Plasmons, polarons, polaritons

- Dielectric function; EM wave in solids
- Plasmon oscillation -- plasmons
- Electrostatic screening
- Electron-electron interaction
- Mott metal-insulator transition
- Electron-lattice interaction -- polarons
- Photon-phonon interaction -- polaritons
- Peierls instability of linear metals

For mobile positive ions

"Particles, particles, particles."

Dept of Phys

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Dielectric function

($\boldsymbol{r}$, t)-space | ($\boldsymbol{k}$, ω)-space

$$\nabla \cdot \vec{E}(\vec{r},t) = 4\pi\rho(\vec{r},t)$$
$$\nabla \cdot \vec{D}(\vec{r},t) = 4\pi\rho_{ext}(\vec{r},t)$$

$\Leftrightarrow$

$$i\vec{k} \cdot \vec{E}(\vec{k},\omega) = 4\pi\rho(\vec{k},\omega)$$
$$i\vec{k} \cdot \vec{D}(\vec{k},\omega) = 4\pi\rho_{ext}(\vec{k},\omega)$$

$$(\rho = \rho_{ext} + \rho_{ind})$$

Take the Fourier "shuttle" between 2 spaces:

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

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

$$\vec{D}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\vec{E}(\vec{k},\omega)$$ (by definition)

or $$\rho_{ext}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\rho(\vec{k},\omega)$$ (easier to calculate)

or $$\phi_{ext}(\vec{k},\omega) = \varepsilon(\vec{k},\omega)\phi(\vec{k},\omega) \quad \because \vec{E}(\vec{k},\omega) = -i\vec{k}\phi(\vec{k},\omega)\ldots \text{ etc}$$

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

EM wave propagation in metal

Maxwell equations

$$\nabla\times\vec{E}=-\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \quad ; \quad \nabla\cdot\vec{D}=4\pi\rho_{ext}$$

$$\nabla\times\vec{B}=+\frac{1}{c}\frac{\partial\vec{D}}{\partial t}+\frac{4\pi}{c}\vec{J}_{ext} \quad ; \quad \nabla\cdot\vec{B}=0$$

⟺

$$i\vec{k}\times\vec{E}=+\frac{i\omega}{c}\vec{B} \quad ; \quad \varepsilon_{ion}\vec{k}\cdot\vec{E}=4\pi\rho_{ext}$$

$$i\vec{k}\times\vec{B}=-\frac{i\omega}{c}\varepsilon_{ion}\vec{E}+\frac{4\pi}{c}\vec{J}_{ext} ; \quad i\vec{k}\cdot\vec{B}=0$$

$$\left(\vec{J}=\sigma\vec{E}\right)$$

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

$$\vec{k}\times\left(\vec{k}\times\vec{E}\right)=\vec{k}\left(\vec{k}\cdot\vec{E}\right)-k^2\vec{E}$$

- Transverse wave

$$k^2=\frac{\omega^2}{c^2}\left(\varepsilon_{ion}+\frac{4\pi i\sigma}{\omega}\right)$$

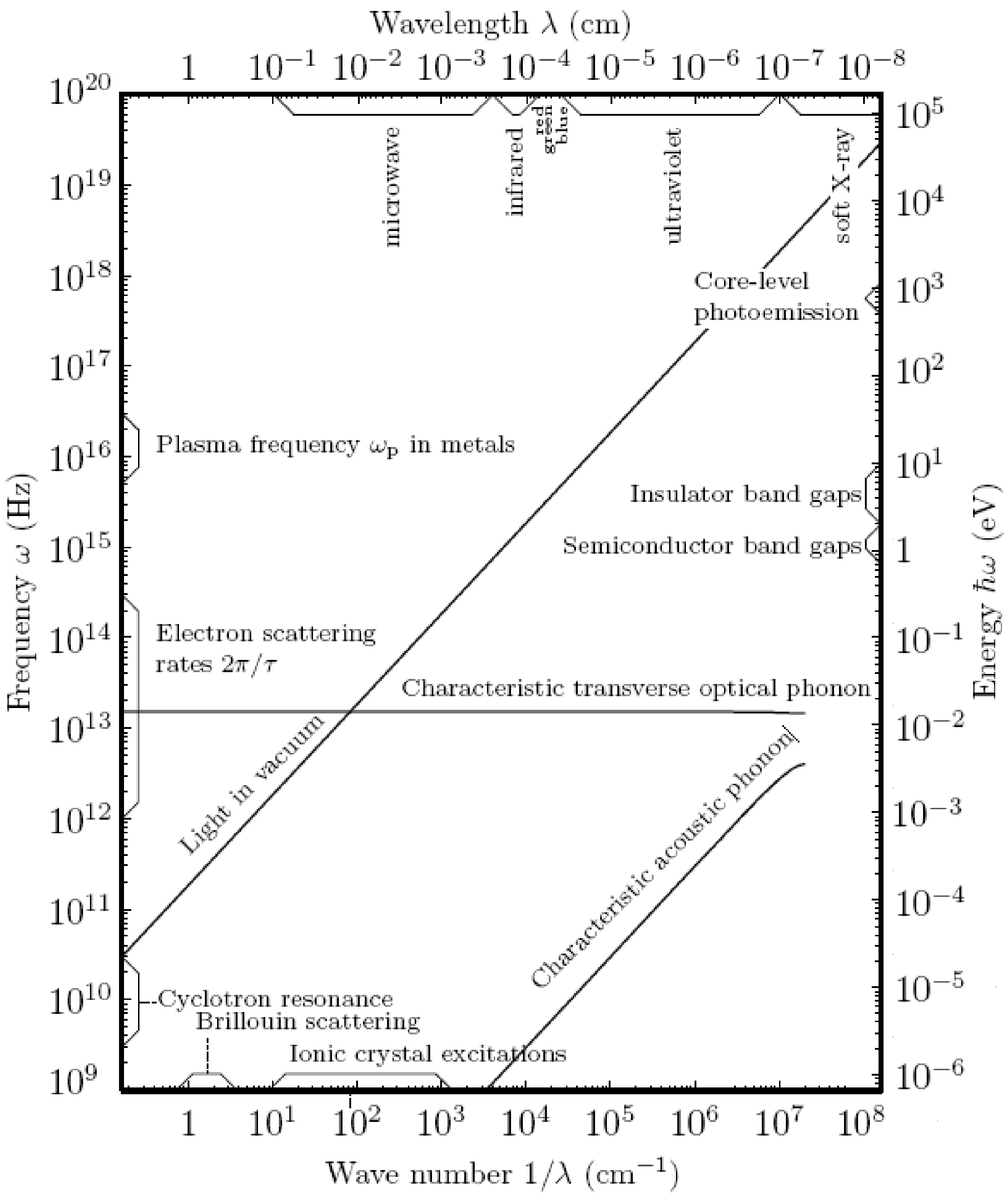
$$\because \upsilon_p=\frac{\omega}{k}=\frac{c}{n}, \text{ refractive index } n=\sqrt{\varepsilon}$$

$$\therefore \varepsilon(\vec{k},\omega)=\varepsilon_{ion}+\frac{4\pi i\sigma}{\omega}$$

(in the following, let $\varepsilon_{ion}\sim 1$)

- Longitudinal wave

$$\varepsilon(\vec{k},\omega)=0$$



Drude model of AC conductivity

$$m_e \frac{d\langle\vec{v}\rangle}{dt} = -e\vec{E}(t) - m_e \frac{\langle\vec{v}\rangle}{\tau}$$

Assume

$$\vec{E}(t) = \vec{E}_0 e^{-i\omega t}$$

then

$$\langle\vec{v}\rangle = \vec{v}_0 e^{-i\omega t}$$

$$\rightarrow \langle\vec{v}\rangle = -\frac{e\tau / m_e}{1-i\omega\tau}\vec{E}(t)$$

$$\rightarrow \vec{j} = -ne\langle\vec{v}\rangle = \sigma(\omega)\vec{E}$$

AC conductivity

$$\sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau}, \quad \sigma_0 \equiv \frac{ne^2\tau}{m_e}$$

