Constantes

$$k_B = 1.381 \times 10^{-23} JK^{-1} = 8.26 \times 10^{-5} eVK^{-1}$$
$$m_e = 9.11 \times 10^{-31} kg = 0.511 MeVc^{-2}$$
$$\varepsilon_0 = \frac{1}{4\pi K} = 8.85 \times 10^{-12} Fm^{-1}$$
$$\hbar = 1.055 \times 10^{-34} Js = 6.58 \times 10^{-16} eVs$$
$$e = 1.602 \times 10^{-19} C$$

1 Estructura cristalina

1.1 Redes de Bravais

a	triclínica
m	monoclínica
o	ortorómbica
t	tetragonal
h	hexagonal
c	cúbica

P	Primitiva
S	Centrada en una cara
I	Centrada en el cuerpo
R	Centrada romboidal
F	Centrada en las caras

14 posibles redes de Bravais

Tric.	Monoc.	Ortor.	Tetra.	Hex.	Cúbico
aP	mP, mS	oP, oS, oF, oI	tP, tI	hP, hR	cP, cF, cI

1.2 Cosas

Base dual y matriz métrica

$$a^* = \frac{b \times c}{V}, \quad b^* = \frac{c \times a}{V}, \quad c^* = \frac{a \times b}{V}, \quad V = \det(\overline{a}, \overline{b}, \overline{c})$$

$$(\overline{a}^*, \overline{b}^*, \overline{c}^*) = \begin{pmatrix} \overline{a}^T \\ \overline{b}^T \\ \overline{c}^T \end{pmatrix}^{-1}, G = \begin{pmatrix} a \cdot a & a \cdot b & a \cdot c \\ b \cdot a & b \cdot b & b \cdot c \\ c \cdot a & c \cdot b & c \cdot c \end{pmatrix}, G^* = G^{-1}$$

Cambio de base

$$(\overline{a}', \overline{b}', \overline{c}') = (\overline{a}, \overline{b}, \overline{c})P, \quad \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$(x, y, z) = (x^*, y^*, z^*)P, \quad \begin{pmatrix} a'^* \\ b'^* \\ z'^* \end{pmatrix} = P^{-1} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}$$

Red recíproca y distancia interplanar $g_{hkl} = \frac{1}{d_{hkl}}$

Transferencia de momento $Q = \frac{4\pi \sin\theta}{\lambda}$

Condiciones de Laue $\overline{Q} = 2\pi \overline{g}_{hkl}$

Ley de Bragg $g_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$

Módulo de Young $\nu_s = \sqrt{\frac{\gamma}{\rho}}$

Factor de estructura

$$F_{hkl} = \sum_p f_p e^{-i2\pi \overline{g}_{hkl} \cdot \overline{r}_p}, \quad I \propto |F_{hkl}|^2$$

1.3 Estructuras comunes

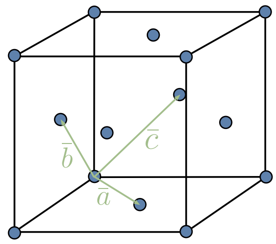
FCC

$$\begin{cases} \overline{a} = \frac{1}{2}(1\ 1\ 0) \\ \overline{b} = \frac{1}{2}(0\ 1\ 1) \\ \overline{c} = \frac{1}{2}(1\ 0\ 1) \end{cases} \qquad \begin{cases} \overline{a}^* = (1\ 1\ -1) \\ \overline{b}^* = (-1\ 1\ 1) \\ \overline{c}^* = (1\ -1\ 1) \end{cases}$$

