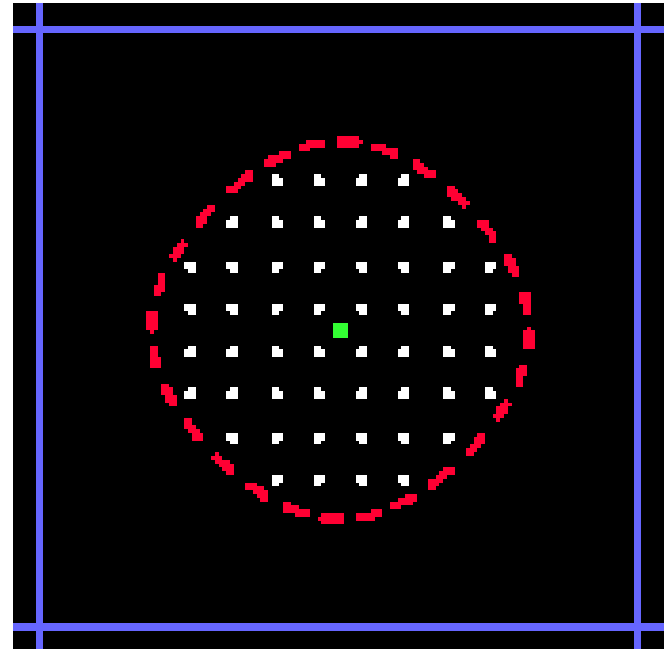
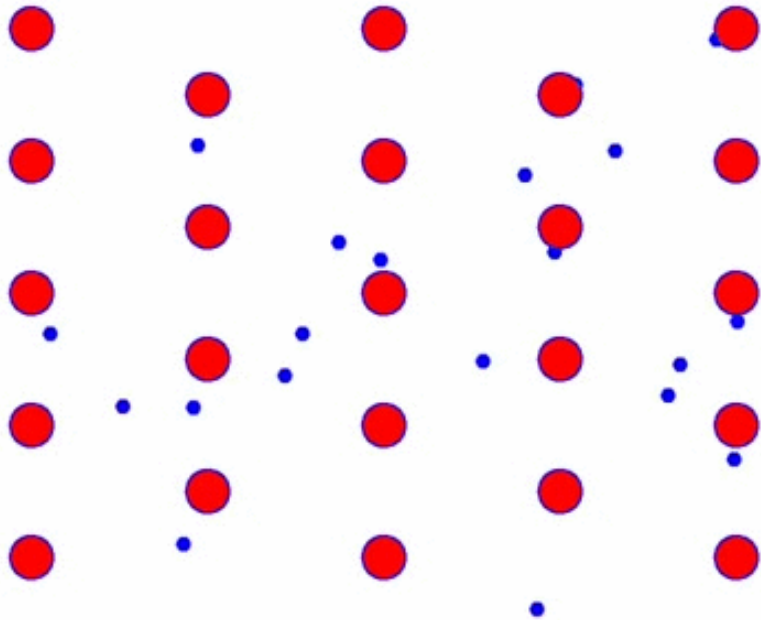
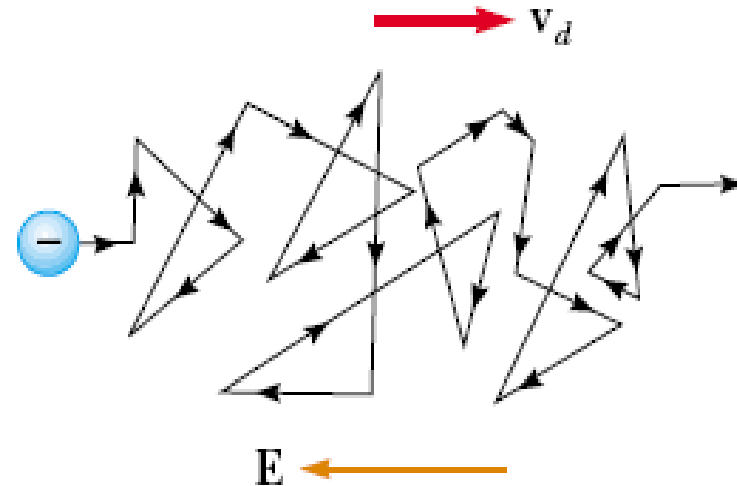
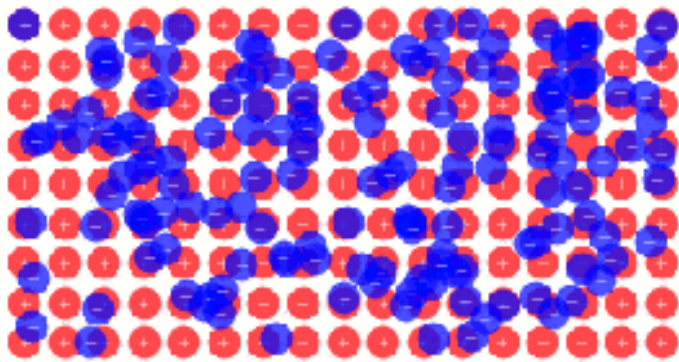


# Capítulo 7: Modelo de Drude - Dinámica semiclassical de electrones en bandas



# Modelo de Drude

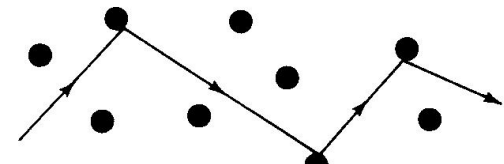
Consideró el gas clásico para estudiar conductividad de los metales



## Hipótesis

1 - movimiento del electrón es sólo perturbado por colisiones que ocurren en promedio cada  $\tau$ .

$1/\tau$  = probabilidad por unidad de tiempo de que un electrón experimente una colisión.



2- Entre colisiones el electrón se mueve siguiendo las leyes de Newton:  $\mathbf{F} = e \mathbf{E}$

3- Después de una colisión el electrón 'olvida' la velocidad que traía y arranca con una dirigida al azar pero cuyo módulo corresponde a la temperatura en ese sitio.

$$m \left( \frac{dv}{dt} + \frac{v}{\tau} \right) = F :$$

Las colisiones introducen un término de amortiguamiento

En ausencia de campo externo:

$$\frac{dv}{dt} + \frac{v}{\tau} = 0 \quad \longrightarrow \quad v(t) = v_0 \exp\left(\frac{-t}{\tau}\right)$$

$\tau$ : tiempo de relajación

$\mathbf{p}(t)$  momento por electrón a tiempo  $t \longrightarrow \mathbf{p}(t + dt) ?$

$dt/\tau$  = probabilidad de que colisione en el tiempo  $t + dt$

$1 - dt/\tau$  = probabilidad de que no colisione

Despreciando la contribución de los electrones que colisionan:

$$\begin{aligned}\mathbf{p}(t + dt) &= \left(1 - \frac{dt}{\tau}\right) \left[ \mathbf{p}(t) + \mathbf{f}(t)dt + O(dt)^2 \right] \\ &= \mathbf{p}(t) - \left(\frac{dt}{\tau}\right) \mathbf{p}(t) + \mathbf{f}(t)dt + O(dt)^2.\end{aligned}$$

$$\mathbf{p}(t + dt) - \mathbf{p}(t) = - \left(\frac{dt}{\tau}\right) \mathbf{p}(t) + \mathbf{f}(t)dt + O(dt)^2.$$

$$\frac{d\mathbf{p}(t)}{dt} = - \frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t).$$

$$e \mathbf{E} = m \mathbf{v}_D / \tau \longrightarrow \mathbf{v}_D = \frac{e \tau}{m} \mathbf{E}$$

$\mu$ : movilidad

$$\bar{\mathbf{v}}_D = \mu \bar{\mathbf{E}}$$

$$\bar{\mathbf{J}} = n e \bar{\mathbf{v}}_D = \frac{n e^2 \tau}{m} \bar{\mathbf{E}} = n e \mu \bar{\mathbf{E}}$$

Ley de  
Ohm

$\sigma$ : conductividad

$$\mathbf{J} = \sigma \mathbf{E}$$

$$\sigma = \frac{n e^2 \tau}{m} = n e \mu$$

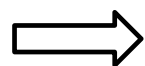
$$\rho = \sigma^{-1}$$

resistividad

$$j = \sigma E = -\sigma \nabla \varphi$$

$$j_Q = -\lambda \nabla T$$

Teoría cinética  
de gases



$$\lambda = \frac{1}{3} l \bar{v} c_{el}$$

Conductividad  
térmica

Usando

$$\bar{v} = \left( \frac{3k_B T}{m_e} \right)^{1/2}$$

$$l = \bar{v} \tau = \left( \frac{3k_B T}{m_e} \right)^{1/2} \tau$$

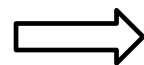
$$c_{el} = \frac{3}{2} n_e k_B$$

Se obtiene

$$\lambda = \frac{3}{2} \frac{n_e \tau}{m_e} k_B^2 T$$

Conductividad  
de Drude

$$\sigma = \frac{n_e e^2 \tau}{m_e}$$



$$\frac{\lambda}{\sigma} = \frac{3}{2} \left( \frac{k_B}{e} \right)^2 T$$

Ley de Wiedemann-Franz

$$L = \frac{3}{2} \left( \frac{k_B}{e} \right)^2 = 1.11 \times 10^{-8} \text{ V}^2 \text{ K}^{-2}$$

**Número de Lorentz**

Metal	$L(0^\circ\text{C})$ ( $10^{-8} \text{ V}^2 \text{ K}^{-2}$ )	$L(100^\circ\text{C})$ ( $10^{-8} \text{ V}^2 \text{ K}^{-2}$ )	Metal	$L(0^\circ\text{C})$ ( $10^{-8} \text{ V}^2 \text{ K}^{-2}$ )	$L(100^\circ\text{C})$ ( $10^{-8} \text{ V}^2 \text{ K}^{-2}$ )
Ag	2.31	2.38	Li	2.22	2.43
Au	2.35	2.36	Mo	2.61	2.79
Al	2.14	2.19	Pb	2.47	2.53
Cu	2.23	2.29	Pt	2.51	2.60
Fe	2.61	2.88	W	3.04	3.20
Ir	2.49	2.49	Zn	2.28	2.30

**A pesar del factor 2 de diferencia, el correcto orden de magnitud de L es sorprendente, ya que el modelo de Drude da estimaciones muy malas de  $l$ ,  $\bar{v}$  y  $c_{el}$**

**Se cancelan errores !!!**

**Gas cuántico**  $\implies L = 2.45 \times 10^{-8} \text{ V}^2 \text{ K}^{-2}$

$$\sigma = \frac{n_e e^2 \tau}{m_e}$$

**Table 16.2.** Resistivity at 77 K and 273 K, and the relaxation (collision) time calculated from it for some metallic elements ( $10^{-15}$  s = 1 fs)

Element	$\rho(77\text{ K})$ (n $\Omega$ m)	$\rho(273\text{ K})$	$\tau(77\text{ K})$ ( $10^{-15}$ s)	$\tau(273\text{ K})$
Ag	2.8	14.7	200	40
Al	2.3	25.0	65	8.0
Au	4.7	20.5	120	30
Ba	67	500	17	3.8
Bi	350	1068	0.72	0.23
Cu	2.0	16.8	210	27
Fe	6.4	89	32	2.4
Ga	27.5	136	8.8	1.7
Na	8	42	170	32
Pb	47	192	5.7	1.4
Sb	80	370	2.7	0.55
Zn	10.4	54.3	24	4.9



$T_{\text{amb}} \longrightarrow \tau$  is typically  $10^{-14}$  to  $10^{-15}$  sec.

mean free path,  $\ell = v_0 \tau$ .

**En la época de Drude:**

$$\frac{1}{2} m v_0^2 = \frac{3}{2} k_B T.$$

**Los e<sup>-</sup> colisionan con los átomos de la red cristalina**

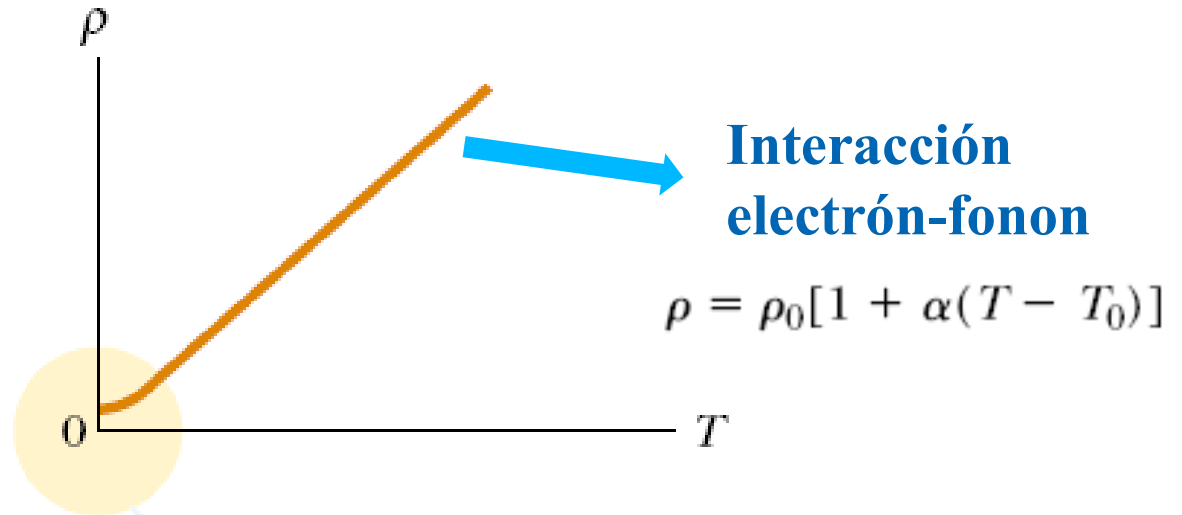
$v_0$  of order  $10^7$  cm/sec  $\longrightarrow$  mean free path of 1 to 10 Å

**Modelo cuántico:  $V_F > 10^8$  cm/sec**

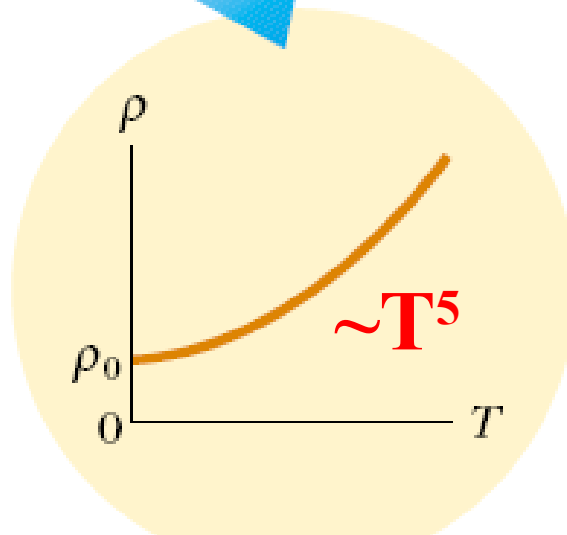
the low-temperature mean free path to  $10^3$  or more angstroms, about a thousand times the spacing between ions. Today, by working at sufficiently low temperatures with carefully prepared samples, mean free paths of the order of centimeters (i.e.,  $10^8$  interatomic spacings) can be achieved. This is strong evidence that the electrons do not simply bump off the ions, as Drude supposed.