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

AC dielectric function (uniform EM wave, k=0)

$$\varepsilon(0,\omega)=1+\frac{4\pi i\sigma_0}{\omega(1-i\omega\tau)}=\begin{cases}1+4\pi i\sigma_0/\omega & \text{for } \omega\tau<<1\\ 1-\omega_p^2/\omega^2 & \text{for } \omega\tau>>1\end{cases}$$

where plasma frequency $\omega_p^2=(4\pi ne^2/m)$

- Low frequency $\omega\tau<<1$

$\tau\sim 10^{-13}$-10^{-14}, $\therefore\ \omega$ can be as large as 100 GHz

$$n=\sqrt{\varepsilon}=n_R+in_I$$

$$\text{where } n_I=\left(-\frac{1}{2}+\frac{1}{2}\sqrt{1+\left(4\pi\sigma_0/\omega\right)^2}\right)^{1/2}=\begin{cases}2\pi\sigma_0/\omega & \text{for } \sigma_0/\omega<<1\\ \sqrt{2\pi\sigma_0/\omega} & \text{for } \sigma_0/\omega>>1\end{cases}$$

- Attenuation of plane wave due to n_I

$$\exp(i\vec{k}\cdot\vec{r})=\exp(in\omega/c\hat{k}\cdot\vec{r})$$
$$=\exp(in_R\omega/c\hat{k}\cdot\vec{r})\exp(-n_I\omega/c\hat{k}\cdot\vec{r})$$

exponential decay

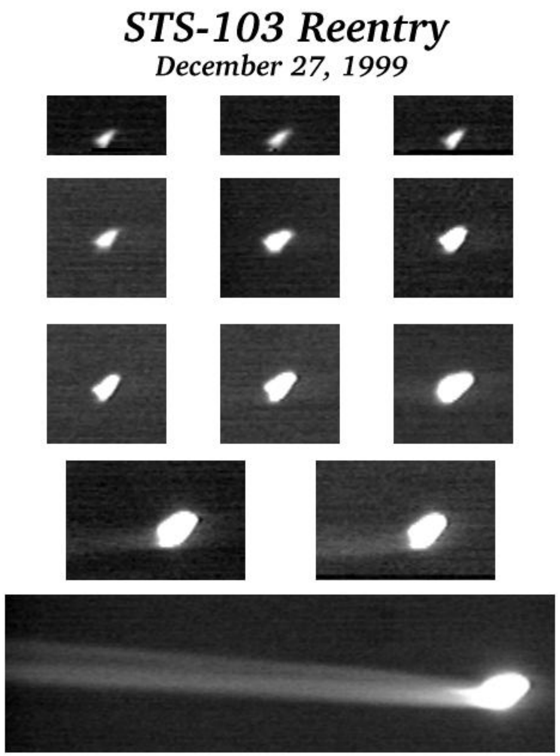
- High frequency

if positive ion charges can be distorted

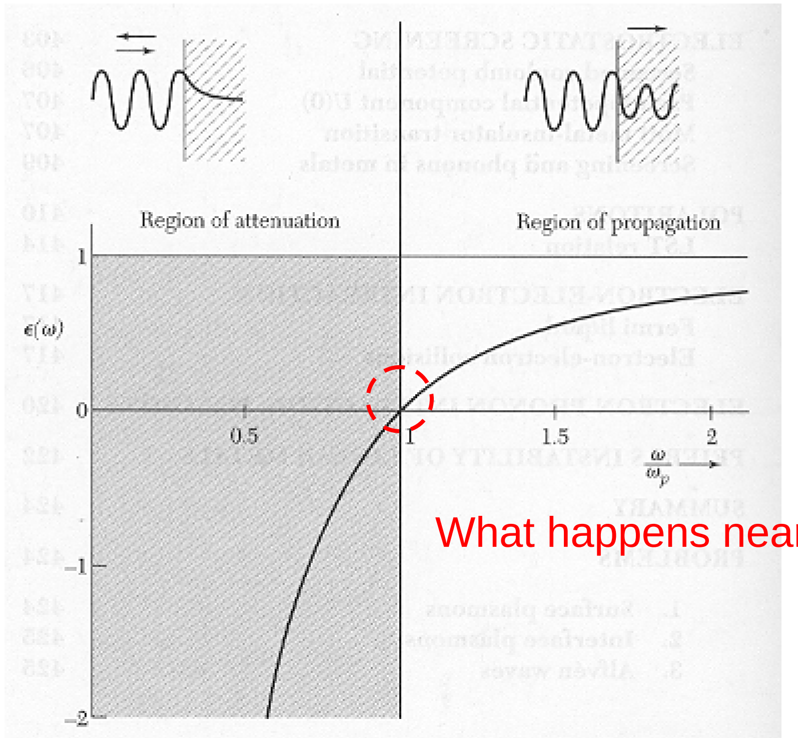
$\omega\tau >> 1$

$$\varepsilon(\omega) = 1 - \omega_p^2 / \omega^2 \rightarrow \varepsilon_{ion} - \omega_p^2 / \omega^2 = \varepsilon_{ion}(1 - \tilde{\omega}_p^2 / \omega^2)$$

$\omega < \tilde{\omega}_p \rightarrow \varepsilon(\omega) < 0$	$\omega > \tilde{\omega}_p \rightarrow 0 < \varepsilon(\omega) < 1$
EM wave is damped	EM wave propagates with phase velocity $C/\sqrt{\varepsilon}$



Shuttle blackout



What happens near $\omega = \omega_p$?

$$\omega = \omega_p \rightarrow \varepsilon(\omega) = 0$$

can have longitudinal EM wave!

Homework:

Assume that $\vec{k} \cdot \vec{E} \neq 0$, then from (a) Gauss' law, (b) equation of continuity, and (c) Ohm's law, show that

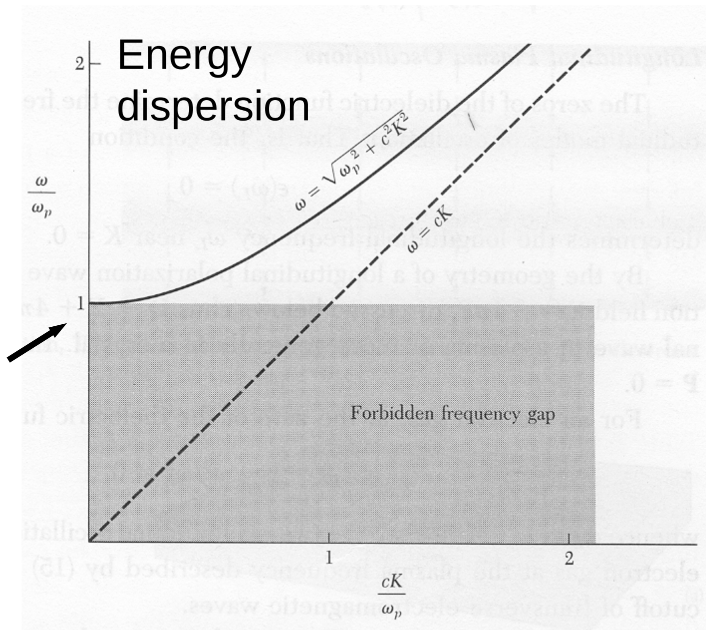
$$4\pi\sigma(\omega)\rho(\omega) = i\omega\rho(\omega)$$

Also show that this leads to $\varepsilon(\omega)$=0.