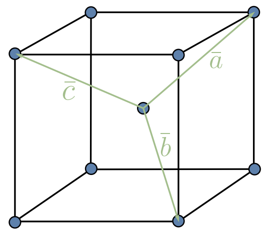
BCC

$$\begin{cases} \overline{a} = \frac{1}{2}(1\ 1\ -1) \\ \overline{b} = \frac{1}{2}(-1\ 1\ 1) \\ \overline{c} = \frac{1}{2}(1\ -1\ 1) \end{cases} \qquad \begin{cases} \overline{a}^* = (1\ 1\ 0) \\ \overline{b}^* = (0\ 1\ 1) \\ \overline{c}^* = (1\ 0\ 1) \end{cases}$$

FCC



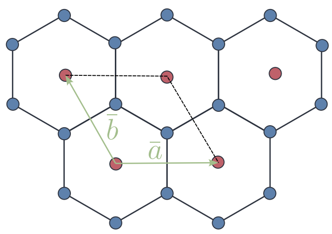
BCC

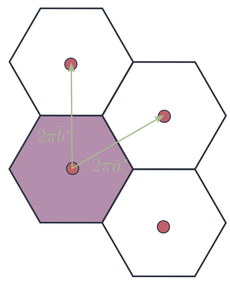


Hexagonal

$$\begin{cases} \overline{a} = (1, 0) \\ \overline{b} = (-\frac{1}{2}, \frac{\sqrt{3}}{2}) \end{cases} \qquad \begin{cases} \overline{a}^* = \frac{2\sqrt{3}}{3}(\frac{\sqrt{3}}{2}, \frac{1}{2}) \\ \overline{b}^* = \frac{2\sqrt{3}}{3}(0, 1) \end{cases}$$

$$G = \begin{pmatrix} a^2 & -\frac{a^2}{2} & 0 \\ -\frac{a^2}{2} & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}, \quad G^* = \begin{pmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & 0 \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$





En una hcp $c = 1.633a$

1.4 Grupos

$$m_{100} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} n_{001} = \begin{pmatrix} \cos\left(\frac{360}{n}\right) & -\sin\left(\frac{360}{n}\right) & 0 \\ \sin\left(\frac{360}{n}\right) & \cos\left(\frac{360}{n}\right) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Cambio de base a $\mathcal{B} = \{\overline{u}, \overline{v}, \overline{w}\}$

$$M_{\mathcal{C}} = M_{\mathcal{B}\to\mathcal{C}} M_{\mathcal{B}} M_{\mathcal{B}\to\mathcal{C}}^{-1}, \quad M_{\mathcal{B}\to\mathcal{C}} = (\overline{u}, \overline{v}, \overline{w})$$

Reflexión vector director (a, b, c)

$$M = \frac{1}{a^2 + b^2 + c^2} \begin{pmatrix} -a^2 + b^2 + c^2 & -2ab & -2ac \\ -2ab & a^2 - b^2 + c^2 & -2bc \\ -2ac & -2bc & a^2 + b^2 - c^2 \end{pmatrix}$$

Rotación respecto $\hat{u} = (u_x, u_y, u_z)$ $(c = \cos\theta, \quad s = \sin\theta)$.
$R =$

$$\begin{pmatrix} c + u_x^2(1-c) & u_x u_y(1-c) - u_z s & u_x u_z(1-c) + u_y s \\ u_y u_x(1-c) + u_z s & c + u_y^2(1-c) & u_y u_z(1-c) - u_x s \\ u_z u_x(1-c) - u_y s & u_z u_y(1-c) + u_x s & c + u_z^2(1-c) \end{pmatrix}$$

Centrosimétricos $(x,y,z) \to (-x,-y,-z)$ no tienen polarización espontánea

2 Dinámica de cristales

2.1 Densidad de estados

$$\overline{k} = \left(\tfrac{2\pi}{L}n \quad \tfrac{2\pi}{L}m \quad \tfrac{2\pi}{L}l\right) \ \forall n,m,l \in \mathbb{Z}$$

Número de estados hasta k

$$N(k) = \int_{(\frac{2\pi}{L})^2(n^2+m^2+l^2)\leq k^2} dV = \frac{L^3}{6\pi^2}k^3 = \frac{V}{6\pi^2}k^3$$