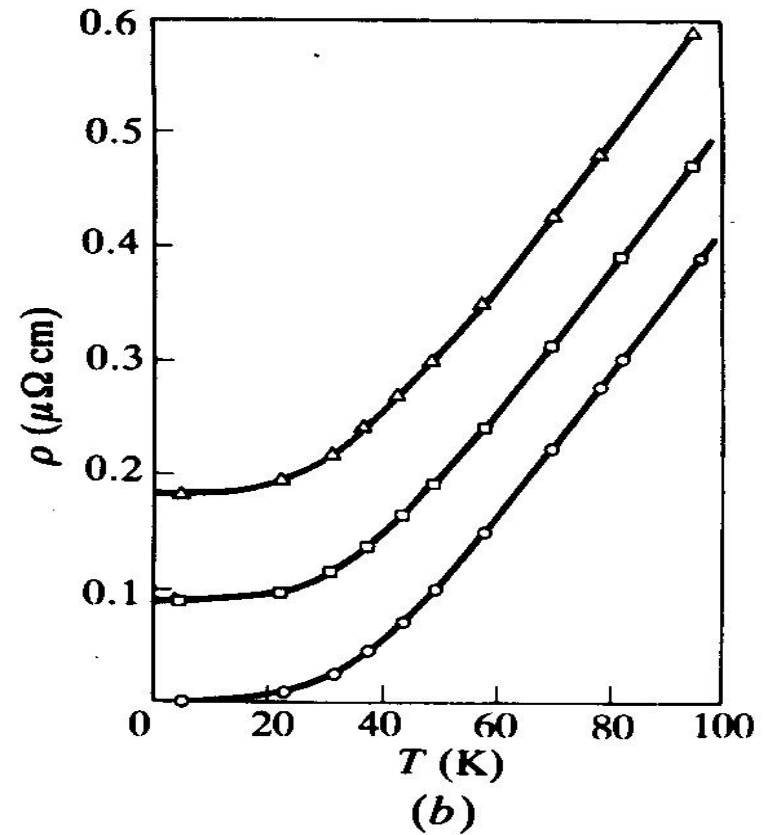
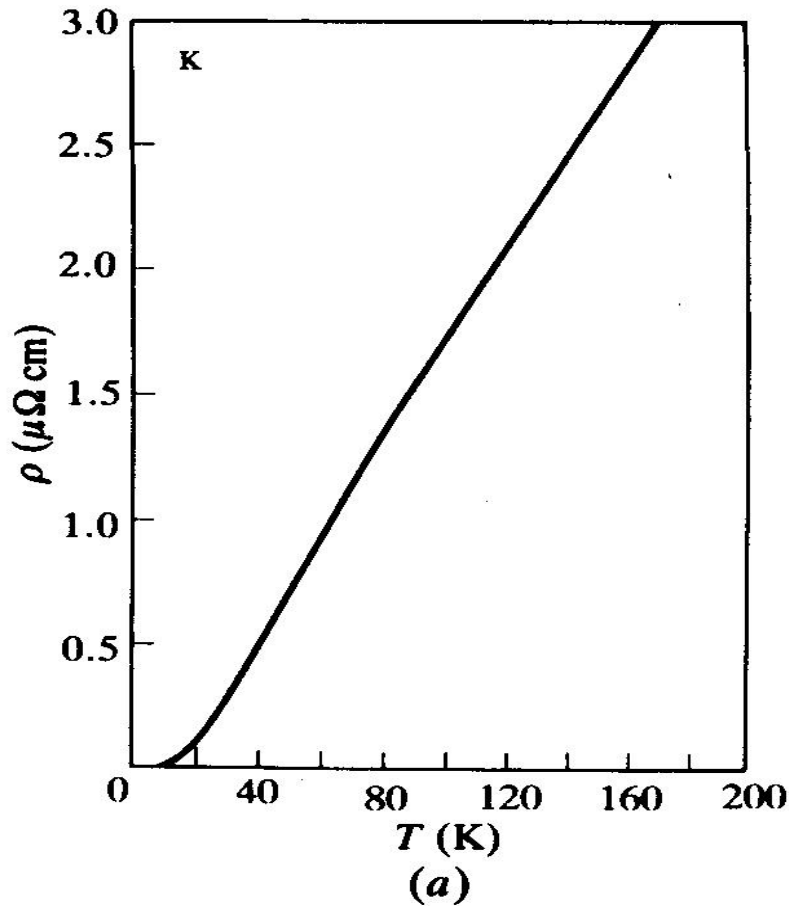
En un metal el comportamiento de la conductividad con T es gobernado por  $\tau$  (T)

$$\sigma = \frac{n_e e^2 \tau}{m_e}$$



Impurezas





**Fig. 9.24** (a) The variation of the electrical resistance of pure potassium as a function of temperature. The behaviour is almost linear over a wide range of temperature, but below about 20 K the resistance becomes constant. At high temperatures, deviations from linearity may arise, particularly for the transition metals. (b) The effect of small amounts of an alloying element (impurity) on the residual resistance of Ag:  $\circ$ , 'pure Ag';  $\square$ , Ag + 0.02 at.% Sn;  $\triangle$ , Ag + 0.5 at.% Au. (After Dugdale (1977).)

# Conductividad en corriente alterna

La ecuación de movimiento en presencia de un campo eléctrico dependiente del tiempo:

$$\frac{d\mathbf{p}}{dt} = -\frac{\mathbf{p}}{\tau} - e\mathbf{E}.$$

Si excitamos con un campo alterno:

$$\mathbf{E}(t) = \text{Re} (\mathbf{E}(\omega)e^{-i\omega t}).$$

Tendremos una solución de la forma

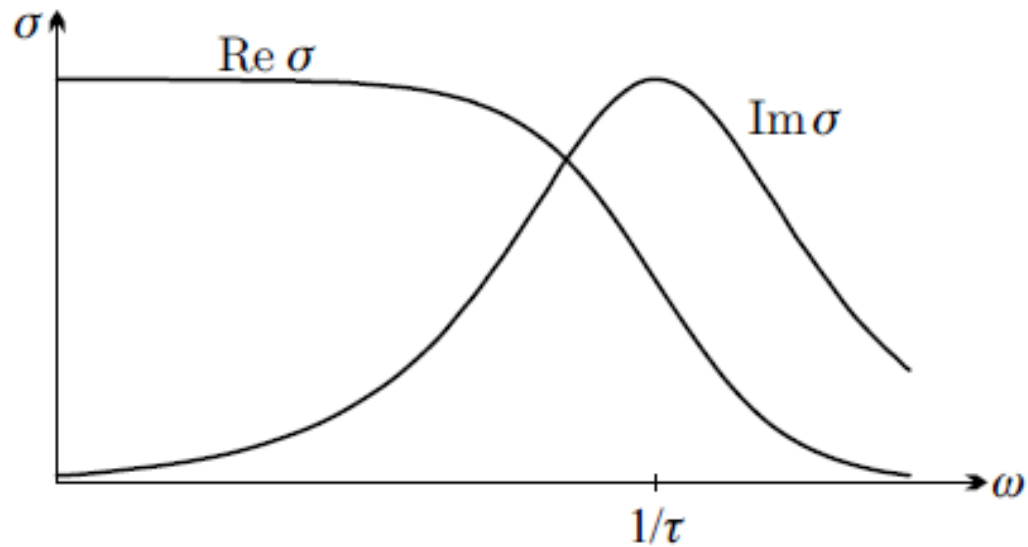
$$\mathbf{p}(t) = \text{Re} (\mathbf{p}(\omega)e^{-i\omega t}).$$

Si sustituimos las formas complejas en la ecuación de movimiento obtenemos la conductividad compleja  $\sigma(\omega)$

$$\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega), \quad (\text{recordemos que } \mathbf{j} = n e \mathbf{v} = n e \mathbf{p}/m)$$

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

$$\text{Re } \sigma(\omega) = \frac{\sigma_0}{1 + (\omega\tau)^2}, \quad \text{Im } \sigma(\omega) = \frac{\sigma_0\omega\tau}{1 + (\omega\tau)^2}$$



**Fig. 16.2.** Semi-logarithmic plot of the frequency dependence of the real and imaginary parts of the conductivity in the Drude model

**La parte real esta asociada a la resistividad (absorción de energía que da lugar a calentamiento Joule).**

**La parte imaginaria es de carácter inductivo (desfasaje) y tiene su máximo en  $\omega\tau = 1$ .**

Utilizando la teoría electromagnética, se encuentra la siguiente relación entre la conductividad y la constante dieléctrica:

$$\epsilon_r(\omega) = 1 + \frac{i\sigma}{\epsilon_0\omega}$$

$$\begin{aligned}\epsilon_r(\omega) &= 1 + \frac{i\sigma_0}{\epsilon_0\omega(1 - i\omega\tau)} = 1 + \frac{in_e e^2 \tau}{\epsilon_0 m_e \omega (1 - i\omega\tau)} \\ &= 1 - \frac{n_e e^2}{\epsilon_0 m_e \omega (\omega + i/\tau)}\end{aligned}$$

**Definimos :**  $\omega_p^2 = \frac{\sigma_0}{\epsilon_0\tau} = \frac{n_e e^2}{\epsilon_0 m_e} = \frac{4\pi n_e \tilde{e}^2}{m_e}$  **Frecuencia de plasma**

donde:  $\tilde{e}^2 = e^2/4\pi\epsilon_0$

$$\epsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i/\tau)}$$

A altas frecuencias ( $\omega\tau \gg 1$ )

$$\epsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$

-  $\omega < \omega_p$     $\epsilon_r(\omega) < 0$     $\longrightarrow$    no se propaga la radiación

-  $\omega > \omega_p$     $\epsilon_r(\omega) > 0$     $\longrightarrow$    la radiación se propaga  
el metal se vuelve transparente



## Recordar: propagación de una onda EM en un medio material

$$\mathbf{E} = \mathbf{E}_0 \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t), \quad \mathbf{B} = \mathbf{B}_0 \exp(i\mathbf{q} \cdot \mathbf{r} - i\omega t),$$

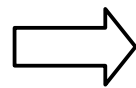
$$\nabla^2 \mathbf{E}(\mathbf{q}, \omega) = \frac{\epsilon_r^{\text{tot}}(\mathbf{q}, \omega) \mu_r^{\text{tot}}(\mathbf{q}, \omega)}{c^2} \frac{\partial^2 \mathbf{E}(\mathbf{q}, \omega)}{\partial t^2}$$

$$q^2 = \frac{\omega^2}{c^2} N^2 \quad \text{donde} \quad N = \sqrt{\epsilon_r^{\text{tot}} \mu_r^{\text{tot}}} \quad \xrightarrow{\text{no magnético}} \quad N \approx \sqrt{\epsilon_r^{\text{tot}}}$$

$$N = n + i\kappa$$

$n$  Índice refracción

$\kappa$  Coef. de extinción



$$\mathbf{E} = \mathbf{E}_0 \exp\left(-\frac{\omega\kappa}{c} \hat{\mathbf{q}} \cdot \mathbf{r}\right) \exp\left(i\frac{\omega n}{c} \hat{\mathbf{q}} \cdot \mathbf{r} - i\omega t\right)$$