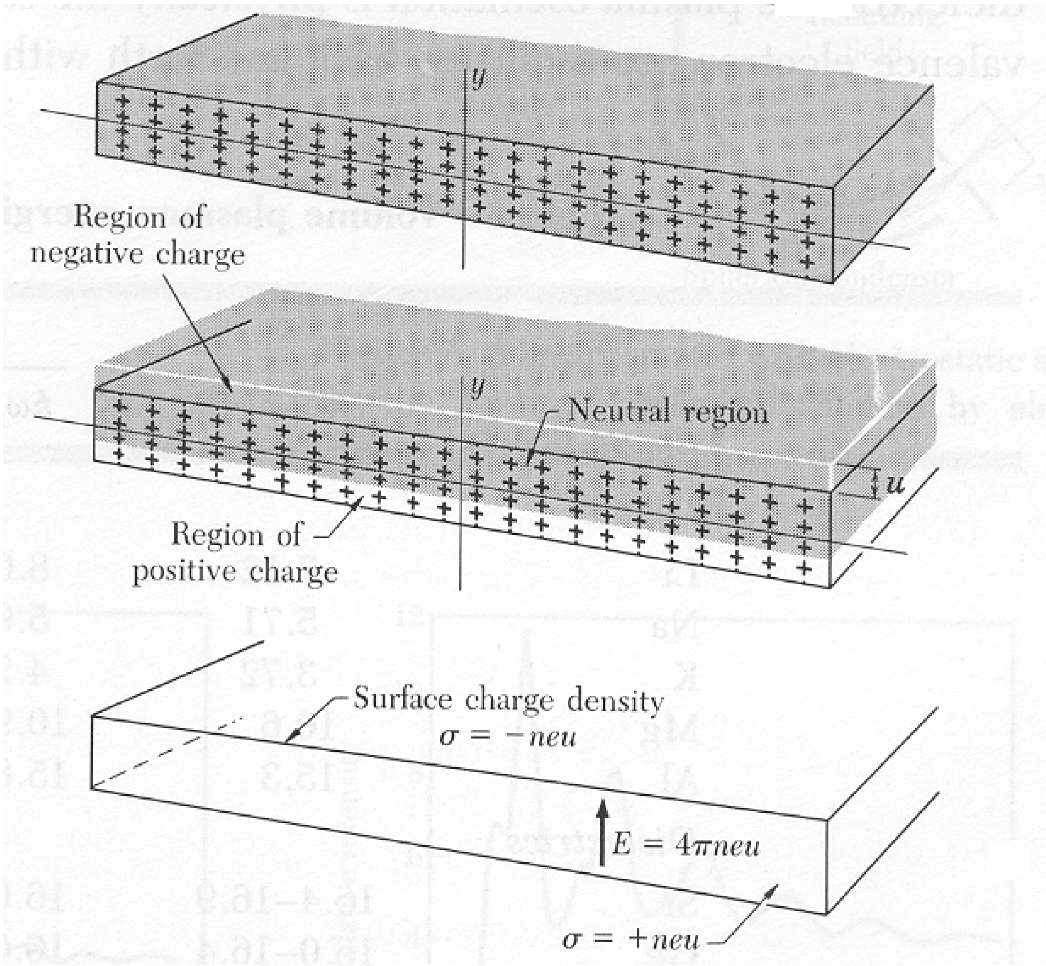
- On the contrary, if $\varepsilon(\omega) \neq 0$, the EM wave can only be transverse.

- When $i\vec{k} \cdot \vec{E} = 4\pi\rho \neq 0$, there exists charge oscillations called plasma oscillation.

(our discussion in the last 2 pages involves only the uniform, or k=0, case)



- A simple picture of (uniform) plasma oscillation



$$m\ddot{u} = -eE = -(4\pi n e^2)u$$

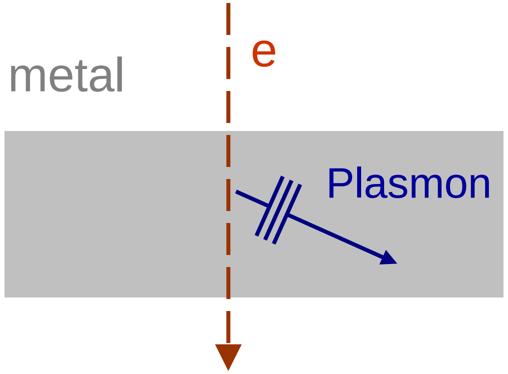
$\therefore u$ oscillates at a frequency

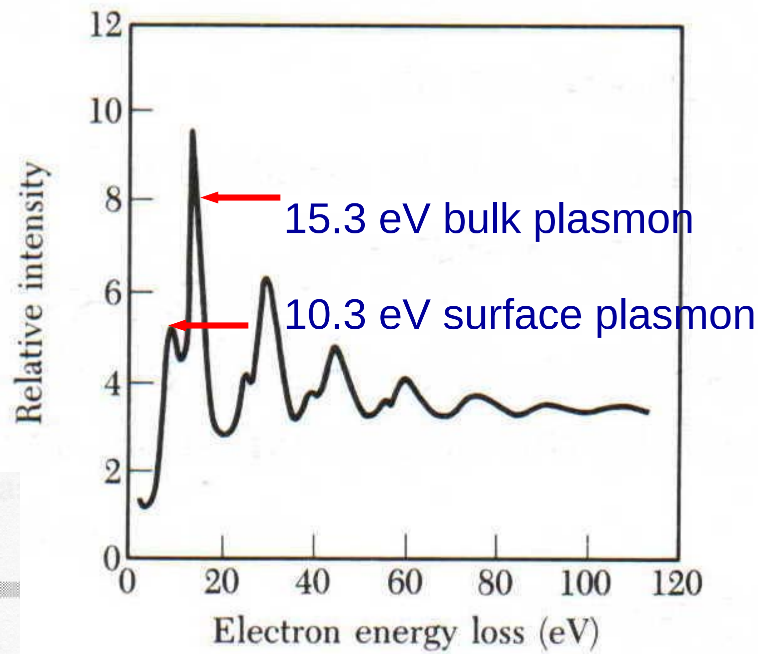
$$\omega = \sqrt{4\pi n e^2 / m}$$

- For copper, $n=8\times10^{22}$ /cm^3

$\omega_p=1.6\times10^{16}$/s, λ_p=1200A, which is ultraviolet light.

Experimental observation: plasma oscillation in Al





Material	Observed	Calculated	
		$\hbar\omega_p$	$\hbar\tilde{\omega}_p$
Metals			
Li	7.12	8.02	7.96
Na	5.71	5.95	5.58
K	3.72	4.29	3.86
Mg	10.6	10.9	
Al	15.3	15.8	
Dielectrics			
Si	16.4–16.9	16.0	
Ge	16.0–16.4	16.0	
InSb	12.0–13.0	12.0	

- The quantum of plasma oscillation is called plasmon.

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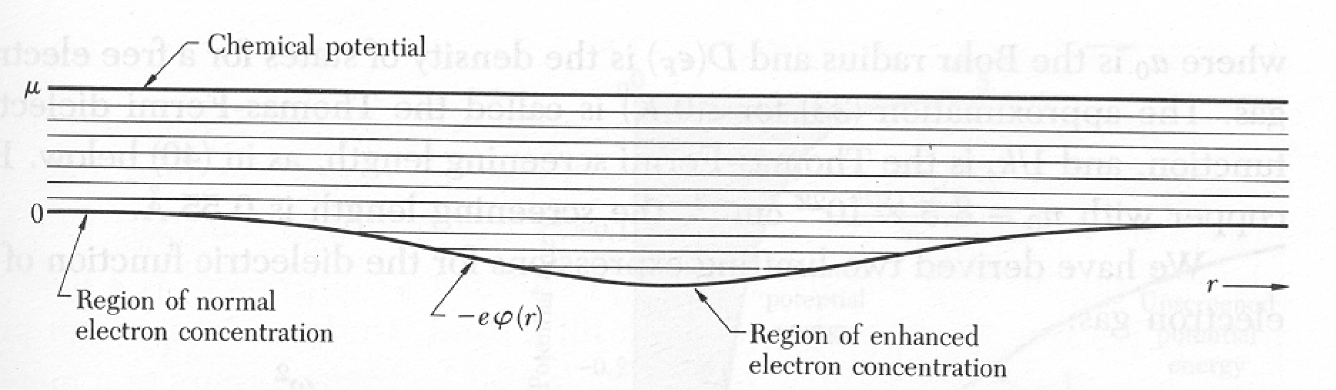
Electrostatic screening: Thomas-Fermi theory (1927)

