The fluctuation-dissipation theorem can thus be used in two ways: it can predict the characteristics of the fluctuation or the noise intrinsic to the system from the known characteristics of the admittance from the impedance, or it can be used as the basic formula to derive the admittance from the analysis of thermal fluctuations of the system. The Nyquist theorem is a classical example of the first category (Nyquist 1928), whereas, perhaps, Onsager's proof of the symmetry of kinetic coefficients is the oldest example of the second (Onsager 1931).

Kubo Rep. Prog. Phys. 1966

Fluctuation-dissipation theorem

- Dynamic structure factor $\begin{aligned}
 \mathbf{S}_{AB}(\vec{k},\omega) &\equiv \int_{-\infty}^{\infty} dt \left\langle A(-\vec{k},t)B(\vec{k},0) \right\rangle e^{i\omega t} \quad \beta &\equiv \frac{1}{k_B T} \\
 \left\langle B(\vec{k},0)A(-\vec{k},t) \right\rangle &= \cdots &= \left\langle A(-\vec{k},t-i\beta\hbar)B(\vec{k},0) \right\rangle \\
 &\therefore \chi_{AB}(\vec{k},\omega) &= \frac{1}{i\hbar} \left(1 - e^{-\hbar\omega/k_B T}\right) S_{AB}(\vec{k},\omega)
 \end{aligned}$
 - ← use cyclic symm of trace (Kubo-Martin-Schwinger identity)

$$\chi_{AB}^{"R}(\omega) = -\frac{1}{2\hbar} (1 - e^{-\hbar\omega/k_BT}) S_{AB}(\omega) \quad \text{if } \eta_A = -\frac{i}{2\hbar} (1 - e^{-\hbar\omega/k_BT}) S_{AB}(\omega) \quad \text{if } \eta_A = +$$

"+" sign if H' ~ -B.h

(aka: Callen-Welton formula)

• Classical form ($\eta_{\scriptscriptstyle A}$ = -)

$$\chi_{AB}^{"R}(\omega) = -\frac{\omega}{2k_BT}S_{AB}(\omega)$$

Close connection between the spontaneous fluctuations in the system (dynamic structure factor), and the response of the system to external perturbations (susceptibility). Johnson noise (1928) Bell Lab

The slope is independent of material, shape, and conduction mechanism Nyquist theorem for electronic noise (1928)

$$\begin{split} H' &= \frac{1}{c} \int d^3 r' \vec{j} \cdot \vec{A}_{\omega} e^{-i\omega t}, \quad \vec{E}_{\omega} = \frac{i\omega}{c} \vec{A}_{\omega} \\ \delta \left\langle j_{\alpha}(\vec{r},t) \right\rangle &= \frac{1}{i\hbar c} \int^t dt' d^3 r' \left\langle \left[j_{\alpha}(\vec{r},t), j_{\beta}(\vec{r}',t') \right] \right\rangle A_{\beta} e^{-i\omega t'} \\ &= -\frac{1}{\hbar \omega} \int^t dt' d^3 r' \left\langle \left[j_{\alpha}(\vec{r},t), j_{\beta}(\vec{r}',t') \right] \right\rangle e^{-i\omega t'} E_{\beta} \\ \rightarrow \sigma_{\alpha\beta}(\vec{k},t-t') &= -\frac{1}{\hbar \omega} \theta(t-t') \left\langle \left[j_{\alpha}(-\vec{k},t), j_{\beta}(\vec{k},t') \right] \right\rangle \\ \sigma_{\alpha\beta}(\vec{k},\omega) &= \frac{1}{i\omega} \chi^{R}_{j_{\alpha}j_{\beta}}(\vec{k},\omega) \\ \rightarrow S_{j_{\alpha}j_{\beta}}(\omega) &= \frac{2\hbar}{1-e^{-\hbar \omega/k_{B}T}} \sigma'_{\alpha\beta}(\vec{k},\omega) \end{split}$$

quantum (shot n.) $\downarrow \qquad \downarrow$ thermal (Johnson n.) or $\sigma'_{\alpha\beta}(\vec{k},\omega) = \frac{1 - e^{-\hbar\omega/k_BT}}{2\hbar} \int_{-\infty}^{\infty} dt \left\langle j_{\alpha}(-\vec{k},t) j_{\beta}(\vec{k},0) \right\rangle e^{i\omega t}$ Non-equil. property Equilibrium property

(This offers one way to determine the Boltzmann constant.)

Zagoskin, p.116

Loudness (left) and pitch (right) fluctuation spectra vs. frequency (Hz) (log-log scale), for a. Scott Joplin piano rags; b. classical radio station; c. rock station; d. news-and-talk station.