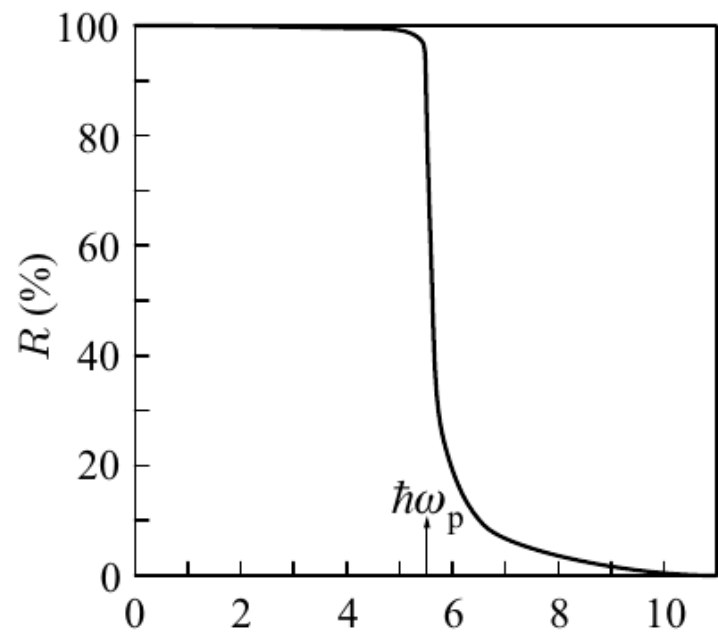
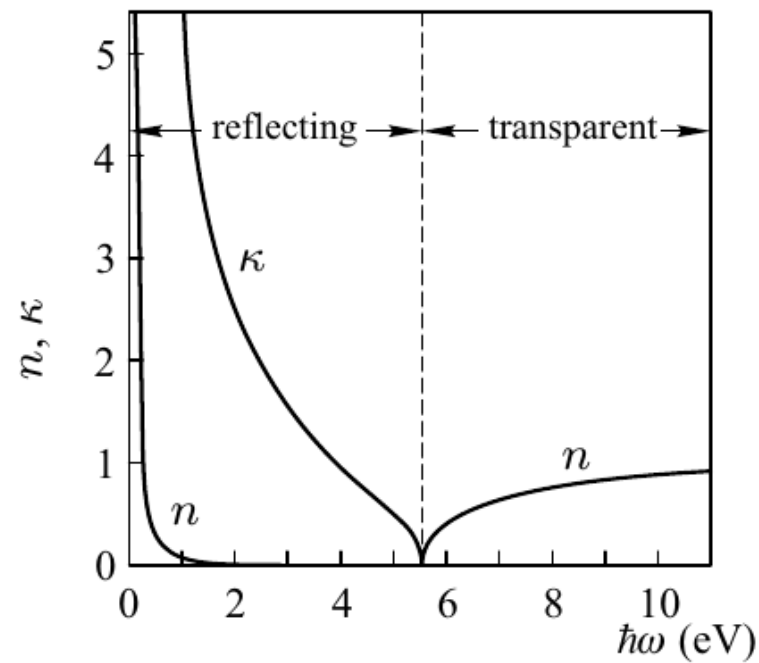
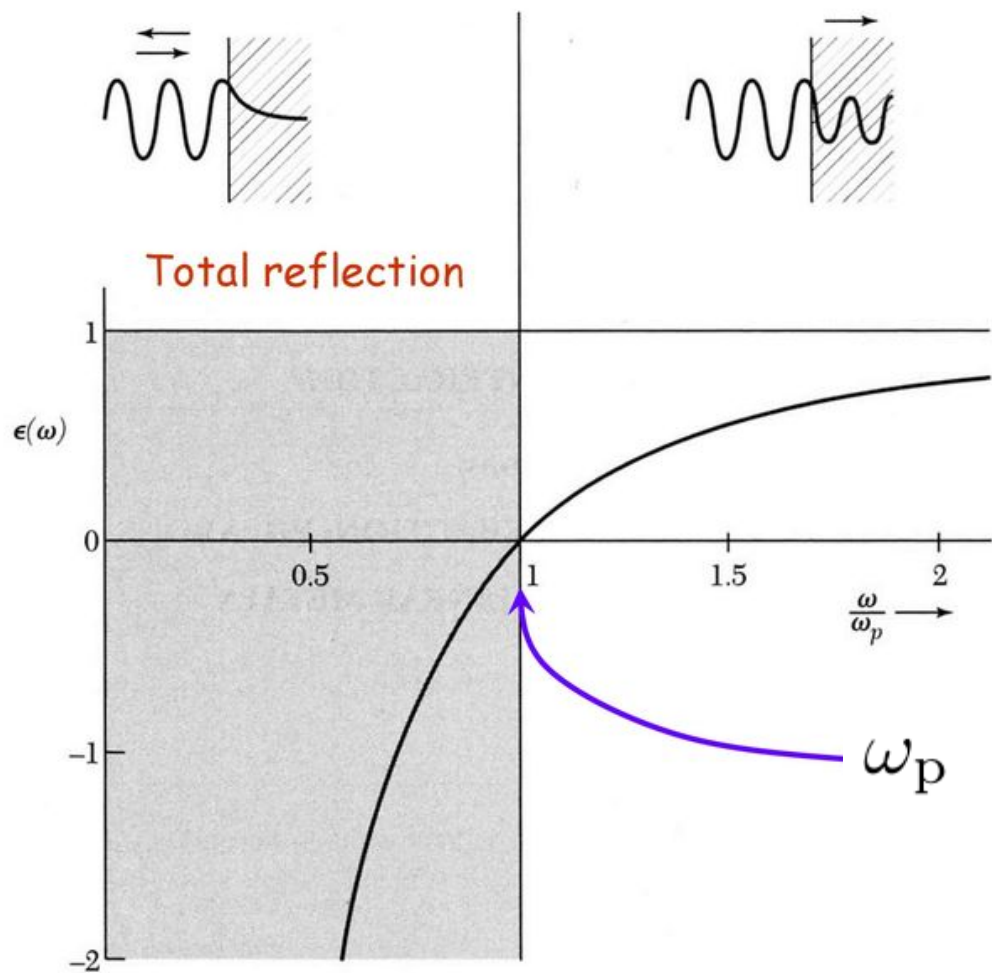
$$\mathbf{B} = \mathbf{B}_0 \exp\left(-\frac{\omega\kappa}{c} \hat{\mathbf{q}} \cdot \mathbf{r}\right) \exp\left(i\frac{\omega n}{c} \hat{\mathbf{q}} \cdot \mathbf{r} - i\omega t\right)$$

**Coeficiente de absorción:**

$$\alpha = -\frac{1}{I} \frac{dI}{dr} \cdot \quad \alpha = \frac{2\kappa\omega}{c} = \frac{4\pi\kappa}{\lambda}.$$

**Reflectancia o Reflectividad:**

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



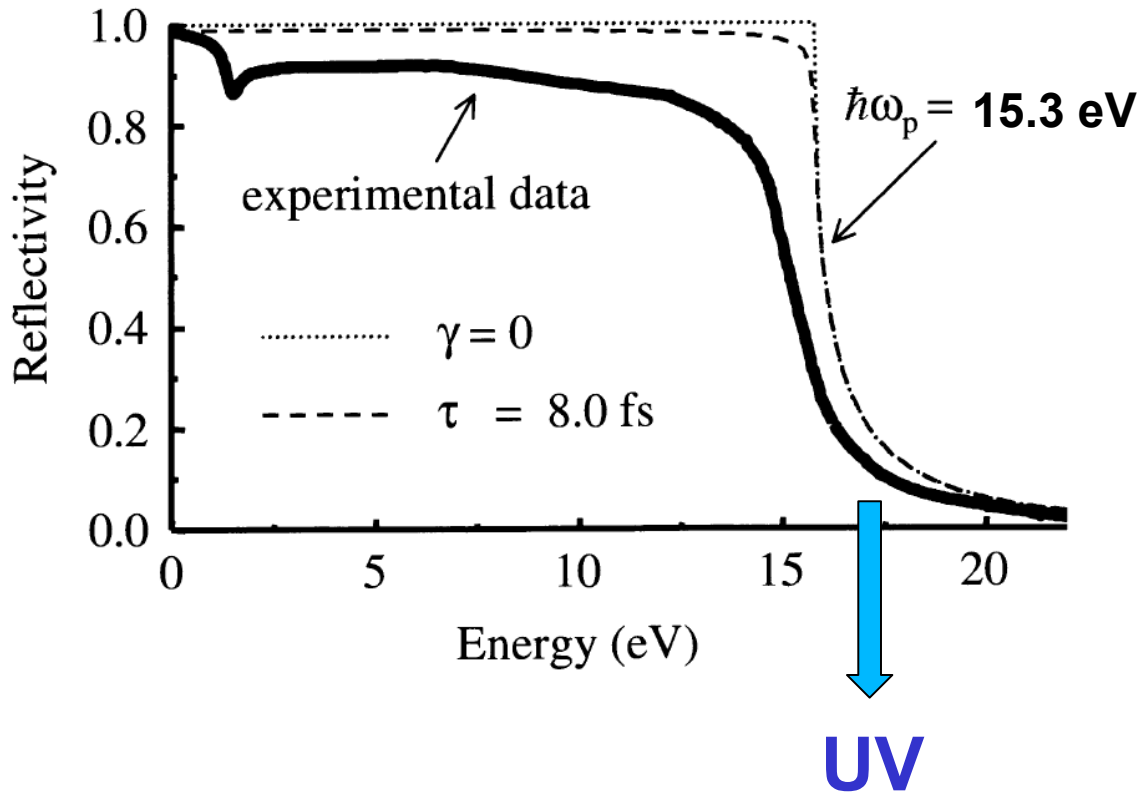
**Por ejemplo, los metales alcalinos se vuelven transparentes en el UV**

$$\nu_p = \frac{\omega_p}{2\pi} = 11.4 \times \left(\frac{r_s}{a_0}\right)^{-3/2} \times 10^{15} \text{ Hz}$$

$$\lambda_p = \frac{c}{\nu_p} = 0.26 \left(\frac{r_s}{a_0}\right)^{3/2} \times 10^3 \text{ \AA.}$$

**OBSERVED AND THEORETICAL WAVELENGTHS BELOW WHICH THE ALKALI METALS BECOME TRANSPARENT**

ELEMENT	THEORETICAL <sup>a</sup> $\lambda$ ( $10^3 \text{ \AA}$ )	OBSERVED $\lambda$ ( $10^3 \text{ \AA}$ )
Li	1.5	2.0
Na	2.0	2.1
K	2.8	3.1
Rb	3.1	3.6
Cs	3.5	4.4



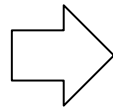
**Fig. 7.2** Experimental reflectivity of aluminium as a function of photon energy. The experimental data is compared to predictions of the free electron model with  $\hbar\omega_p = 15.8 \text{ eV}$ . The dotted curve is calculated with no damping. The dashed line is calculated with  $\tau = 8.0 \times 10^{-15} \text{ s}$ , which is the value deduced from DC conductivity. The experimental data is taken from reference [3], copyright 1963 American Institute of Physics, reprinted with permission.

**Los metales reflejan en el visible y son transparentes en el ultravioleta**

# Ondas de densidad de carga: Plasmones

En lo anterior supusimos  $\rho=0$ . Si  $\rho(x,t)\neq 0$  es posible que se propague una onda de densidad de carga. Veamos que esto sólo ocurre a  $\omega=\omega_p$ .

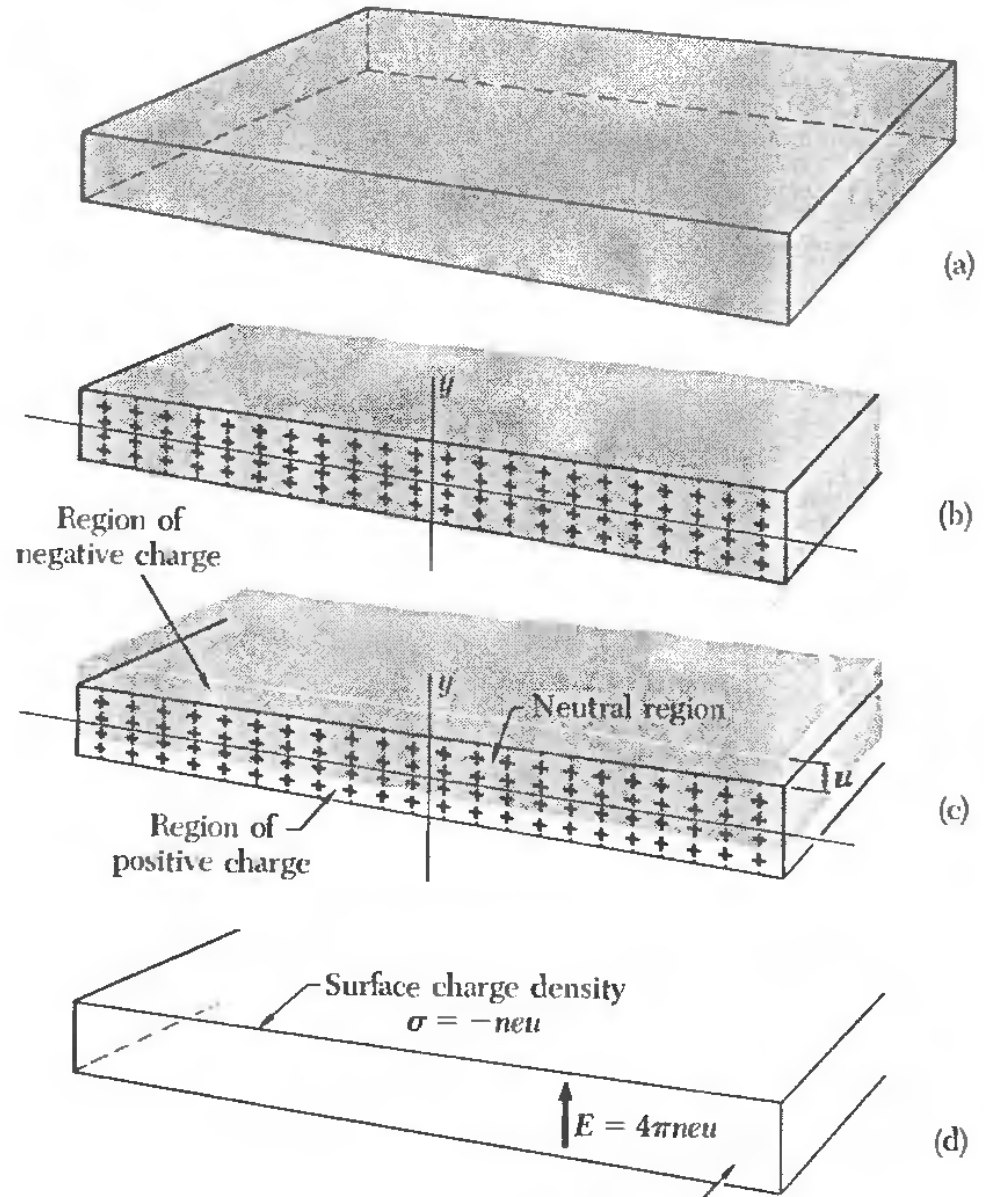
Experimento imaginario



$$Q = neu \cdot A$$

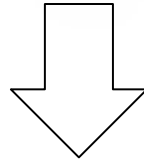
$$\sigma = neu$$

$$E = neu/\epsilon_0$$



La ecuación de movimiento para la unidad de volumen de electrones del gas es:

$$nm \frac{d^2 u}{dt^2} = -neE = -4\pi n^2 e^2 u ,$$

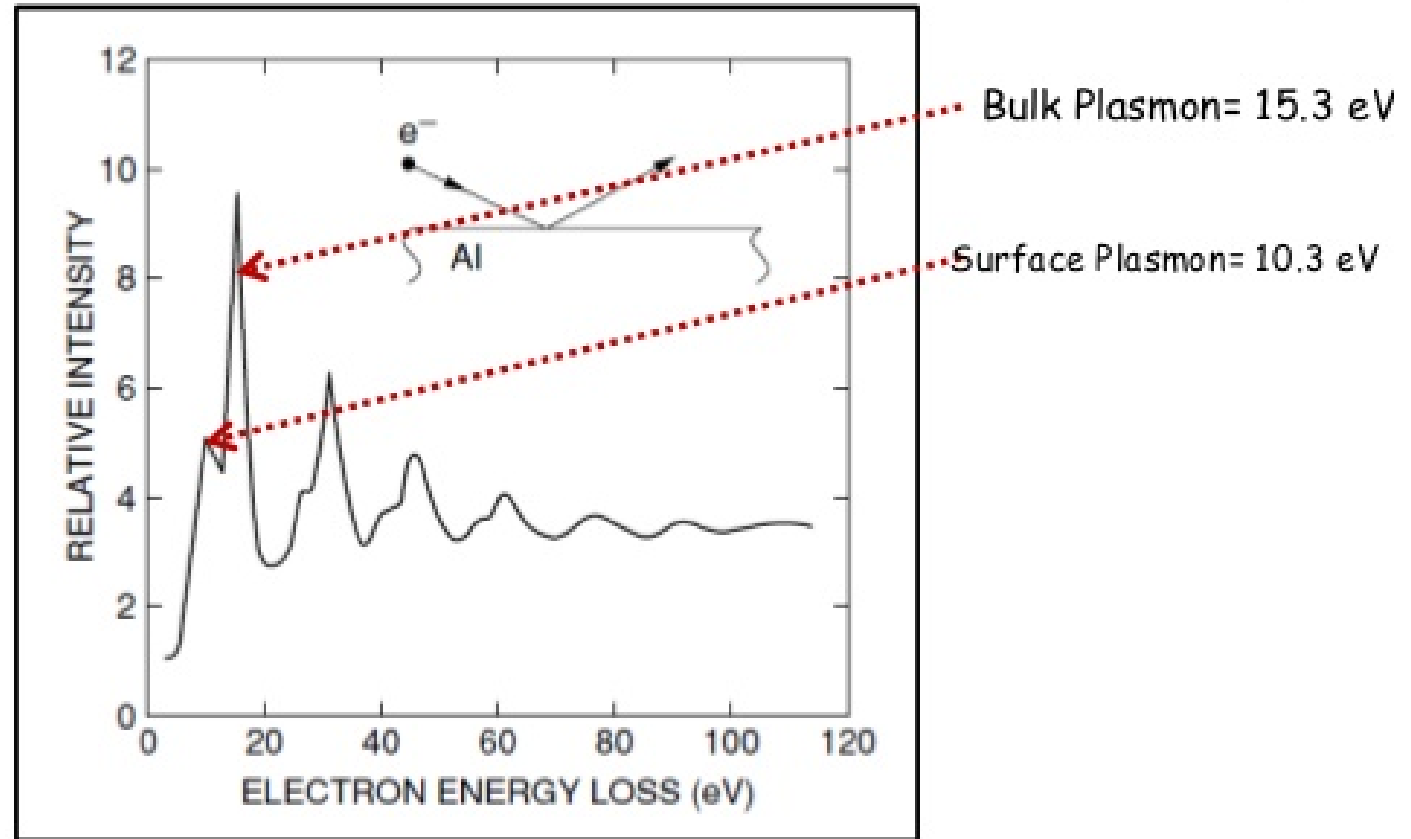


$$\frac{d^2 u}{dt^2} + \omega_p^2 u = 0 ; \quad \omega_p = \left( \frac{4\pi n e^2}{m} \right)^{1/2} .$$

Oscilador armónico de frecuencia  $\omega_p$

Es una onda de densidad de carga o **plasmón**

# Electron energy loss spectra of Al



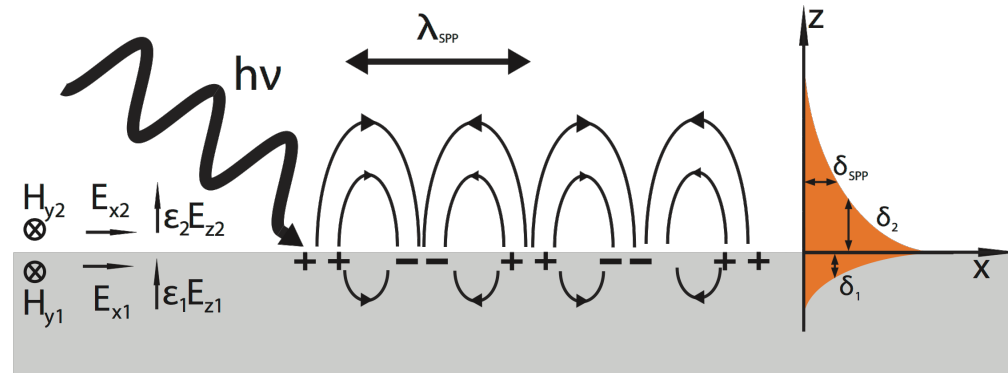
Energy loss spectrum for electrons reflected from Al for incident primary electron energy of 2 keV. The loss peaks are made up of a combination of surface and bulk plasmon

# Bulk

Table 2 Volume plasmon energies, in eV

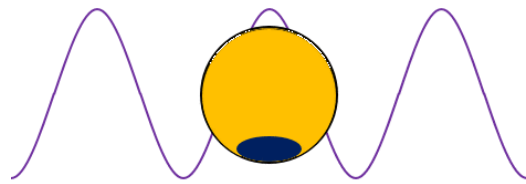
Material	Observed	Calculated	
		$\hbar\omega_p$	$\hbar\tilde{\omega}_p$
<i>Metals</i>			
Li	7.12	8.02	7.96
Na	5.71	5.95	5.58
K	3.72	4.29	3.86
Mg	10.6	10.9	
Al	15.3	15.8	

# Superficie



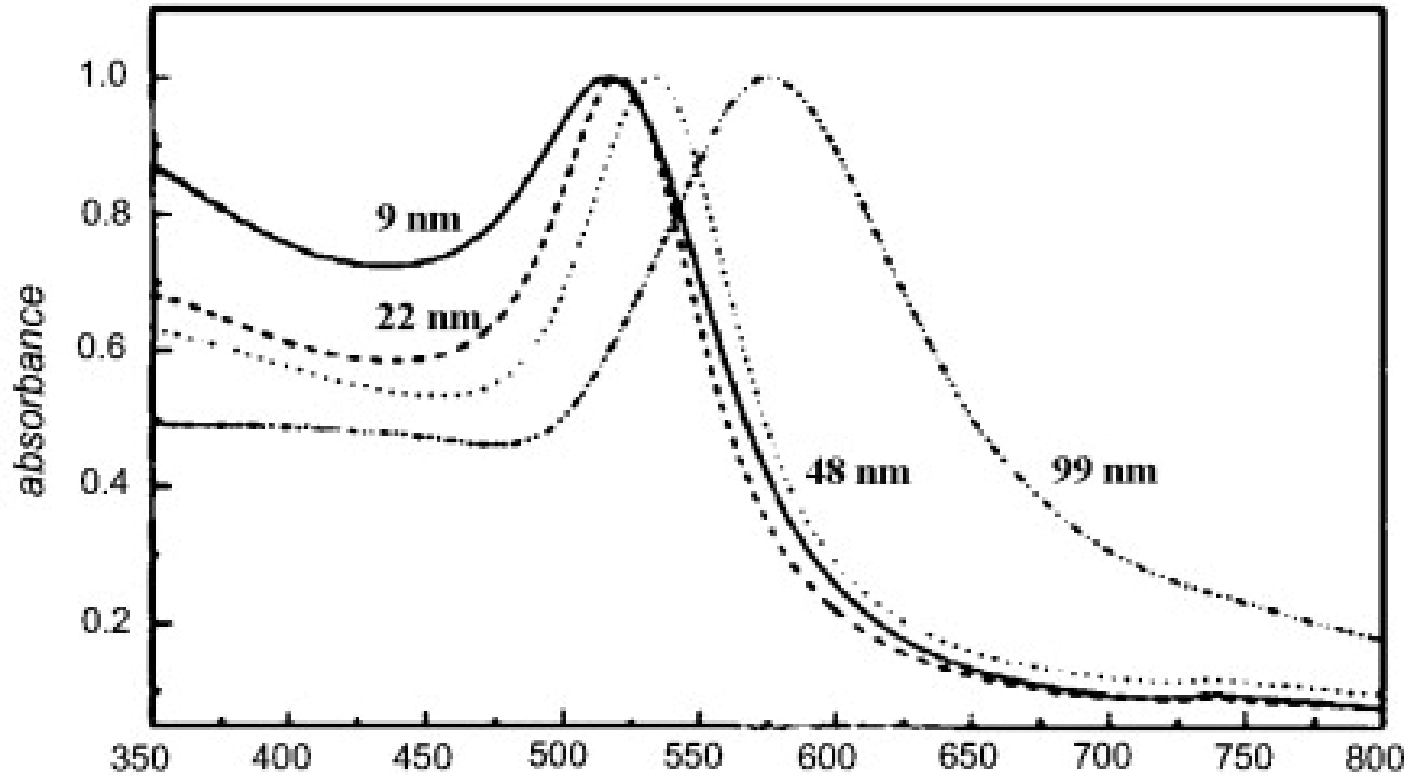
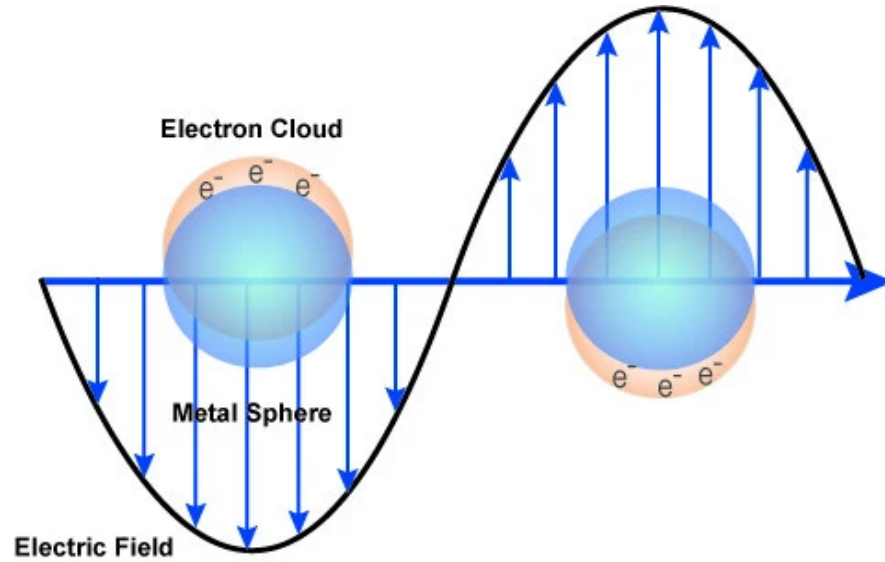


# Nanopartículas



Electric Field (E):  
(experienced by particle)

Electrons: ●



# **Modelo semiclásico para la dinámica de electrones en bandas**

Que ocurre con los electrones en los sólidos cuando aplicamos campos EM ?

~~$$\mathcal{H} = \frac{1}{2m_e} \left[ \frac{\hbar}{i} \nabla + e\mathbf{A}(\mathbf{r}) \right]^2 + U(\mathbf{r}) - e\varphi(\mathbf{r})$$~~

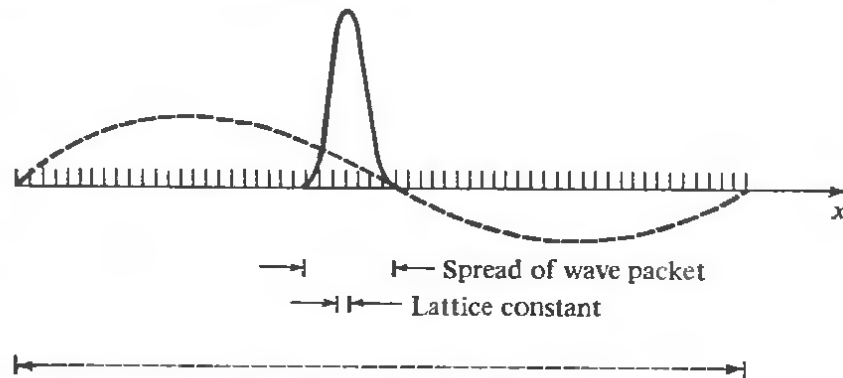
**Modelo semiclásico:** movimiento de un paquete de onda

$$\phi_{n\mathbf{k}}(\mathbf{r}, t) = \sum_{\mathbf{k}'} g(\mathbf{k}') \psi_{n\mathbf{k}'}(\mathbf{r}) e^{-i\varepsilon_{n\mathbf{k}'} t / \hbar}$$

$$g(\mathbf{k}') \approx 0, \quad |\mathbf{k}' - \mathbf{k}| > \Delta k \quad |\Delta k| \cdot |\Delta r| \sim 1$$

Figure 12.1

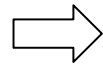
Schematic view of the situation described by the semiclassical model. The length over which the applied field (dashed line) varies is much greater than the spread in the wave packet of the electron (solid line), which in turn is much larger than the lattice constant.