Valid if ϕ (r) is very smooth within λ_F

- Fermi energy: $$\varepsilon_F(\vec{r}) \approx \frac{\hbar^2}{2m}\left(3\pi^2 n(\vec{r})\right)^{2/3}$$

- Electrochemical potential: $$\mu = \varepsilon_F(\vec{r}) - e\phi(\vec{r}) = \frac{\hbar^2}{2m}\left(3\pi^2 n_0\right)^{2/3}$$



$$\rho_{ind}(\vec{r}) = -e(n(\vec{r}) - n_0) \approx -\frac{3}{2}\frac{n_0 e^2}{\mu}\phi(\vec{r})$$

or

$$\rho_{ind}(\vec{k}) = -\frac{3}{2}\frac{n_0 e^2}{\mu}\phi(\vec{k})$$

Dielectric function $\varepsilon(k,0) = \frac{\rho_{ext}(k)}{\rho(k)} = 1 - \frac{\rho_{ind}(k)}{\rho(k)} = 1 + \frac{3}{2}\frac{n_0 e^2}{\mu}\frac{\phi(k)}{\rho(k)}$

but $k^2\phi(k) = 4\pi\rho(k)$

$$\therefore \varepsilon(k) = 1 + \frac{k_s^2}{k^2} \quad \text{where } k_s^2 \equiv \frac{6\pi n_0 e^2}{\mu}\left(= 4\pi e^2 D(\mu), D(\mu) = \frac{3}{2}\frac{n_0}{\mu}\right)$$

- For free electron gas, $D(\varepsilon_F) = mk_F/\hbar^2\pi^2$, $a_0 = \frac{\hbar^2}{me^2}$

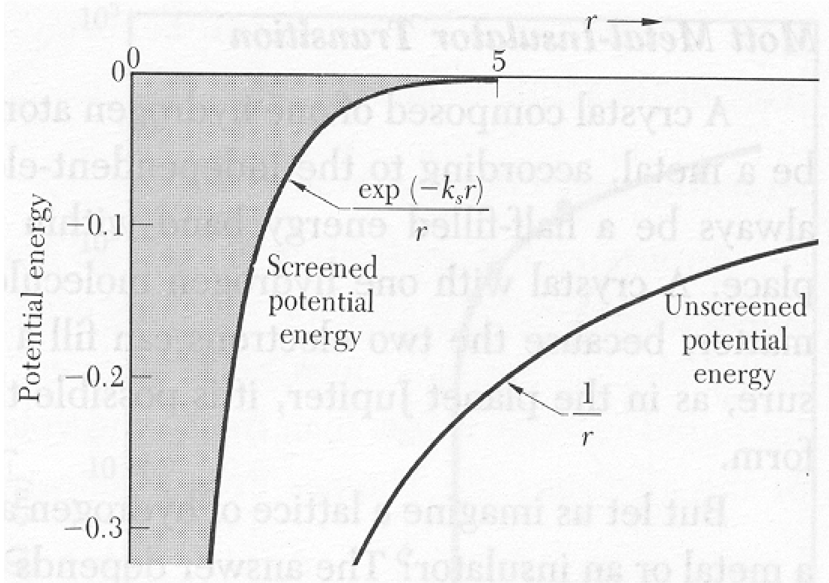
$\rightarrow (k_s/k_F)^2 = (4/\pi)(1/k_F a_0) \sim O(1)$

- Screening of a point charge

For $\phi_{ext}(\vec{r}) = Q/r \Leftrightarrow \phi_{ext}(\vec{k}) = 4\pi Q/k^2$

$$\phi(\vec{k}) = \frac{\phi_{ext}(\vec{k})}{\varepsilon(\vec{k})} = 4\pi\frac{Q}{k^2 + k_s^2}$$

$$\Rightarrow \phi(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3}\phi(\vec{k})e^{i\vec{k}\cdot\vec{r}} = \frac{Q}{r}e^{-k_s r}$$



Comparison: $\varepsilon(0,\omega) = 1 - \omega_p^2/\omega^2; \varepsilon(k,0) = 1 + k_s^2/k^2$

Why e-e interaction can usually be ignored in metals?

- $$K \approx \frac{\hbar^2}{m}\frac{1}{r^2}, \quad U \approx \frac{e^2}{r}$$

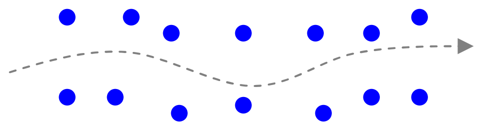
$$\frac{U}{K} \approx \frac{me^2}{\hbar^2} r = \frac{r}{a_B}$$

Typically, 2 < U/K < 5

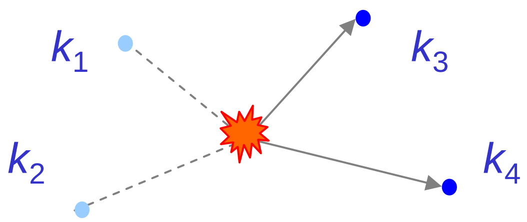
- Average e-e separation in a metal is about 2 A

Experiments find e mean free path about 10000 A (at 300K)

At 1 K, it can move 10 cm without being scattered! Why?



- A collision event:



- Calculate the e-e scattering rate using Fermi's golden rule:

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\sum_{i,f}\left|\langle f \,|V_{ee}|\, i\rangle\right|^2 \delta(E_i - E_f)$$

Scattering amplitude $\left|\langle f \,|V_{ee}|\, i\rangle\right|^2 = \left|\langle k_3, k_4 \,|V_{ee}|\, k_1, k_2\rangle\right|^2$

$$E_i = E_1 + E_2; \quad E_f = E_3 + E_4$$

The summation is over all possible initial and final states that obey energy and momentum conservation.

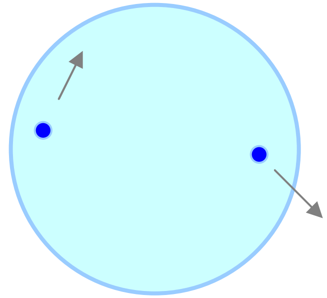
Pauli principle reduces available states for the following reasons:

Assume the scattering amplitude $|V_{ee}|^2$ is roughly of the same order for all k's, then

$$\tau^{-1} \approx \frac{2\pi}{\hbar} |V_{ee}|^2 \sum_{k_1,k_2} \sum_{k_3,k_4} 1$$

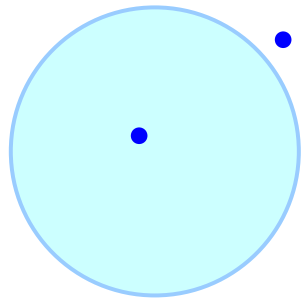
$E_1+E_2=E_3+E_4$; $\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4$

• Two e's inside the FS cannot scatter with each other (energy conservation + Pauli principle). At least one of them must be outside of the FS.



Let electron 1 be outside the FS:

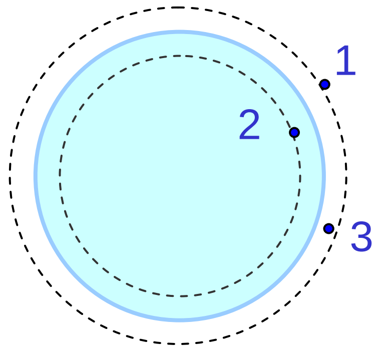
• One e is "shallow" outside, the other is "deep" inside also cannot scatter with each other, since the "deep" e has nowhere to go.



