Optical and Transport properties in metals (G and P ch. XI)

- We have mostly focused on ground-state properties
- We will now consider solids excited by electromagnetic fields

* Assume non-magnetic material, no external charges or currents

* Assume "linear response" regime: induced responses, e.g., density (ρ_{ind}) or current ($\vec{J}_{ind}$) proportional to driving fields, and have same spatial/temporal dependence

* Assume homogeneous material

* Fields in a material govered by Maxwell equations (Gauss units):

$$\nabla \cdot \vec{E} = 4\pi \rho_{ind}, \quad \nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}, \quad \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\vec{J}_{ind}$$

* Assume field is of the form of a monochromatic transverse EM wave propagating in $\hat{z}$ in isotropic material:

$$\vec{E}(\vec{r},t) = E(z)\,\hat{x}\, e^{-i\omega t} \quad \rightarrow \quad \vec{E} \parallel x$$

$$\vec{B}(\vec{r},t) = B(z)\,\hat{y}\, e^{-i\omega t} \quad \rightarrow \quad \vec{B} \parallel y$$

$$\vec{J}_{ind}(\vec{r},t) = J(z)\,\hat{x}\, e^{i\omega t} \quad \rightarrow \quad \vec{J} \parallel x$$

x	y	z
$\frac{\partial}{\partial x}$	$\frac{\partial}{\partial y}$	$\frac{\partial}{\partial z}$
$\cancel{0}$	$\cancel{0}$	0

* Apply Maxwell's equations:

  - $\nabla \cdot \vec{E} = 0$, so $\rho_{ind} = 0$
  - $\nabla \cdot \vec{B} = 0$ as expected
  - $\frac{dE(z)}{dz} = \frac{i\omega}{c} B(z)$ and $-\frac{dB(z)}{dz} = -\frac{i\omega}{c} E(z) + \frac{4\pi}{c} J(z)$

- so:

$$\frac{d^2E(z)}{dz^2} = \frac{i\omega}{c}\frac{dB(z)}{dz} = -\frac{\omega^2}{c^2}E(z) - \frac{4\pi i\omega}{c^2}J(z)$$

* Now we need to include the behavior of the fields in a solid

relates physical quantities for given solid

- General constitutive relation between $\vec{J}$ and $\vec{E}$ for homogeneous medium:

$$J(z) = \int \sigma(z-z', \omega)\, E(z')\, dz'$$

conductivity

multiply by $e^{iq\cdot z}$ and integrate:

$$\int J(z)e^{iqz}dz = \iint \sigma(z-z',\omega)E(z')\,e^{iqz}\,dz'dz$$

$$= \iint \sigma(z-z',\omega)\,e^{iq(z-z')}\,E(z')e^{iqz'}\,dz'dz$$

$$= \int E(z')e^{iqz'}\underbrace{\left[\int \sigma(z-z',\omega)\,e^{iq(z-z')}\,dz\right]}_{\equiv\, \sigma(q,\omega)}dz'$$

In terms of Fourier transforms of J, E, σ:

$$J(q) = \sigma(q,\omega)\,E(q)$$

* We now assume a local response $\sigma(z-z',\omega) = \sigma(\omega)\,\delta(z-z')$ which is independent of q

- Then: $$\frac{d^2E(z)}{dz^2} = -\frac{\omega^2}{c^2}\left[1 + \frac{4\pi i\sigma(\omega)}{\omega}\right]E(z)$$

so $E(z) = E_0 \exp\left[i\frac{\omega}{c}N(\omega)\,z\right]$

with: $N^2(\omega) = 1 + \dfrac{4\pi i\sigma(\omega)}{\omega}$ ← complex refractive index

* If we write $N(\omega) = n(\omega) + i\,k(\omega)$

refractive index (n); extinction coefficient (k)

$$E(z) = E_0 \exp\left[i \frac{\omega}{c} n z\right] \exp\left[-\frac{\omega}{c} k z\right]$$