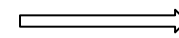
Velocidad ?  $\Longrightarrow$  Velocidad de grupo del paquete

$$v(k) = \frac{\partial \omega(k)}{\partial k}$$

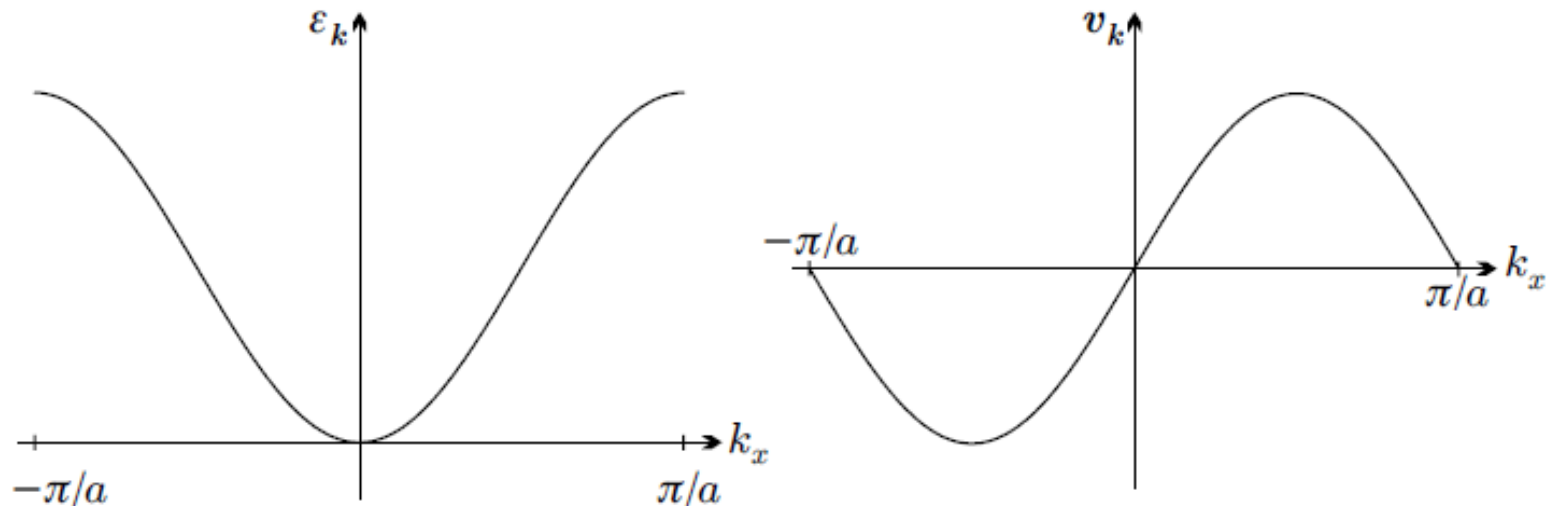
$$\epsilon = \hbar \omega$$



$$v_{nk} = \frac{1}{\hbar} \frac{\partial \epsilon_{nk}}{\partial k}$$



Gradiente



**Fig. 21.1.** Dispersion curve for electrons in the tight-binding approximation and their velocity in a cubic crystal along a high-symmetry direction of the Brillouin

# Ecuación de movimiento

El trabajo hecho en un tiempo  $dt$  sobre un electrón en el estado  $n\mathbf{k}$  debido a una campo eléctrico es

$$dW = -e\mathbf{E} \cdot \mathbf{v}_{n\mathbf{k}} dt \quad (1)$$

Al diferencial de energía lo puedo escribir como  $\frac{d\varepsilon_{n\mathbf{k}}}{dt} dt$

$$dW = \frac{d\varepsilon_{n\mathbf{k}}}{dt} dt = \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial \mathbf{k}} \frac{d\mathbf{k}}{dt} dt = \hbar \mathbf{v}_{n\mathbf{k}} \frac{d\mathbf{k}}{dt} dt \quad (2)$$

Comparando (1) con (2)  $\implies \hbar \dot{\mathbf{k}} = -e\mathbf{E}$

$$\hbar \dot{\mathbf{k}} = -e \left[ \mathbf{E}(\mathbf{r}, t) + \mathbf{v}_{n\mathbf{k}} \times \mathbf{B}(\mathbf{r}, t) \right]$$

# Postulados del modelo semiclásico

$\varepsilon_n(\mathbf{k})$   $\longrightarrow$  posición  $\mathbf{r}$   
vector de onda  $\mathbf{k}$   
índice de banda  $n$

- 1- El índice de banda  $n$  es una constante de movimiento
- 2- La evolución temporal para  $\mathbf{r}$  y  $\mathbf{k}$  de un electrón perteneciente a la banda  $n$  esta dada por

$$\dot{\mathbf{r}} = \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}},$$
$$\hbar \dot{\mathbf{k}} = -e \left[ \mathbf{E}(\mathbf{r}, t) + \frac{1}{c} \mathbf{v}_n(\mathbf{k}) \times \mathbf{H}(\mathbf{r}, t) \right].$$

- 3-  $(n, \mathbf{r}, \mathbf{k})$  y  $(n, \mathbf{r}, \mathbf{k} + \mathbf{G})$  describen el mismo electrón

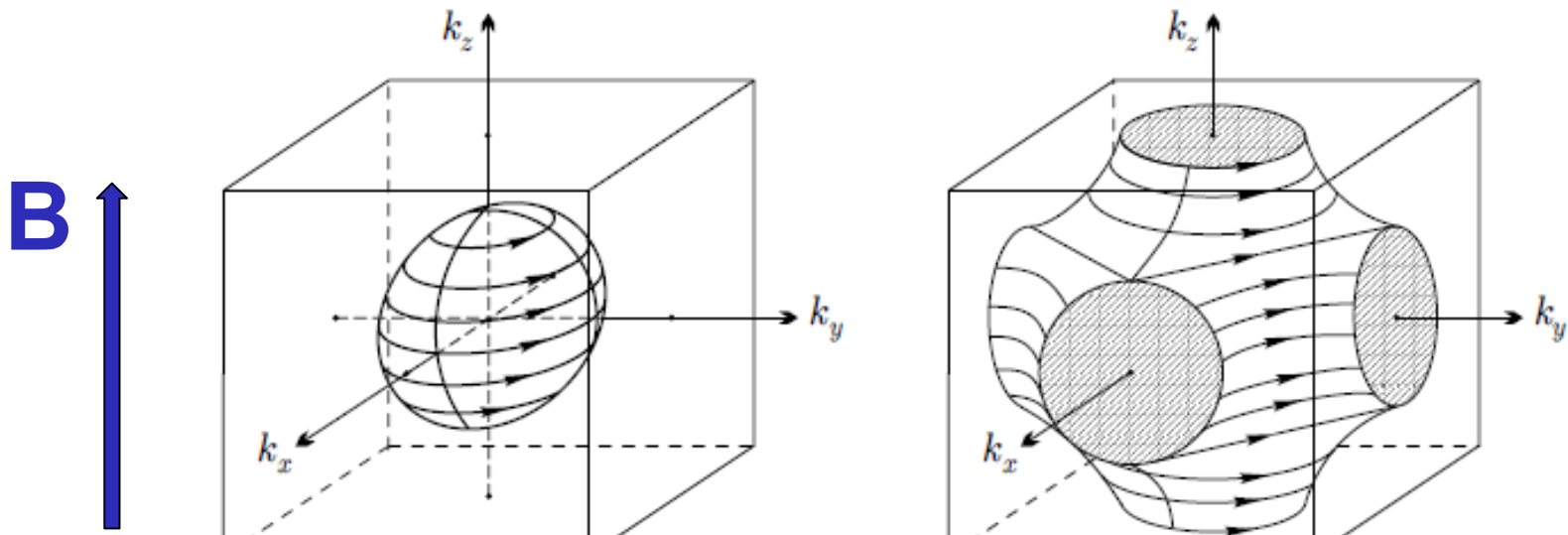
# Consecuencias del modelo semiclásico

## 1- Electrones de Bloch en un campo magnético uniforme

$$\frac{dk}{dt} = -\frac{e}{\hbar} \mathbf{v}_{\mathbf{k}} \times \mathbf{B} \quad \mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}$$

$$\frac{d\varepsilon_{\mathbf{k}}}{dt} = \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt} = -e \mathbf{v}_{\mathbf{k}} \cdot (\mathbf{v}_{\mathbf{k}} \times \mathbf{B}) = 0$$

Los electrones de Bloch no absorben energía del campo



**Las órbitas en el espacio  $k$  están sobre planos perpendiculares a  $B$  y en superficies de  $E$  constante.**

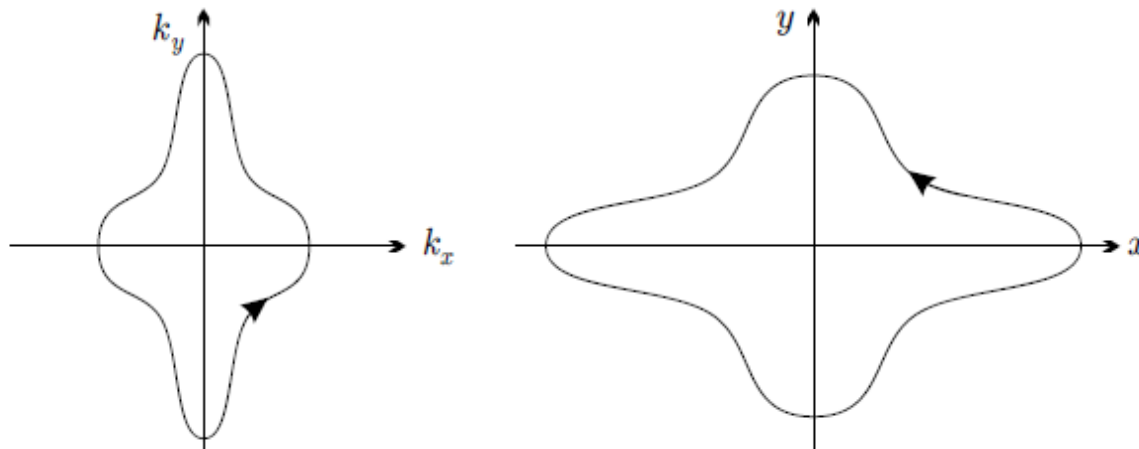
$$\frac{dk}{dt} = -\frac{e}{\hbar} \left( \frac{dr}{dt} \times B \right) \implies k(t) - k(0) = -\frac{e}{\hbar} [r(t) - r(0)] \times B$$

$$[r(t) - r(0)]_{\perp} \times \hat{z} = -\frac{\hbar}{eB} [k(t) - k(0)]$$

$$x(t) - x(0) = \frac{\hbar}{eB} [k_y(t) - k_y(0)],$$

$$y(t) - y(0) = -\frac{\hbar}{eB} [k_x(t) - k_x(0)].$$

**La proyección en el espacio real perpendicular a  $B$  es la órbita del espacio  $k$  rotada  $90^\circ$  y multiplicada por el factor  $\hbar/eB$**





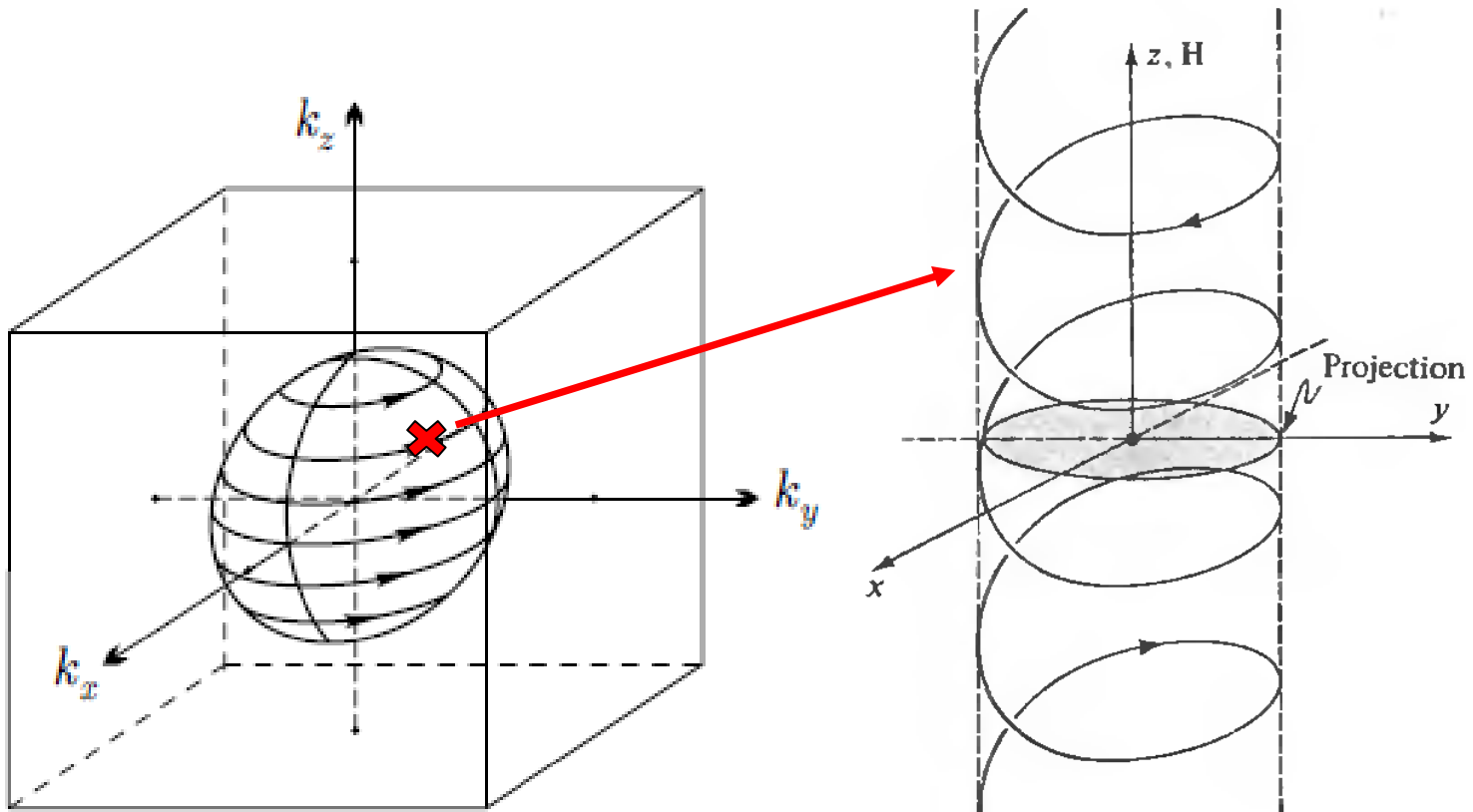
Para la componente paralela al campo B

$$dk_z/dt = 0$$

$$k_z = \text{cte}$$

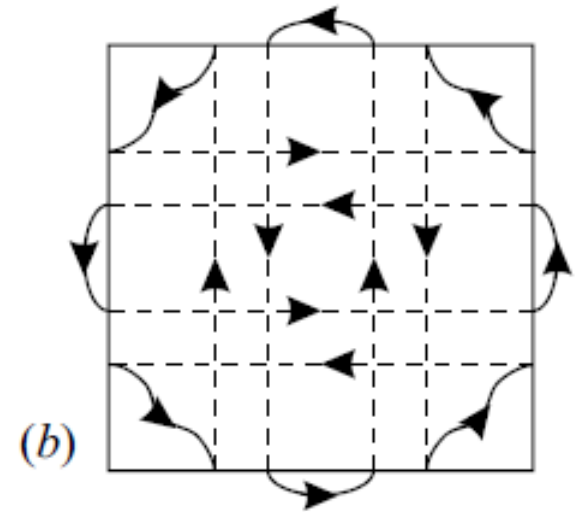
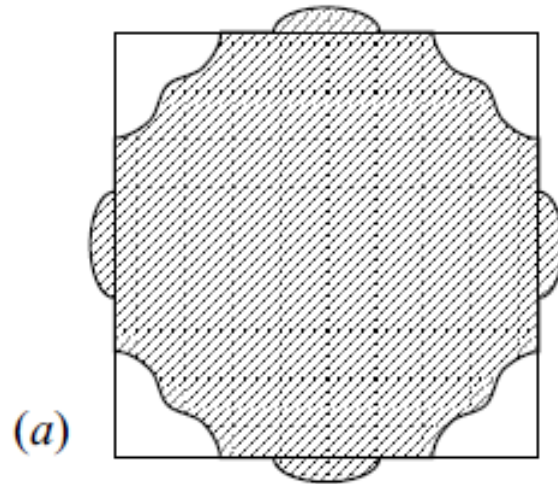
$$z(t) = z(0) + \int_0^t v_z(t) dt; \quad v_z = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial k_z}$$

Al contrario de lo que ocurre con electrones libres, puede ser que  $v_z$  no sea constante

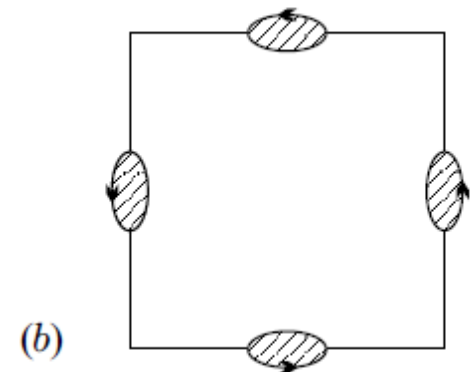
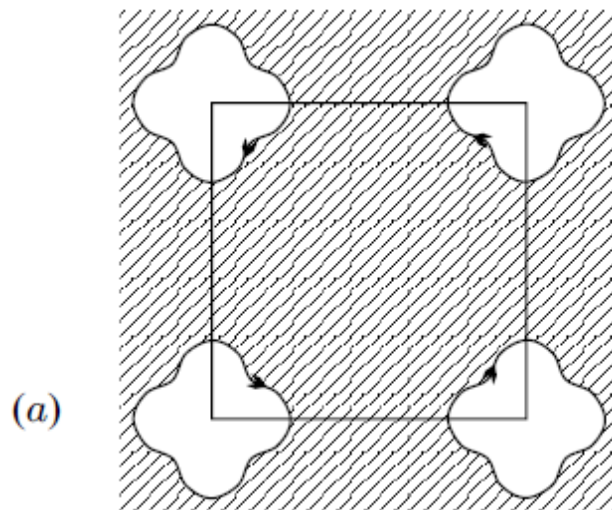


Las trayectorias en el espacio  $k$  pueden ser cerradas o abiertas, dependiendo de la forma que tenga la superficie de energía constante.