• If $|E_2| < E_1$, then $E_3+E_4 > 0$ (let $E_F=0$)

But since $E_1+E_2 = E_3+E_4$, 3 and 4 cannot be very far from the FS if 1 is close to the FS.

Let's fix E_1, and study possible initial and final states.



(let the state of electron 1 be fixed)

- number of initial states = (volume of E_2 shell)/ Δ^3k

number of final states = (volume of E_3 shell)/ Δ^3k

(E_4 is uniquely determined)

- $\tau^{-1} \sim$ V(E_2)/ Δ^3k x V(E_3)/ Δ^3k $\leftarrow$ number of states for scatterings

$$V(E_2) \cong 4\pi k_F^2 \,|\, k_2 - k_F \,|$$
$$V(E_3) \cong 4\pi k_F^2 \,|\, k_3 - k_F \,|$$

$\therefore\ \tau^{-1} \sim (4\pi/\Delta^3 k)^2\, k_F^2 |k_2-k_F| \times k_F^2 |k_3-k_F|$

Total number of states for particle 2 and 3 = $[(4/3)\pi\, k_F^3/\ \Delta^3 k]^2$

- The fraction of states that "can" participate in the scatterings

$= (9/k_F^2)\ |k_2-k_F| \times |k_3-k_F|$

$\sim (E_1/E_F)^2$ (1951, V. Wessikopf)

Finite temperature:

$\sim (kT/E_F)^2 \sim 10^{-4}$ at room temperature

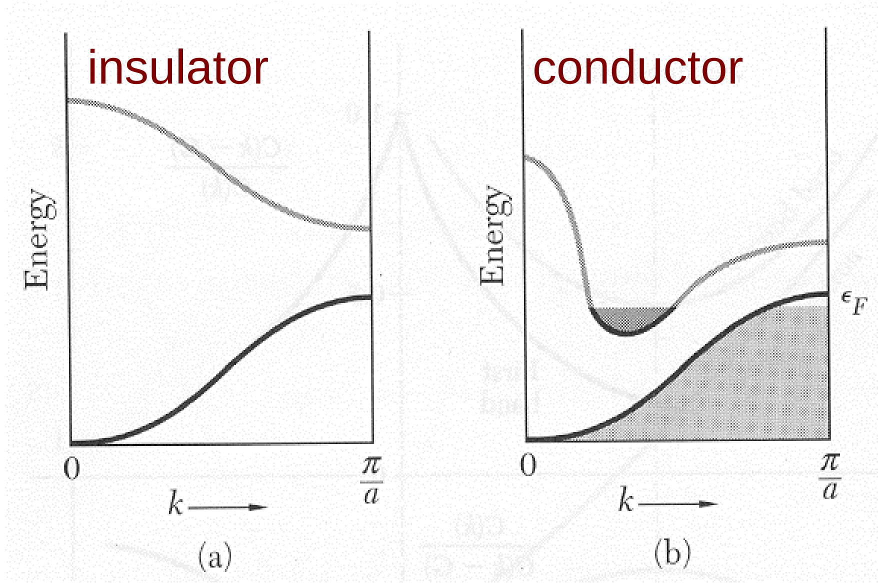
$\rightarrow$ e-e scattering rate $\propto T^2$

- need very low T (a few K) and very pure sample to eliminate thermal and impurity scatterings before the effect of e-e scattering can be observed.

3 types of insulator:

1. Band insulator (1931)

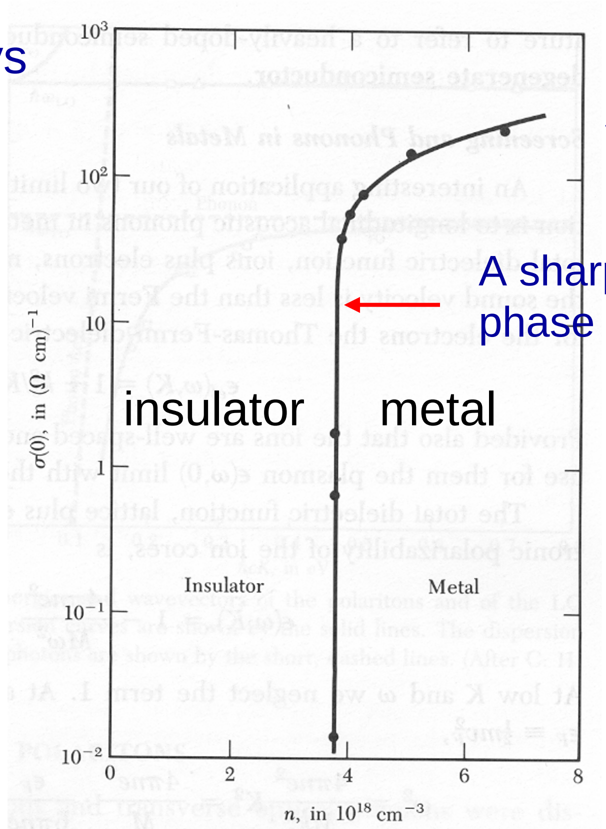
[due to e-lattice interaction]



e-e interaction is not always unimportant!

2. Mott insulator (1937)

[due to e-e interaction]