1, 2 y 3 dimensiones respectivamente (y se cumple $\omega = \nu_s k$)

$$\begin{cases} g(k) = \frac{L}{\pi} \\ g(\omega) = \frac{L}{\pi\nu} \end{cases} \quad \begin{cases} g(k) = \frac{L^2}{2\pi}k \\ g(\omega) = \frac{L^2}{2\pi\nu^2}\omega \end{cases} \quad \begin{cases} g(k) = \frac{V}{2\pi^2}k^2 \\ g(\omega) = \frac{V}{2\pi^2\nu_s^3}\omega^2 \end{cases}$$

2.2 Dispersión

Oscilador con masa m y constante k_s

$$F_n = m\ddot{x}_n = k_s(x_{n+1} + x_{n-1} - 2x_n)$$

$$-m\omega^2 A e^{i(kna-\omega t)} = k_s A e^{i(kna-\omega t)}(e^{ika} + e^{-ika} - 2) =$$

$$= -4k_s\sin^2\left(\frac{ka}{2}\right) \Rightarrow \boxed{\omega = 2\sqrt{\frac{k_s}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|}$$

Oscilador con masa m y constantes alternadas k_1, k_2

$$\begin{cases} m\ddot{x}_n = k_1(y_{n-1} - x_n) + k_2(y_n - x_n) \\ m\ddot{y}_n = k_1(x_{n+1} - y_n) + k_2(x_n - y_n) \end{cases}$$

Ansatz

$$x_n = Ae^{i(kna-\omega t)} \qquad y_n = Be^{i(kna-\omega t)}$$

Ecuaciones

$$\begin{cases} -m\omega^2 A = -A(k_1+k_2) + B(k_1e^{ika} + k_2) \\ -m\omega^2 B = -A(k_1e^{ika} + k_2) + B(-k_1 - k_2) \end{cases}$$

Forma matricial

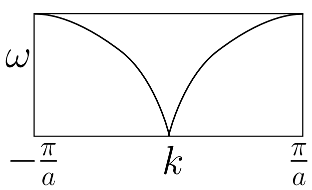
$$m\omega^2\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1+k_2) & -k_2 - k_1e^{ika} \\ -k_2 - k_1e^{ika} & (k_1+k_2) \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = K\begin{pmatrix} A \\ B \end{pmatrix}$$

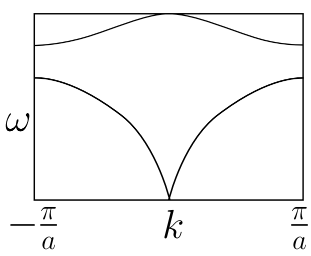
$$0 = \det(K - m\omega^2 I) = |(k_1+k_2) - m\omega^2|^2 - |k_2 + k_1e^{ika}|^2$$

$$\boxed{\omega_\pm(k) = \sqrt{\frac{k_1+k_2}{m} \pm \frac{1}{m}\sqrt{(k_1+k_2)^2 - 4k_1k_2\sin^2(ka/2)}}}$$

Si $m_1 \neq m_2$ y k_s es la misma, sea $K_i = \frac{k}{m_i}$, entonces

$$\boxed{\omega_\pm(k) = \sqrt{(K_1+K_2) \pm \sqrt{(K_1+K_2)^2 - 4K_1K_2\sin^2(ka/2)}}}$$





2.3 Modelo de Einstein

$$E_n = \hbar\omega(n + \frac{1}{2}) \quad \Rightarrow \quad Z_1 = \frac{1}{2\sinh(\frac{\beta\hbar\omega}{2})}$$

$$\langle E_1\rangle = -\frac{\partial}{\partial\beta}\ln Z_1 = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

Energía y capacidad calorífica

$$\langle E\rangle = \frac{3}{2}N\hbar\omega\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

$$C_v = \frac{\partial\langle E\rangle}{\partial T} = 3Nk_B(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