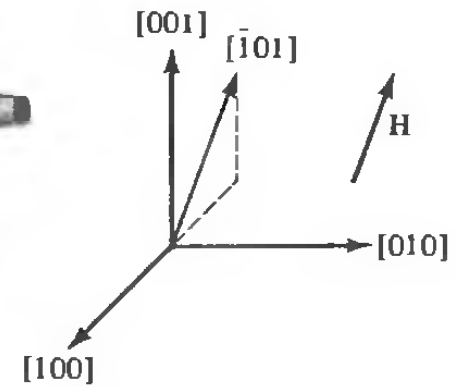
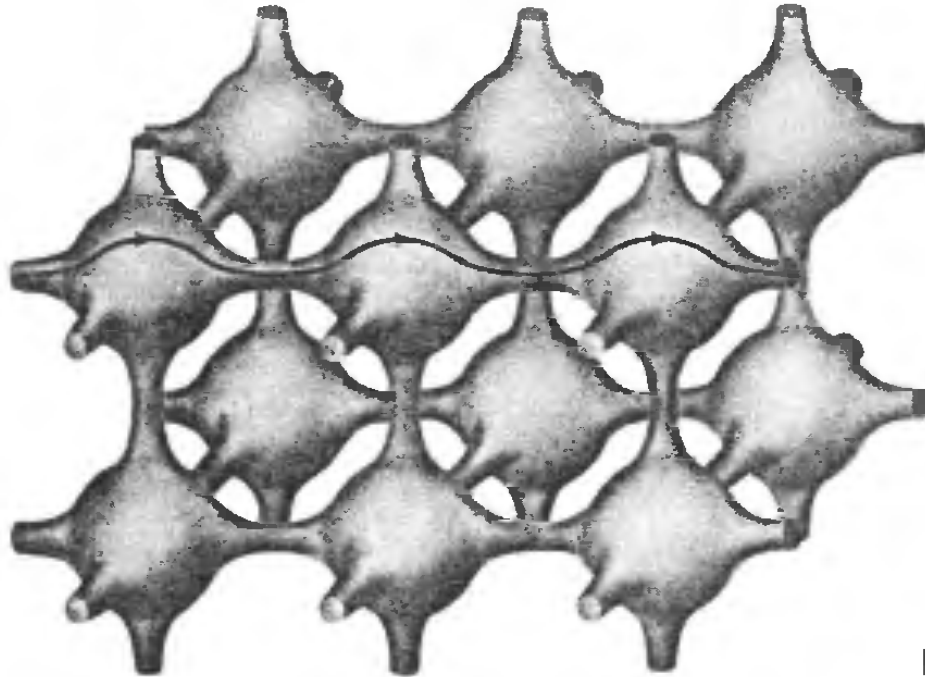
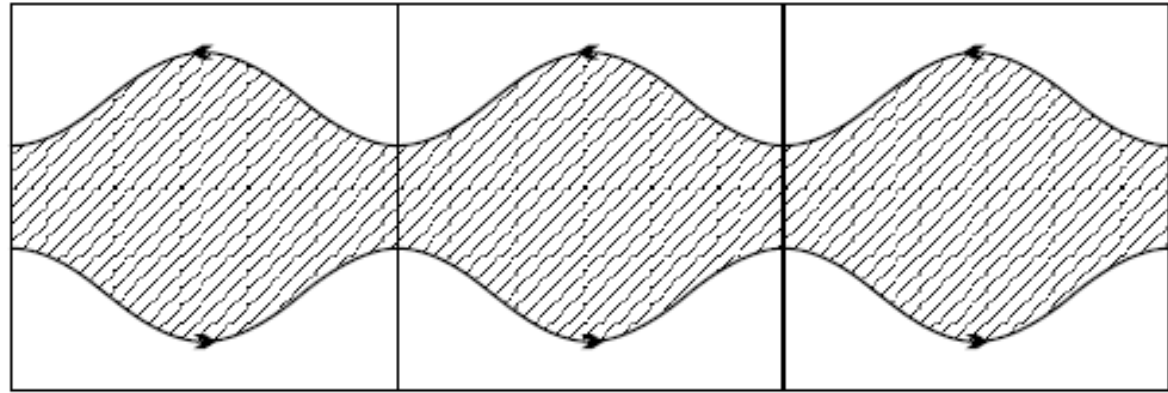
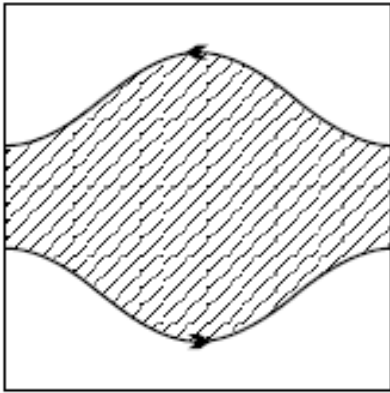
## Cerradas



Comparar el sentido de giro !!!



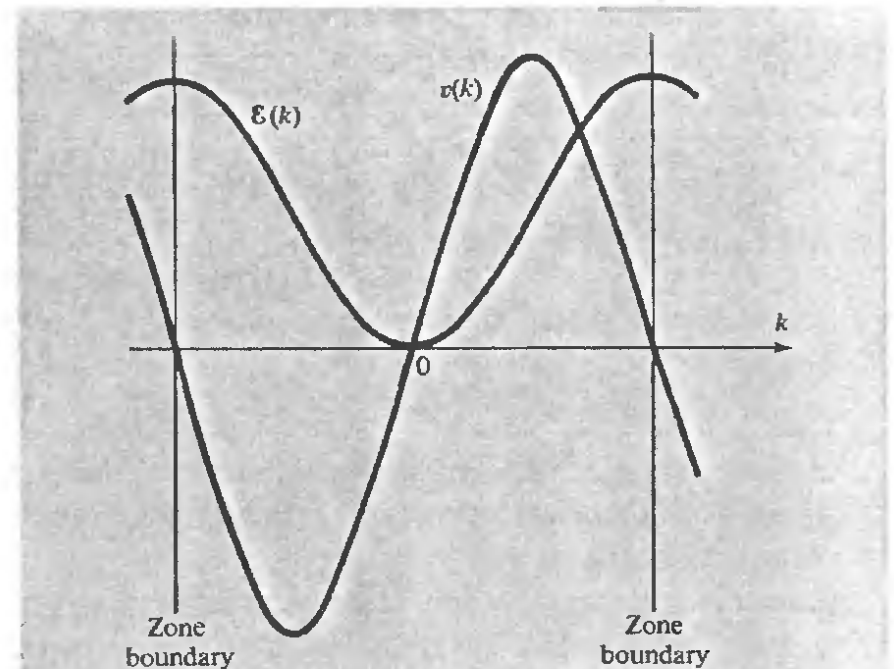
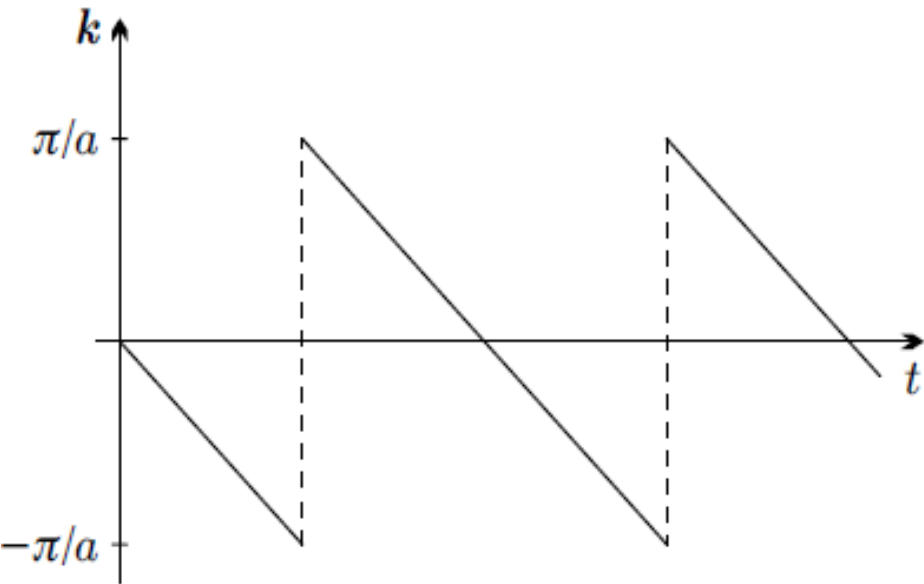
# Abiertas

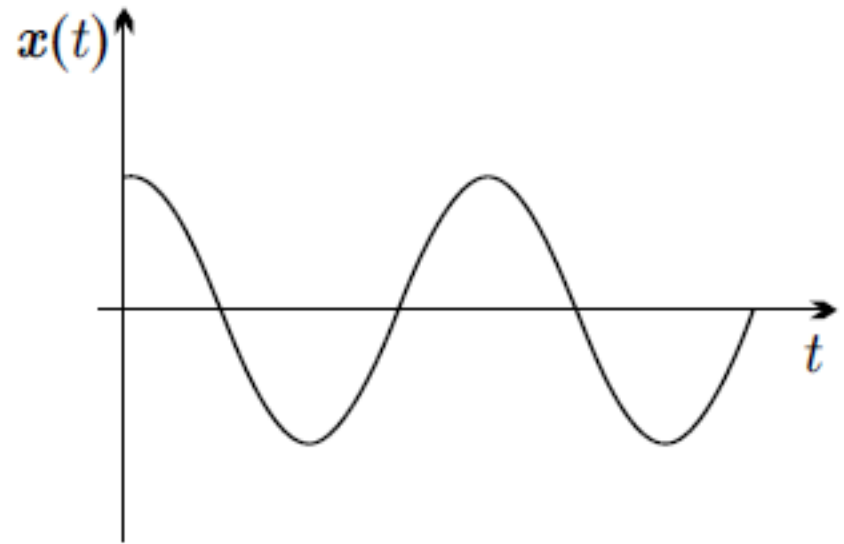
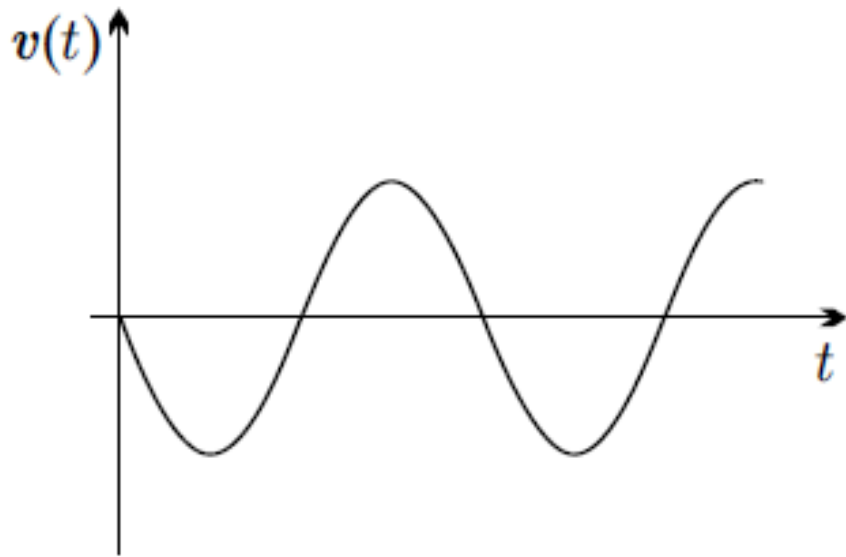


## 2- Oscilaciones en un campo eléctrico DC

$$\hbar \dot{k} = -eE \quad \Longrightarrow \quad \hbar k(t) = \hbar k(0) - eEt$$

$$\dot{r}(t) = v_n[k(t)]$$





Para un campo  $E \sim 10^{-2} \text{ V/cm}$ , el cambio del vector  $k$  entre colisiones ( $\tau \sim 10^{-14} \text{ s}$  a  $T_{\text{amb}}$ ) es del orden de  $10^{-1} \text{ cm}^{-1}$

Este valor es muy pequeño respecto a las dimensiones de la 1ZB ( $1/a \sim 10^8 \text{ cm}^{-1}$ )

Si bien esta oscilación no se detecta experimentalmente hay evidencia de que los electrones en el tope de una banda se desaceleran con el campo.