Si:P alloy

A sharp (quantum) phase transition

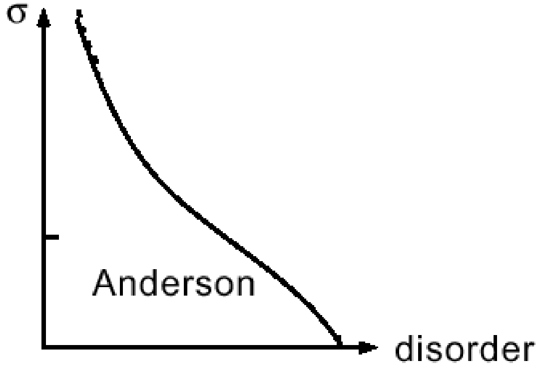
insulator

metal

1977

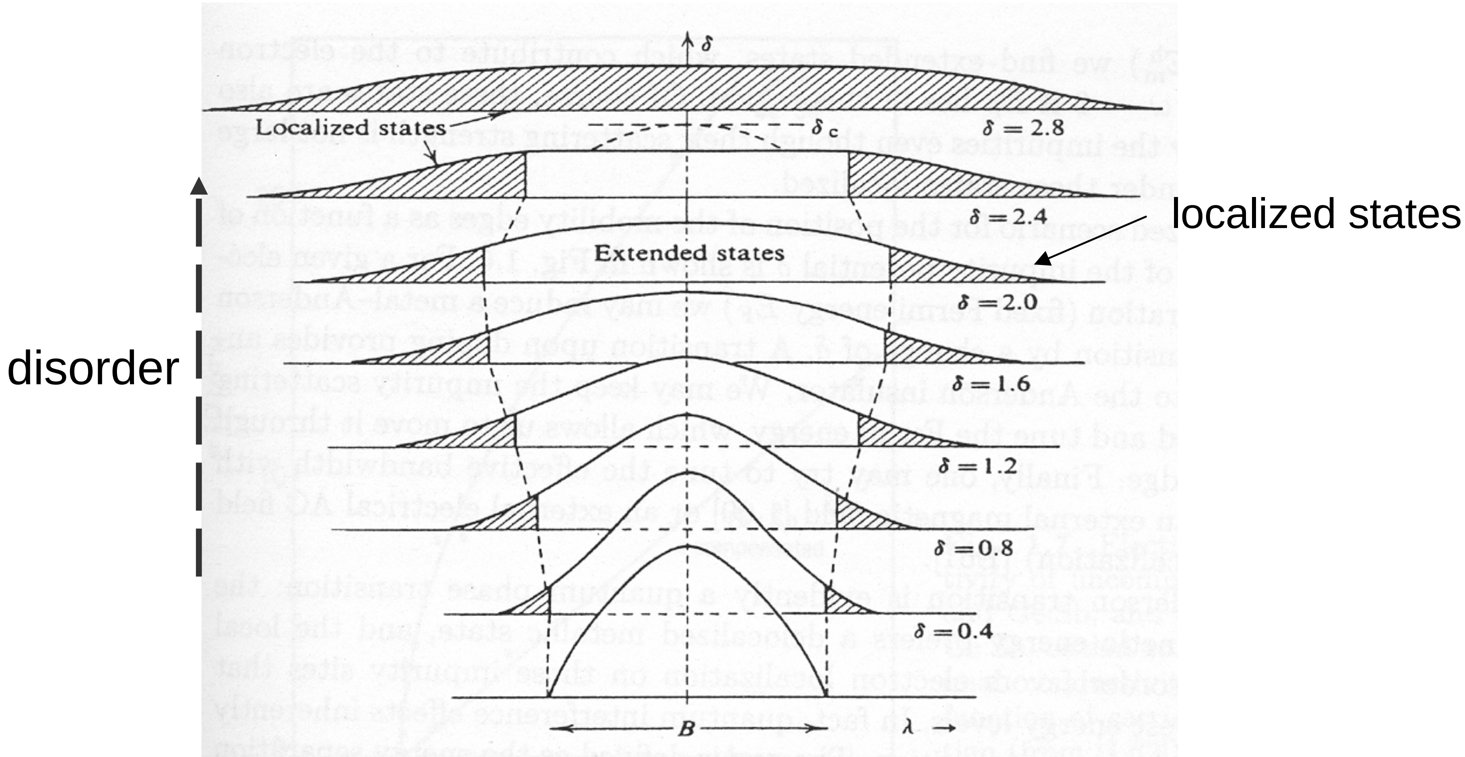
3. Anderson insulator (1958)

[due to disorder]

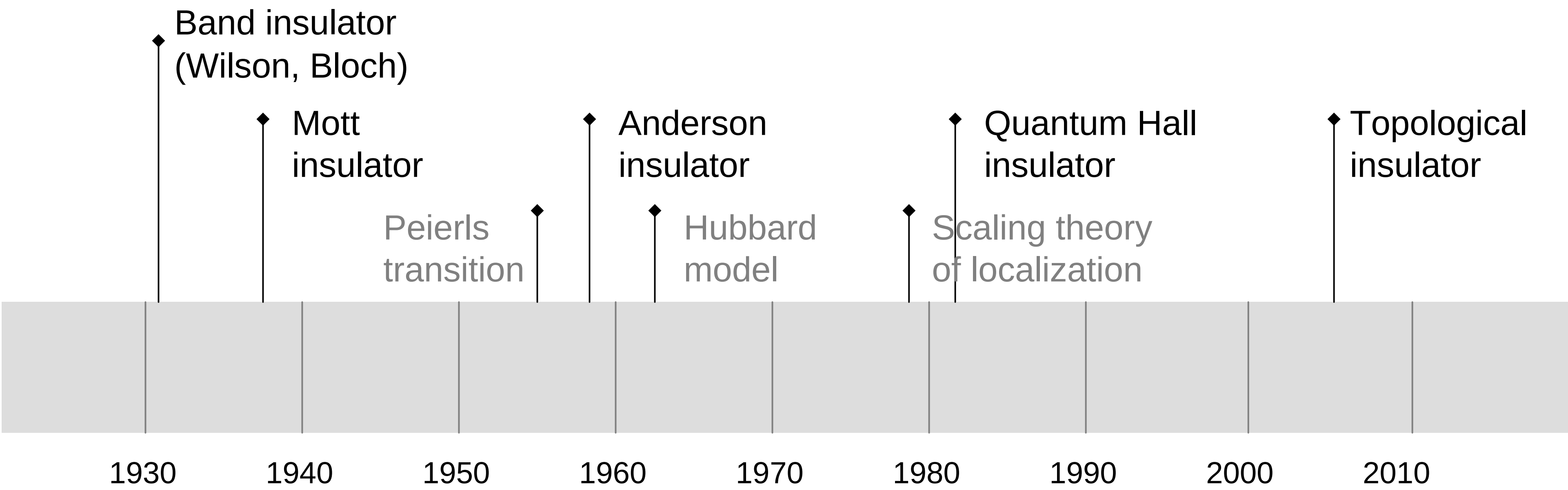


1977

- Localized states near band edges



Insulators, boring as they are (to the industry), have many faces.



2D TI is also called QSHI

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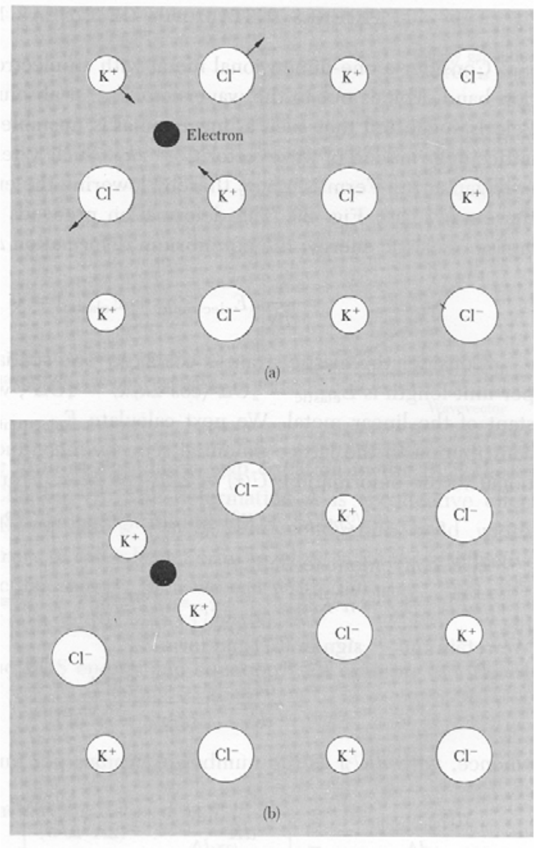
Electron-lattice interaction - polarons 極化子

- rigid ions: band effective mass m*
- movable ions: drag and slow down electrons
  - larger effect in polar crystal such as NaCl, smaller effect in covalent crystal such as GaAs



- The composite object of

"an electron + deformed lattice (phonon cloud)" is called a polaron.

- # of phonons surrounding the electron

$$\frac{\text{deformation energy}}{\hbar\omega_L(k \to 0)} \equiv \frac{1}{2}\alpha$$

$$m^*_{pol} \approx \frac{m^*}{1-\alpha/6} \quad \text{for small } \alpha$$

	KCl	KBr
α	3.97	3.52
m^*/m_e	0.50	0.43
m^*_{pol}/m_e	1.25	0.93

Phonons in metals

• Regard the metal as a gas of electrons (mass m) and ions (mass M)

The ion vibrating frequency appears static to the swift electrons

$$\therefore \text{use} \quad \varepsilon_{el}(k,0) = 1 + k_s^2 / k^2$$

However, to the ions, $\varepsilon_{ion}(0,\omega) = 1 - 4\pi n e^2 / M\omega^2$

$$\text{total} \quad \boxed{\varepsilon(k,\omega) = \varepsilon_{el} + \varepsilon_{ion} - 1}$$

$$= 1 + \frac{k_s^2}{k^2} - \frac{4\pi n e^2}{M\omega^2}$$

For a derivation, see A+M, p.515.

• The longitudinal charge oscillation (ion+electron) at ε =0 is interpreted as LA phonons in the Fermi sea.