Definimos ahora $T_E = \frac{\hbar\omega_E}{k_B}$. En los límites

- Si $T \gg T_E \quad \Rightarrow \quad C_v = 3Nk_b$
- Si $T \ll T_E \quad \Rightarrow \quad C_v = 3Nk_b(\frac{T_E}{T})^2\frac{1}{\sinh^2(\frac{T_E}{2T})}$

2.4 Modelo de Debye

Aproximamos la ecuación de dispersión para k baja como $\omega = \nu k$

$$3N = \int_0^{\omega_D} 3g(\omega)d\omega = \frac{V}{2\pi^2\nu^3}\omega_D^3 \Rightarrow \boxed{\omega_D = \sqrt[3]{\frac{6\pi^2\nu^3 N}{V}}}$$

donde hemos contado cada partícula y cada estado 3 veces y hemos usado

$$\omega = \nu k, \qquad g(k) = \frac{V}{2\pi^2}k^2, \qquad g(\omega) = \frac{V}{2\pi^2\nu^3}\omega^2$$

La energía y la capacidad calorífica

$$\langle E\rangle = \int_0^{\omega_D}\hbar\omega 3g(\omega)\left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\right)d\omega =$$

$$= E_0 + \frac{3V\hbar}{2\pi^2\nu^3}\int_0^{\omega_D}\frac{\hbar\omega^3}{e^{\beta\hbar\omega}-1}d\omega \qquad (x = \frac{\hbar\omega}{k_BT})$$

$$T_D := \frac{\hbar\omega}{k_B} \quad \Rightarrow \boxed{\langle E\rangle = \frac{3Vk_B^4T^4}{2\pi^2\nu^3\hbar^3}\int_0^{\frac{T_D}{T}}\frac{x^3}{e^x-1}dx}$$

La capacidad calorífica $C_v = \frac{\partial\langle E\rangle}{\partial T}$ en los extremos:

- Si $T \gg T_D \quad \Rightarrow \quad \langle E\rangle \sim 3Nk_BT \quad \Rightarrow \quad C_v \sim 3Nk_B$
- Si $T \ll T_D \quad \Rightarrow \quad \langle E\rangle \sim \frac{3\pi^4 Nk_BT^4}{5T_D^3} \quad \Rightarrow \quad C_v \sim \frac{12\pi^4}{5}Nk_B\left(\frac{T}{T_D}\right)^3$

3 No se, cuanticocosas

3.1 Drude model

$$n = \frac{N}{V}; \quad \frac{dp}{dt} = F - \frac{p}{\tau}, \bar{j} = -ne\bar{v} = \sigma\bar{E}$$
$$mv = p = -e\tau E; \quad R_H = \frac{-1}{ne} = \frac{\rho_{yx}}{|B|}$$
$$\bar{E} = \tilde{\rho}\bar{j}; \quad \rho_{xx} = \rho_{yy} = \rho_{zz}\frac{m}{ne^2\tau}$$

Hall resistivity $\rho_{xy} = -\rho_{yx} = \frac{B}{ne}$ $(\bar{B} \propto \hat{z})$

Peltier coefficient $\Pi = -\frac{k_B T}{2e} = \frac{-c_v T}{3e}$

Seebeck coefficient $S = \frac{\Pi}{T}$

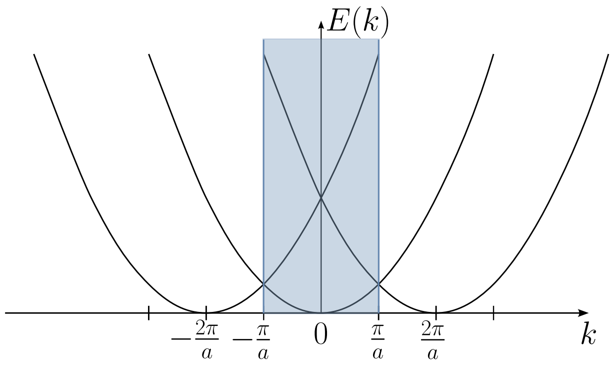
$$< v >_{gasid.} = \sqrt{\frac{8k_BT}{\pi m}}; \quad \kappa = \frac{1}{3}nc < v >^2 \tau = \frac{4}{\pi}\frac{n\tau k_B^2 T}{m}$$