### 3- Las bandas llenas no conducen

La densidad de corriente y de energía transportadas por los electrones que ocupan la banda  $n$  se calcula:

$$j = -e \frac{1}{V} \sum_{k,\sigma} v_{nk} = -e \int \frac{dk}{4\pi^3} \frac{1}{\hbar} \frac{\partial \varepsilon_{nk}}{\partial k}$$

$$j_\varepsilon = \frac{1}{V} \sum_{k,\sigma} \varepsilon_{nk} v_{nk} = \int \frac{dk}{4\pi^3} \varepsilon_{nk} \frac{1}{\hbar} \frac{\partial \varepsilon_{nk}}{\partial k} = \frac{1}{2} \int \frac{dk}{4\pi^3} \frac{1}{\hbar} \frac{\partial \varepsilon_{nk}^2}{\partial k}$$

$$\varepsilon_{nk} \quad \varepsilon_{nk}^2 \implies \text{periódicas en el espacio } k$$

La integral en la 1ZB de la derivada de una función periódica se anula.

**Un sólido en el cual sus bandas están completamente llenas es un aislante eléctrico y térmico (respecto a los  $e^-$ )**

**Si la banda esta  
parcialmente llena**

$$j = -e \int_{\text{filled}} \frac{dk}{4\pi^3} v_{nk}$$

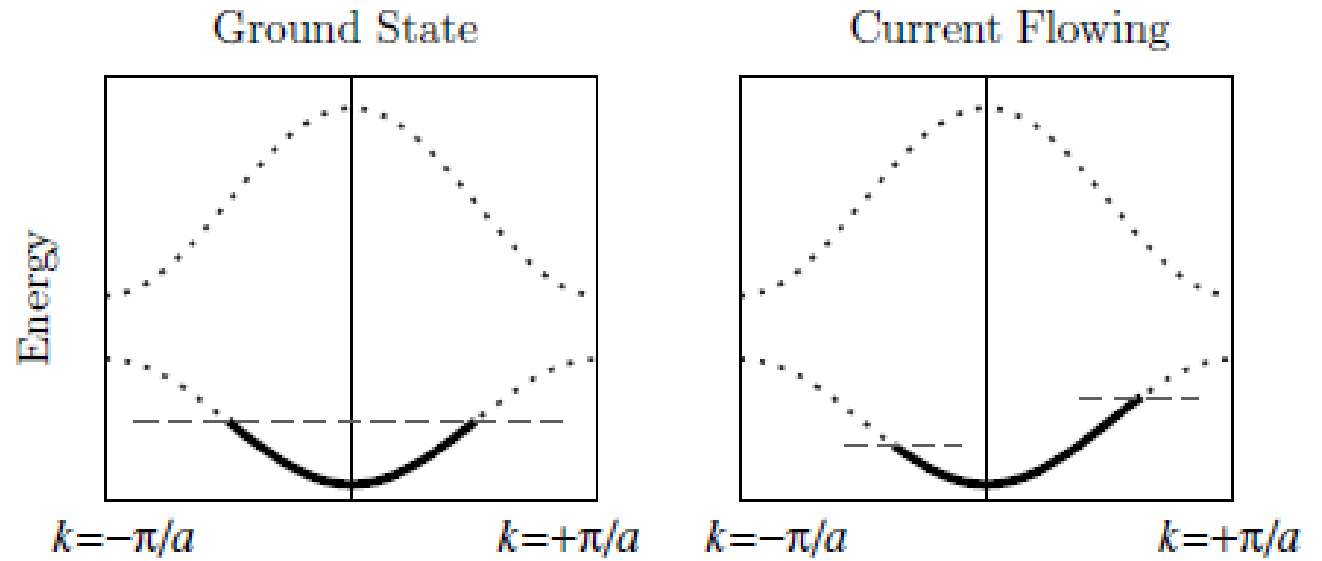
**pero**

$$\int_{\text{filled}} \frac{dk}{4\pi^3} v_{nk} + \int_{\text{empty}} \frac{dk}{4\pi^3} v_{nk} = 0$$

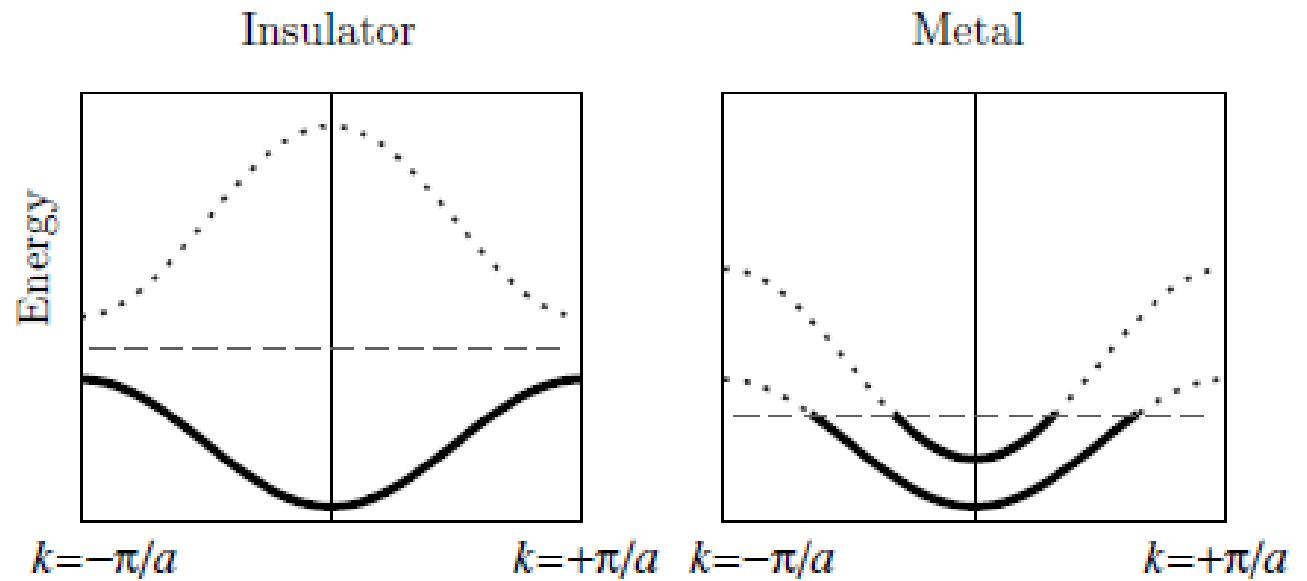
$$j = -e \int_{\text{filled}} \frac{dk}{4\pi^3} v_{nk} = +e \int_{\text{empty}} \frac{dk}{4\pi^3} v_{nk}$$

**La corriente puede ser interpretada a partir de portadores con carga positiva (agujeros o holes)**

# 1 e<sup>-</sup> /celda



# 2 e<sup>-</sup> /celda





4- Los niveles desocupados de una banda evolucionan en el tiempo bajo la influencia de un campo eléctrico como si fueran electrones con carga positiva

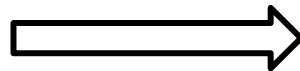
$$\hbar \dot{k} = -eE$$

$$E(k) \approx E(k_0) - A(k - k_0)^2$$

$$\frac{\hbar}{2m^*} \equiv A > 0$$

$$v = \frac{1}{\hbar} \frac{\partial E}{\partial k} \approx -\frac{\hbar}{m^*} (k - k_0)$$

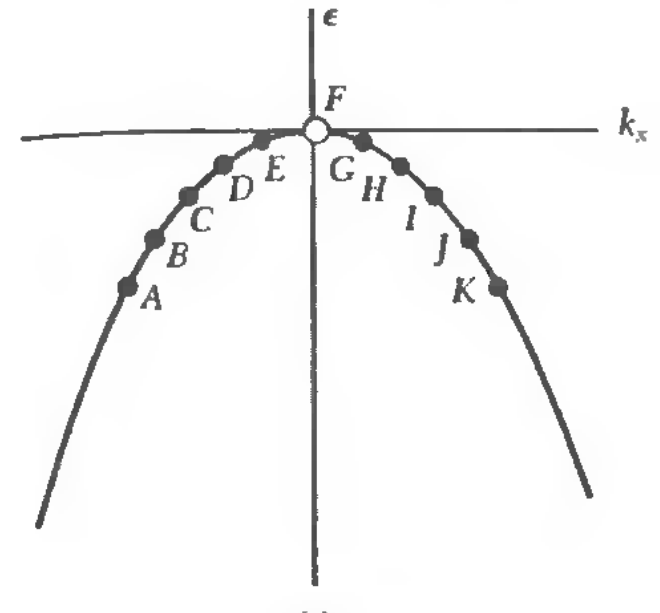
$$a = \frac{dv}{dt} = -\frac{\hbar}{m^*} \dot{k}$$



$$-m^*a = F_{\text{ext}} = -eE$$

$$m^*a = eE$$

Tope de una banda



## 5- Masa efectiva

$$\dot{v}_{n\mathbf{k}} = \frac{d}{dt} \left( \frac{1}{\hbar} \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial \mathbf{k}} \right).$$

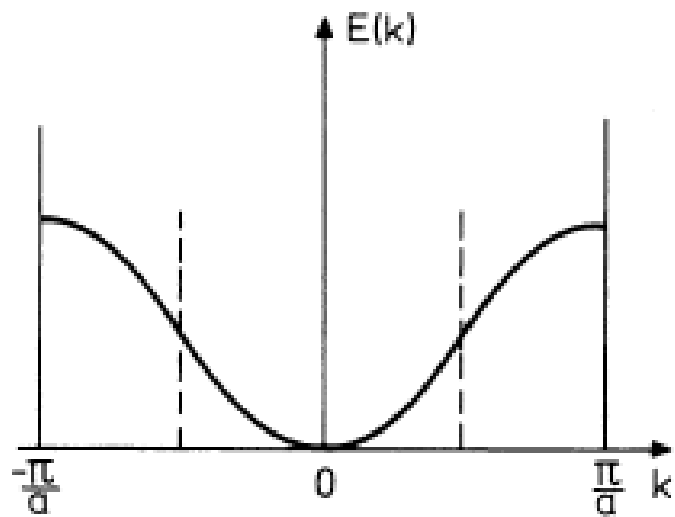
$$\dot{v}_{\mathbf{k}} = \frac{\partial}{\partial \mathbf{k}} \left( \frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \right) \frac{d\mathbf{k}}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k^2} \hbar \dot{\mathbf{k}}.$$

$$\dot{v} = \frac{1}{M} F$$

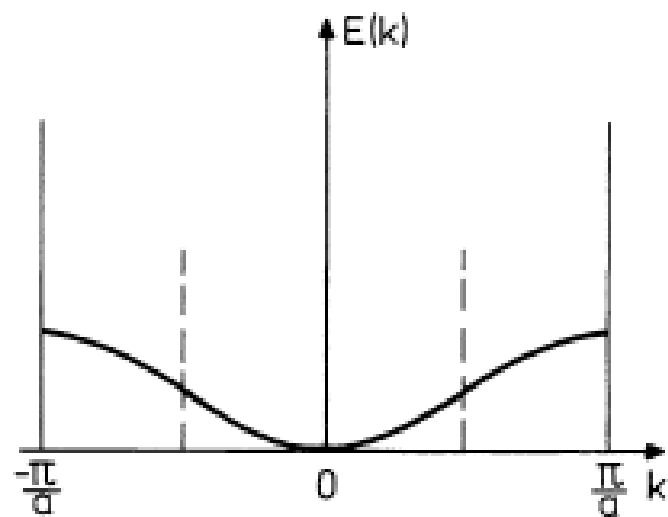


$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k^2},$$

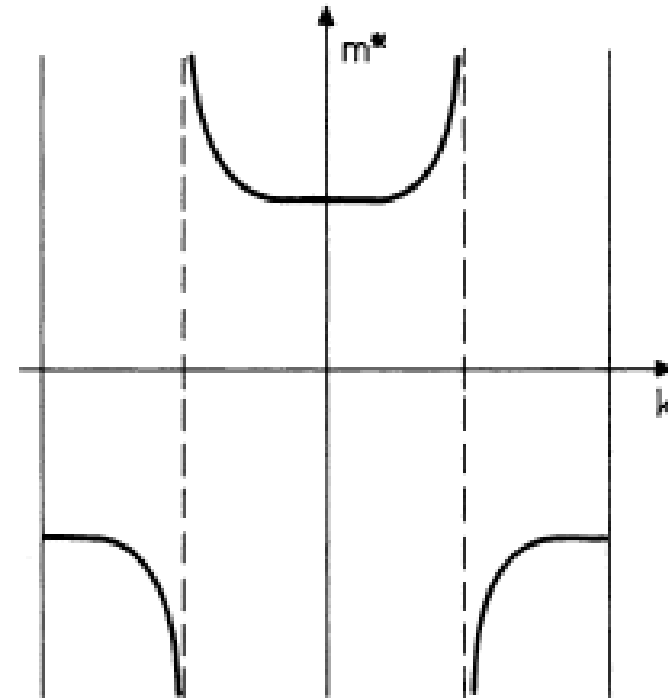
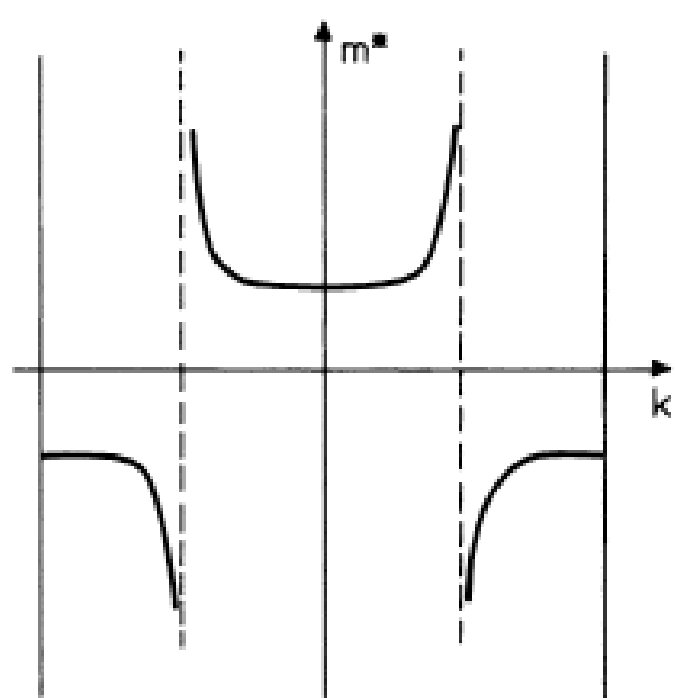
**Masa efectiva**



a



b



En el caso general donde la relación de dispersión no es isotrópica,

$$\dot{v}_\alpha = \left( \frac{1}{M^*} \right)_{\alpha\beta} F_\beta$$

## Tensor masa efectiva

$$\left( \frac{1}{m^*} \right)_{\alpha\beta} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_\alpha \partial k_\beta} \quad \alpha, \beta = x, y, z$$