- velocity of waves in medium is $\frac{c}{n}$
- "Classical skin depth," z where $E(z)$ drops by $\frac{1}{e}$:

$$\delta(\omega) = \frac{c}{\omega k(\omega)}$$

- Intensity of field is proportional to $|E|^2$ so

$$I(z) = I_0 \exp\left[-2 \frac{\omega k(\omega)}{c}\right] \equiv I_0 \exp\left[-\alpha(\omega)\right]$$

so "absorption coefficient" is

$$\alpha(\omega) = \frac{2\omega k(\omega)}{c} = \frac{2}{\delta(\omega)}$$

* If we write $N^2 = \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, where $D = \varepsilon E_{tot}$

induced field due to exteral E (D): $\equiv \varepsilon_0 E + P$

total E field in medium (E_{tot})

- $\varepsilon(\omega)$ determines how the material screens fields
- $\varepsilon_1 = n^2 - k^2$, $\varepsilon_2 = 2nk$
- $\varepsilon(\omega) = 1 + \frac{4\pi i \sigma(\omega)}{\omega} \Rightarrow \varepsilon_1(\omega) = \frac{1 - 4\pi\sigma_2(\omega)}{\omega}$ and $\varepsilon_2(\omega) = \frac{4\pi\sigma_1(\omega)}{\omega}$

where $\sigma(\omega) = \sigma_1(\omega) + i\,\sigma_2(\omega)$

* If we take the surface of material at $z=0$, reflectivity is (see G and P Sec. XI 1):

$$R = \left|\frac{1-N}{1+N}\right|^2 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

Drude and Boltzmann theory of transport

- Consider free electron gas, $N = \frac{n}{V}$ carriers with effective mass m, uniform background positive charge

* Classical EOM for electrons with field $\vec{E}$

$$m\ddot{\vec{r}} = -\frac{m}{\tau}\dot{\vec{r}} + (-e)\vec{E}_0 e^{i(\vec{q}\cdot\vec{r}-\omega t)}$$

↑ some viscous damping term

- Take long wavelength limit of field:

$$m\ddot{\vec{r}} = -\frac{m}{\tau}\dot{\vec{r}} + (-e)\vec{E}_0 e^{-i\omega t}$$

↳ valid for short scattering times or high frequencies

- Anzatz: $\vec{r}(t) = \vec{A}_0 \exp[-i\omega t]$:

$$\vec{A}_0 = \frac{e\tau}{m}\frac{1}{\omega(i+\omega\tau)}\vec{E}_0$$

- Current density is:

$$\vec{J} = n(-e)\dot{\vec{r}} = n(-e)(-i\omega)\vec{A}_0 e^{-i\omega t}$$

$$= \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau}\vec{E}_0 e^{-i\omega t}$$

so: $$\sigma(\omega) = \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau} \equiv \sigma_0 \frac{1}{1-i\omega\tau}$$

static conductivity

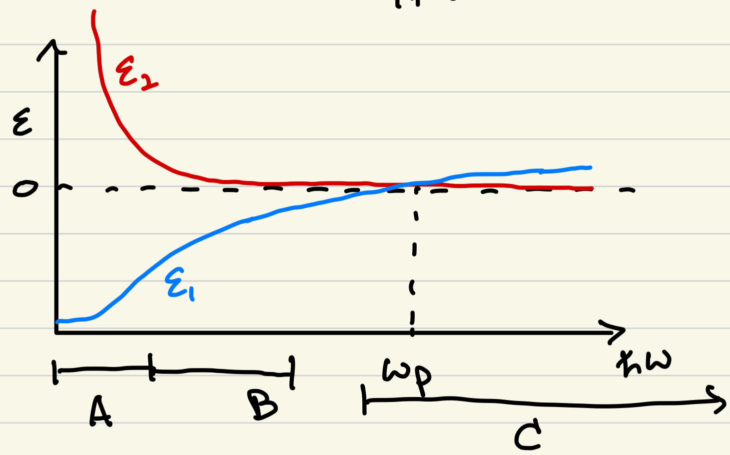
and: $$\varepsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega) = 1 + 4\pi i\frac{ne^2\tau}{m}\frac{1}{\omega(1-i\omega\tau)}$$

$$= 1 - \underbrace{\frac{4\pi ne^2}{m}}_{\equiv \omega_p}\frac{1}{\omega(\omega+i/\tau)}$$