• For long wave length (both ω and k are small), we have

$$k_s^2 \equiv \frac{6\pi n e^2}{\varepsilon_F}$$

$$\omega = \upsilon k, \quad \upsilon = (m/3M)^{1/2} \upsilon_F$$

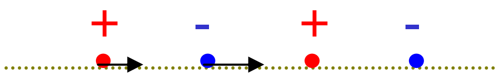
Longitudinal sound velocity

For K, v=1.8$\times$10^5 cm/s (theory), vs 2.2$\times$10^5 cm/s (exp't)

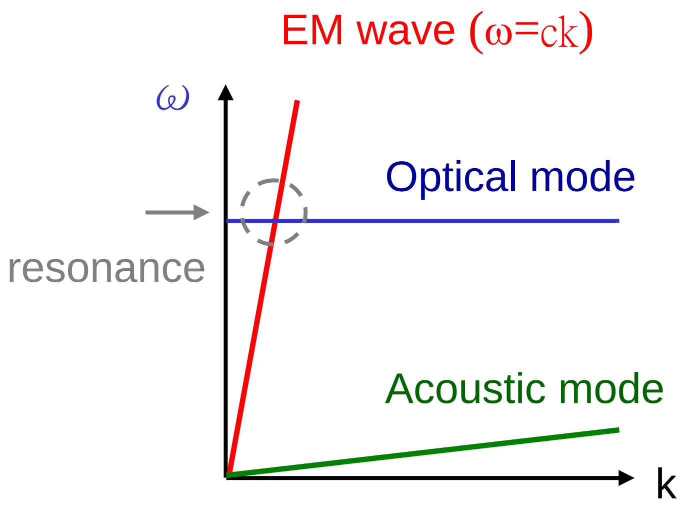
Resonance between photons and TO phonons: polaritons 電磁極化子

(LO phonons do not couple with transverse EM wave. Why?)

- dispersion of $\omega_T(k)$ ignored in the active region
- ignore the charge cloud distortion of ions
- assume there are 2 ions/unit cell



Dipole moment of a unit cell



$$\vec{p} = e(\vec{u}_+ - \vec{u}_-) \equiv e\vec{u}$$

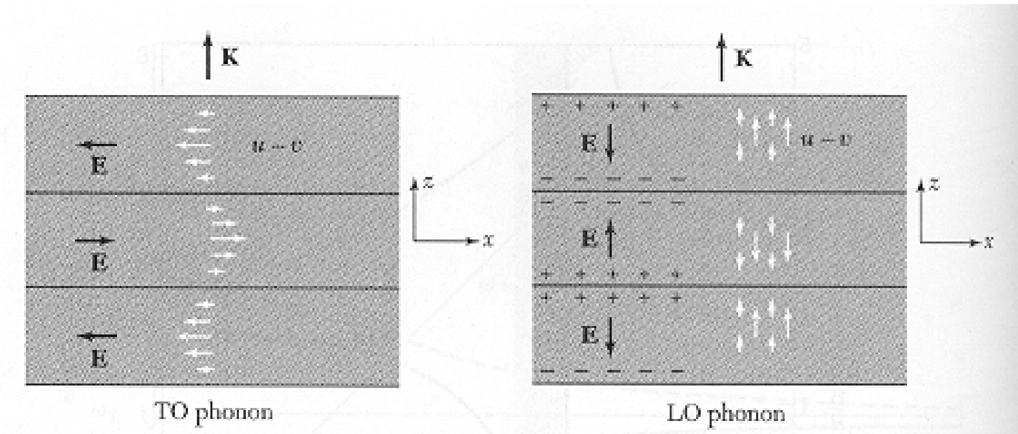
then $$M_+\ddot{\vec{u}}_+ + k(\vec{u}_+ - \vec{u}_-) = e\vec{E}(t)$$

$$M_-\ddot{\vec{u}}_- - k(\vec{u}_+ - \vec{u}_-) = -e\vec{E}(t)$$

$$\rightarrow \quad M\ddot{\vec{u}} + k\vec{u} = e\vec{E},$$

where $M^{-1} = M_+^{-1} + M_-^{-1}$

is the reduced mass



Consider a single mode of uniform EM wave

$$\vec{E}(t) = \vec{E}_0 e^{-i\omega t}, \text{ then } \vec{u} = \vec{u}_0 e^{-i\omega t}$$

$$\rightarrow -\omega^2 \vec{u} + \omega_T^2 \vec{u} = \frac{e}{M}\vec{E}, \quad \text{where } \omega_T^2 \equiv k / M$$

- Total polarization *P=Np/V, N* is the number of unit cells

$$\therefore \vec{P} = \frac{ne^2 / M}{\omega_T^2 - \omega^2}\vec{E}, \vec{D} = \vec{E} + 4\pi\vec{P}$$

$$\text{Therefore, } \varepsilon(\omega) = 1 + \frac{4\pi ne^2 / M}{\omega_T^2 - \omega^2}$$

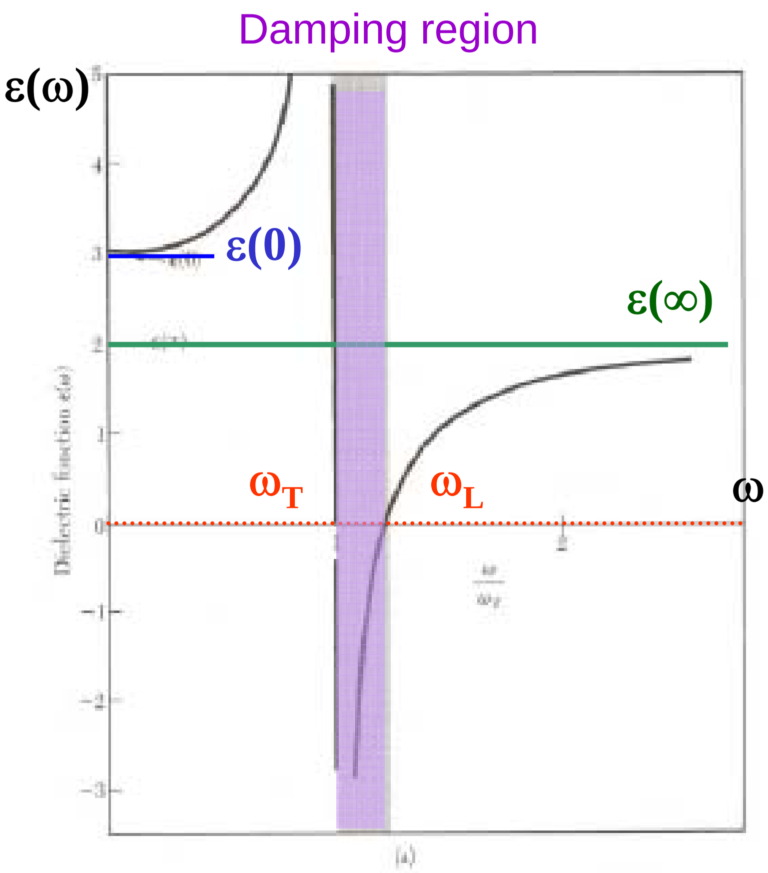
If charge cloud distortion of ions is considered,

$$\rightarrow \varepsilon_\infty + \frac{4\pi ne^2 / M}{\omega_T^2 - \omega^2}$$

- Static dielectric const. $\varepsilon_0 = \varepsilon_\infty + \frac{4\pi ne^2}{M\omega_T^2} > \varepsilon_\infty$

$$\therefore \varepsilon(\omega) = \frac{\omega_T^2 \varepsilon_0 - \omega^2 \varepsilon_\infty}{\omega_T^2 - \omega^2} \equiv \varepsilon_\infty \left(\frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2} \right)$$