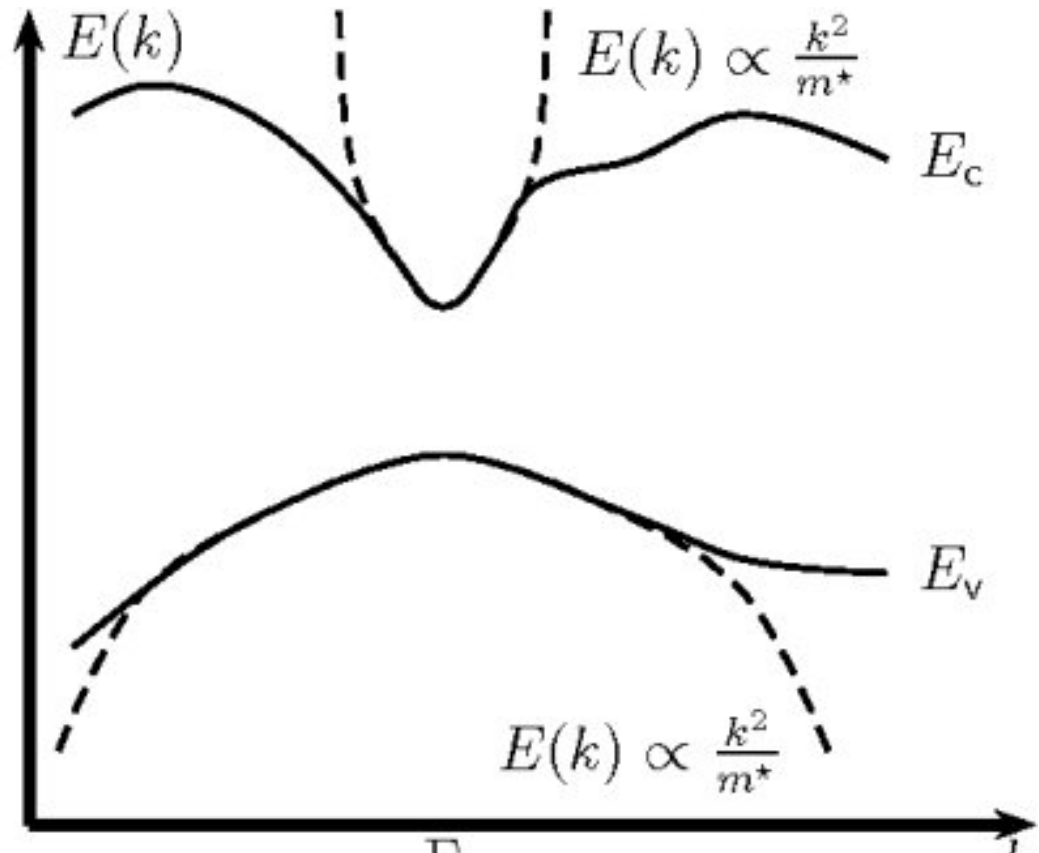
Para el caso de electrones libres

$$E = \hbar^2 k^2 / 2m \quad \Longrightarrow \quad \left( \frac{1}{m^*} \right)_{\alpha\beta} = \frac{\delta_{\alpha\beta}}{m}$$

El fondo y el tope de una banda se pueden aproximar con relaciones de dispersión cuadráticas de la forma

$$\varepsilon_{\mathbf{k}} \approx \varepsilon_{\mathbf{k}_0} + \frac{\hbar^2}{2} \sum_{\alpha\beta} \left( \frac{1}{M^*} \right)_{\alpha\beta} (k_\alpha - k_{0\alpha})(k_\beta - k_{0\beta})$$

**Muy útil en  
semiconductores  
(banda de valencia  
casi llena y banda de  
conducción casi vacía)**



**Conductividad de Drude  
para electrones libres**

$$\sigma = \frac{n_e e^2 \tau}{m_e}$$

**Para electrones en una banda de conducción **casi vacía**  
cambiamos la masa  $m_e$  por la masa efectiva**

$$\sigma_0 = \frac{n_e e^2 \tau}{m^*}$$

$$\sigma_{\alpha\beta} = n_e e^2 \tau \left( \frac{1}{M^*} \right)_{\alpha\beta}$$

**Para una banda de valencia **casi llena****

$$\sigma_0 = \frac{n_h e^2 \tau}{m_h^*}$$

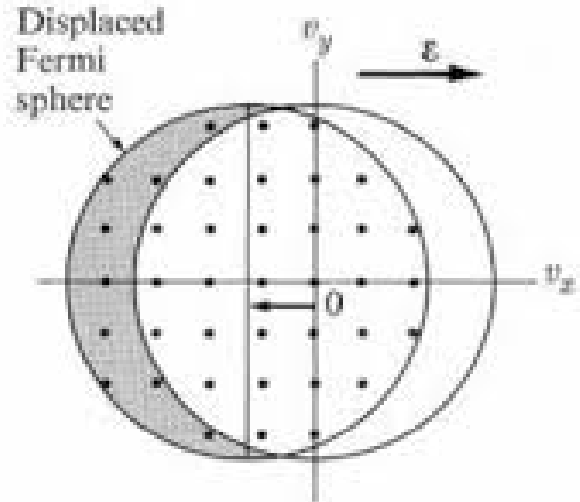
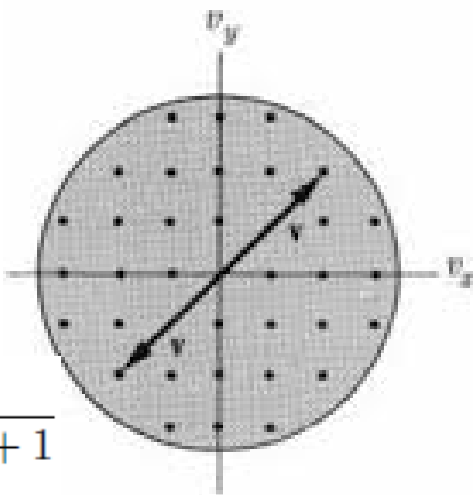
# 6- Teoría de la conducción en sólidos

$$j = -e \int \frac{dk}{4\pi^3} v_k f(k) \quad j_E = \int \frac{dk}{4\pi^3} \epsilon_k v_k f(k)$$

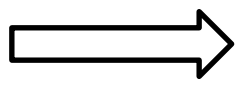
Probabilidad de ocupación con campo

$$\hbar k(t) = \hbar k(0) - eEt$$

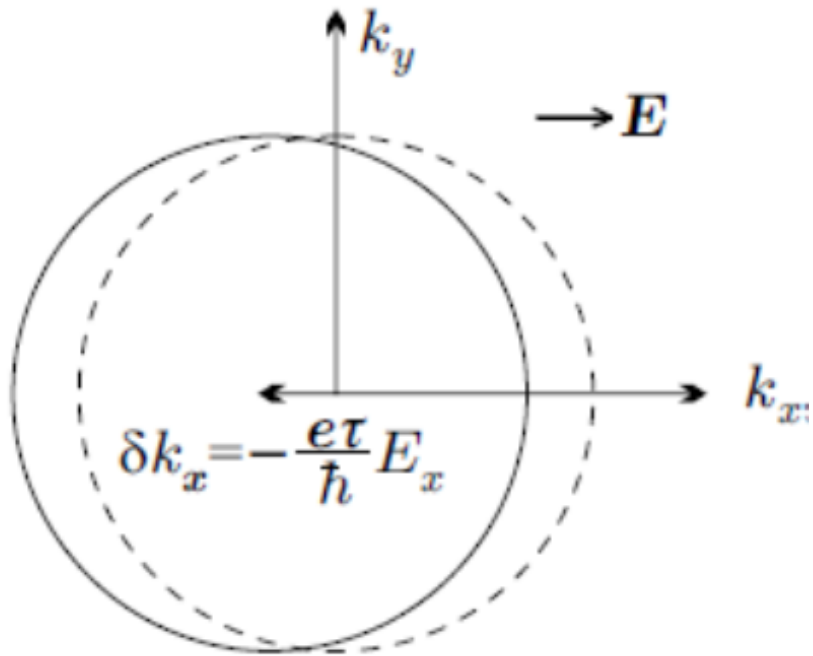
$$f_0(k) = \frac{1}{\exp[(\epsilon_k - \mu) / k_B T] + 1}$$



Debido a los procesos de scattering

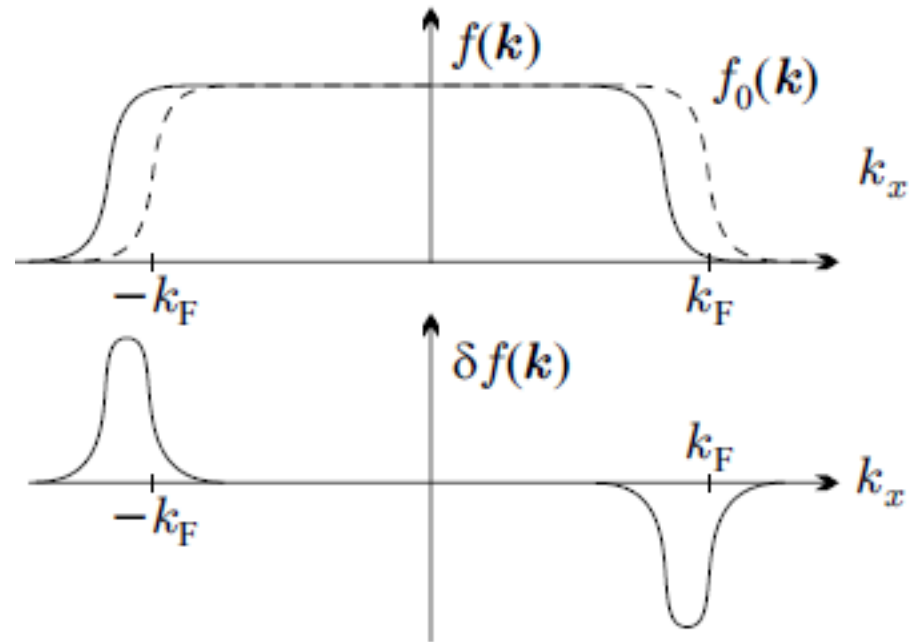


$$f(k) = f_0(k') = f_0\left(k + \frac{e\tau}{\hbar} E\right)$$



$$f(\mathbf{k}) = f_0(\mathbf{k}) + \frac{\partial f_0}{\partial \epsilon_{\mathbf{k}}} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k} \frac{e\tau}{\hbar} \mathbf{E}$$

$$= f_0(\mathbf{k}) + \left( -\frac{\partial f_0}{\partial \epsilon_{\mathbf{k}}} \right) \mathbf{v}_{\mathbf{k}} \cdot (-e\mathbf{E}) \tau$$



$$\sigma = e^2 \int \frac{dk}{4\pi^3} \mathbf{v}_{\mathbf{k}} \circ \mathbf{v}_{\mathbf{k}} \tau(\epsilon_{\mathbf{k}}) \left( -\frac{\partial f_0}{\partial \epsilon_{\mathbf{k}}} \right)$$



$$v_{\mathbf{k}} \left( -\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) = -\frac{1}{\hbar} \frac{\partial f_0(\varepsilon_{\mathbf{k}})}{\partial \mathbf{k}} \longrightarrow \sigma = -\frac{1}{\hbar} e^2 \tau(\varepsilon_F) \int \frac{d\mathbf{k}}{4\pi^3} v_{\mathbf{k}} \circ \frac{\partial f_0(\varepsilon_{\mathbf{k}})}{\partial \mathbf{k}}$$

**Integrando por partes y asumiendo que la dispersión se puede escribir en función de una masa efectiva escalar  $\sigma_{\alpha\beta} = \delta_{\alpha\beta} \sigma$**

$$\sigma_0 = e^2 \tau(\varepsilon_F) \int \frac{d\mathbf{k}}{4\pi^3} \frac{1}{\hbar} \frac{\partial v_{\mathbf{k}}}{\partial \mathbf{k}} f_0(\varepsilon_{\mathbf{k}}) = e^2 \tau(\varepsilon_F) \int_{\text{occupied}} \frac{d\mathbf{k}}{4\pi^3} \frac{1}{m_{\mathbf{k}}^*}.$$

**Si la masa efectiva es independiente de  $\mathbf{k}$ , se obtiene la formula de Drude**

$$\sigma_0 = \frac{n_e e^2 \tau}{m^*}$$

**Si la integral se realiza sobre los estados desocupados**

$$\sigma_0 = e^2 \tau(\varepsilon_F) \int_{\text{empty}} \frac{d\mathbf{k}}{4\pi^3} \left( -\frac{1}{m_{\mathbf{k}}^*} \right) \Longrightarrow \sigma_0 = \frac{n_h e^2 \tau}{m_h^*}$$

Volvamos a la expresión general

$$\sigma = e^2 \int \frac{dk}{4\pi^3} v_{\mathbf{k}} \circ v_{\mathbf{k}} \tau(\varepsilon_{\mathbf{k}}) \left( -\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right)$$

Para un sistema isotrópico

$$\sigma_0 = e^2 \int \frac{dk}{4\pi^3} \frac{1}{3} v_{\mathbf{k}}^2 \tau \left( -\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right)$$

$$\sigma_0 = n_e e^2 \tau / m_{\text{opt}} \quad \Longrightarrow \quad m_{\text{opt}}^{-1} = \frac{1}{3n_e} \int \frac{dk}{4\pi^3} v_{\mathbf{k}}^2 \left( -\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right)$$

$$\int dk \rightarrow \int d\varepsilon$$

Uso la densidad  
de estados

$$\rho_n(\varepsilon) = \frac{2}{(2\pi)^3} \int_{S(\varepsilon)} \frac{dS}{|\nabla_{\mathbf{k}} \varepsilon_{n\mathbf{k}}|}$$

$$m_{\text{opt}}^{-1} = \frac{1}{12\pi^3 \hbar n_e} \int_{S(\varepsilon_F)} v_{\mathbf{k}} dS$$

$$\sigma_0 = \frac{n_e e^2 \tau}{12\pi^3 \hbar n_e} \int_{S(\varepsilon_F)} v_{\mathbf{k}} dS$$