ω_p, "plasma frequency"

• So:

$$\varepsilon_1(\omega) = 1 - \frac{\omega_p^2 \tau^2}{1+\omega^2\tau^2}, \quad \varepsilon_2(\omega) = \frac{\omega_p^2 \tau}{\omega(1+\omega^2\tau^2)}$$



A: Non relaxation regime: $\omega\tau \ll 1 \ll \omega_p \tau$

$$\varepsilon_1(\omega) \approx -\omega_p^2\tau^2, \quad \varepsilon_2(\omega) \approx \frac{\omega_p^2\tau^2}{\omega}$$

and $\quad n \approx k \approx \sqrt{\frac{\varepsilon_2(\omega)}{2}} = \sqrt{\frac{\omega_p \tau}{2\omega}}$ ← also diverges

⇒ large $n(\omega)$ means very reflective

B: relaxation regime: $1 \ll \omega\tau \ll \omega_p\tau$

⇒ still large $n(\omega)$, very reflective

C: "Ultraviolet" region: $\omega \approx \omega_p$ or $\omega > \omega_p$

$$\varepsilon_1(\omega) \approx 1 - \frac{\omega_p^2}{\omega^2}, \quad \varepsilon_2(\omega) \approx \frac{\omega_p^2}{\omega^3\tau} \approx 0$$

⇒ reflectivity almost 0, metal is transparent

- What happens in a crystal?

* Still consider a metal w/ single partially-filled band

- Occupation in equilibrium:

$$f_0(\vec{k}) = \frac{1}{e^{E(k)-E_F(T)/k_BT}+1}$$

- Applying external perturbation changes distribution

$f_0(\vec{k}) \longrightarrow f(\vec{r},\vec{k},t)$ ← gives # of electrons in volume element $(\vec{r},\vec{k})$

- From semi-classical dynamics $t \to dt$:

$$\vec{r} \to \vec{r} + \underbrace{\frac{1}{\hbar}\frac{\partial E(\vec{k})}{\partial \vec{k}}}_{\vec{v}_{\vec{k}}} dt \ , \quad \vec{k} \longrightarrow \vec{k} + \frac{1}{\hbar}\frac{d(\hbar\vec{k})}{dt} dt$$

$$\vec{F} = \frac{d(\hbar\vec{k})}{dt}$$

- If we include scattering term $[\partial f/\partial t]_{coll}$:

$$f(\vec{r}+\vec{v}\,dt, \vec{k} + \vec{F}/\hbar\, dt, t+dt) = f(\vec{r},\vec{k},t) + \left[\frac{\partial f}{\partial t}\right]_{coll} dt$$

- Assume small deviations from f_0, and

$$\left[\frac{\partial f}{\partial t}\right]_{coll} = -\frac{f-f_0}{\tau}$$ ← relaxation time approximation

- Expand LHS to first order:

$$\frac{\partial f}{\partial \vec{r}}\cdot\vec{v} + \frac{\partial f}{\partial \vec{k}}\cdot\frac{\vec{F}}{\hbar} + \frac{\partial f}{\partial t} = -\frac{f-f_0}{\tau}$$

* Now we can calculate current density:

$$\vec{J} = \frac{\overset{\text{spin}}{2}}{(2\pi)^3}\int(-e)\,\vec{v}_{\vec{k}}\, f\, d\vec{k}$$