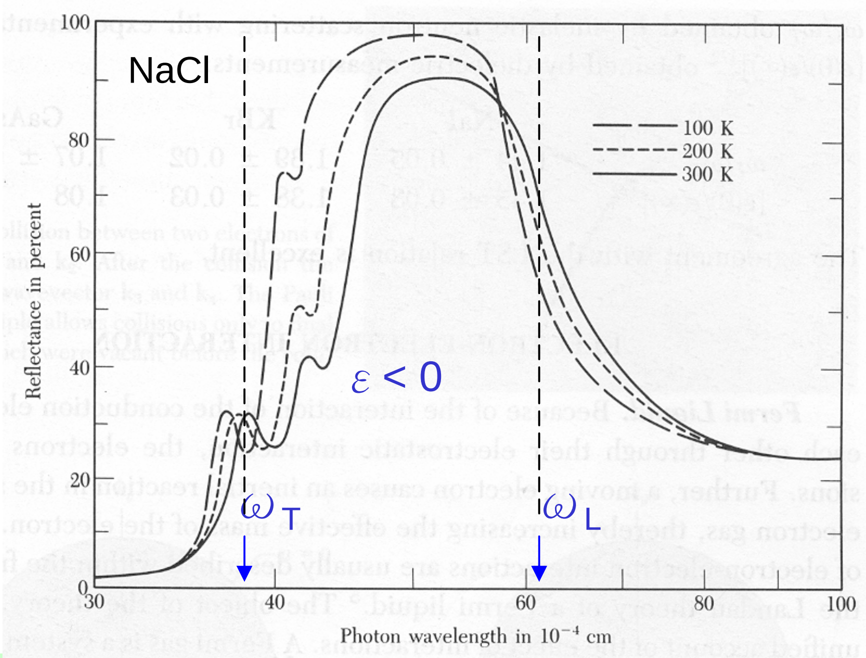
$$\text{where } \omega_L^2 \equiv \frac{\varepsilon_0}{\varepsilon_\infty}\omega_T^2, \text{ such that } \varepsilon(\omega_L) = 0$$



• LST relation $\frac{\omega_L^2}{\omega_T^2} = \frac{\varepsilon_0}{\varepsilon_\infty} (>1)$

Experimental results

	NaCl	KBr	GaAs
ω_L/ω_T	1.44	1.39	1.07
$[\varepsilon(0)/\varepsilon(\infty)]^{1/2}$	1.45	1.38	1.08



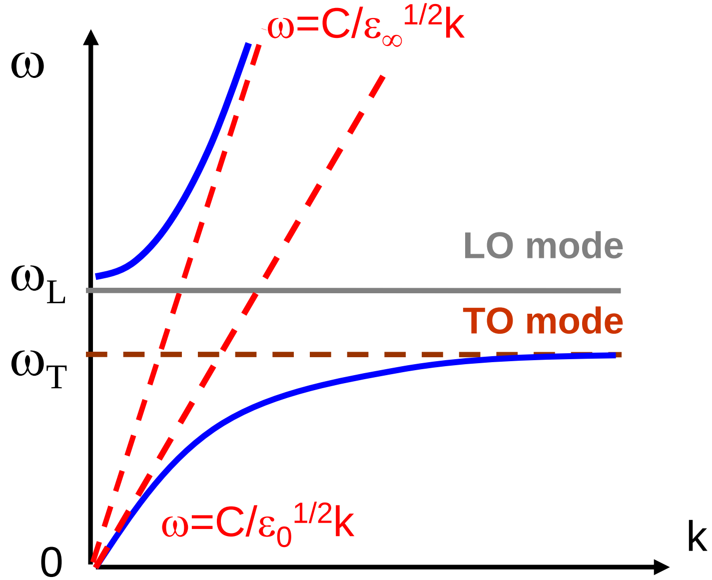
Dispersion relation

$$\omega^2 = \frac{C^2k^2}{\varepsilon(\omega)} = \frac{(Ck)^2}{\varepsilon_\infty}\frac{\omega^2 - \omega_T^2}{\omega^2 - \omega_L^2}$$

$$\omega >> \omega_{L,T} \rightarrow \quad \omega = (C/\sqrt{\varepsilon_\infty})k$$

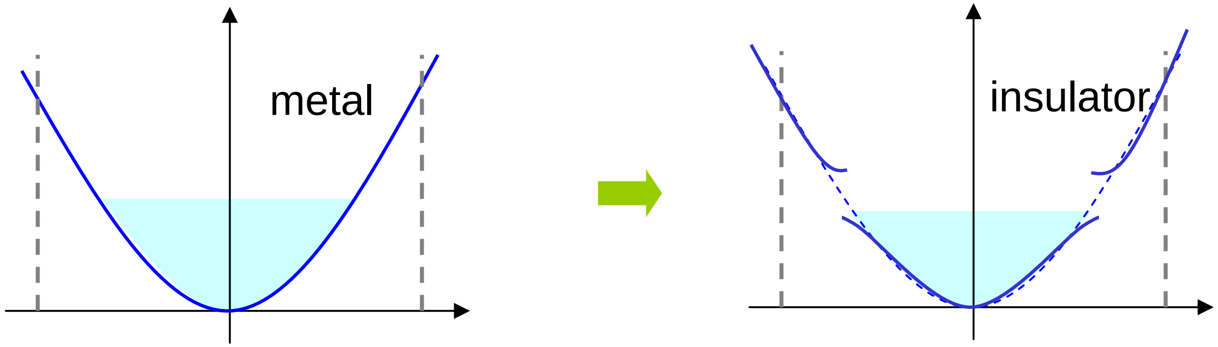
$$\omega << \omega_{L,T} \rightarrow \quad \omega = (C/\sqrt{\varepsilon_0})k$$

$$\omega_T < \omega < \omega_L \rightarrow \quad \text{no solution}$$

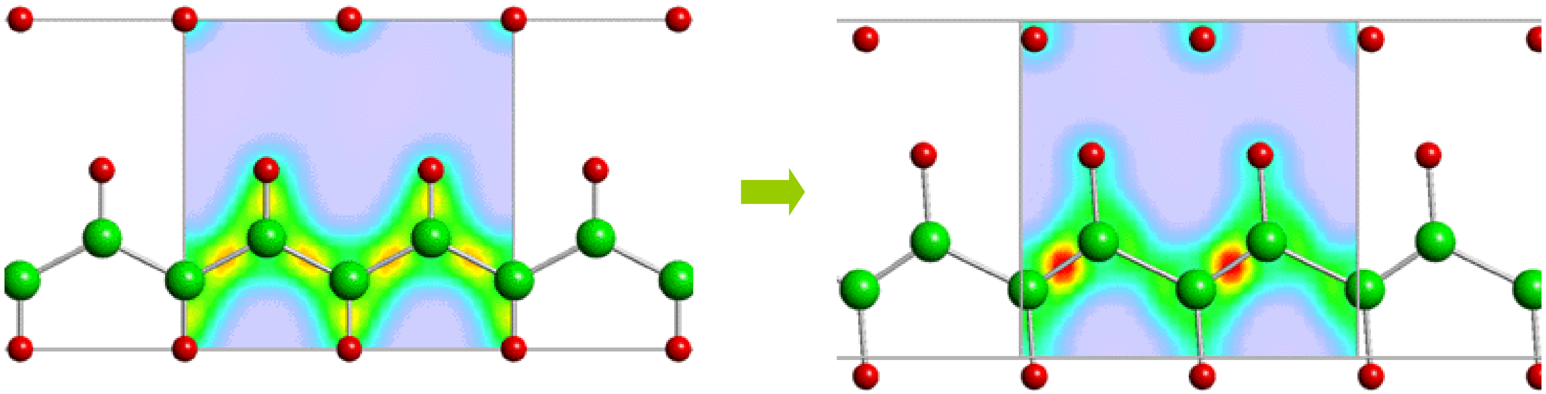


• The composite object of photon+TO phonon is called polariton.

Peierls instability of 1-dim metal chain



• An example of 1-d metal: poly-acetylene (1958) 聚乙炔



• sp^2 bonding

• π - electrons delocalized along the chain

• Dimerization opens an energy 二聚[作用] gap 2-3 eV (Peierls instability) and becomes a semiconductor.