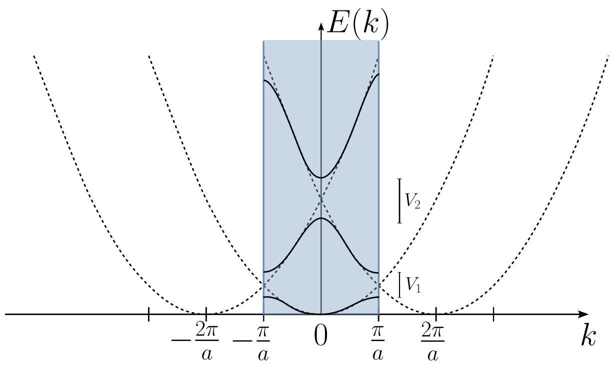
3.2 Capacidad calorífica

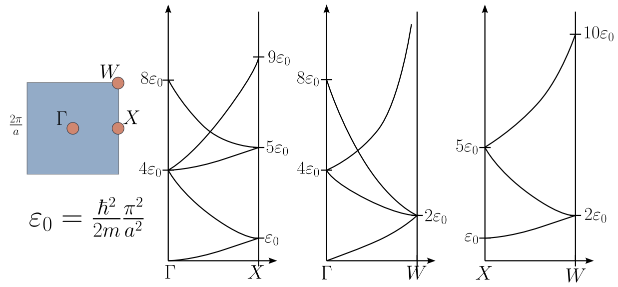
g densidad de estados / V

$$g(\varepsilon) = \frac{3n}{2(E_F)^{\frac{3}{2}}}\varepsilon^{\frac{1}{2}} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\varepsilon^{\frac{1}{2}}, \quad k = \sqrt{\frac{2\varepsilon m}{\hbar^2}}$$
$$N = \int_0^\infty d\varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu)), \quad E_T = \int_0^\infty d\varepsilon\varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu))$$
$$C = \frac{\pi^2}{3}\left(\frac{3Nk_B}{2}\right)\left(\frac{T}{T_F}\right)$$

$$\bar{M} = g(E_F)\mu_B^2\bar{B}; \quad \mu_B = 0.67\left(\frac{K}{Tesla}\right)k_B$$







Teorema de Bloch ($V(\bar{r})$ periódico)

$$\psi_{\bar{k}}(\bar{r}) = u_{\bar{k}}(\bar{r})e^{i\bar{k}\cdot\bar{r}}, \quad E(\bar{k}) = E(\bar{k} + \bar{G})$$

(1D) Fourier del potencial de dos formas

$$V(x) = V_0 + \sum_{j=1}^{\infty} V_j \cos\left(\frac{2\pi j}{a}x\right) \quad \text{ó} \quad V(x) = \sum_{j=-\infty}^{\infty} V_{\frac{2\pi j}{a}} e^{\frac{2\pi j}{a}ix}$$

Con las relaciones $V_j = 2V_{\frac{2\pi j}{a}}$, y donde los coeficientes son

$$V_j = \frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x)\cos\left(\frac{2\pi}{a}jx\right); \quad V_{\frac{2\pi j}{a}} = \frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x) e^{\frac{-2\pi}{a}ijx}$$

<u>Gas de electrones libres</u>

$$\bar{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \quad E(\bar{k}) = \frac{\hbar^2}{2m}|\bar{k}|^2, \quad n_F(x) = \frac{1}{e^x + 1}$$
$$N = 2\sum_{\bar{k}} n_F(\beta(E(\bar{k}) - \mu)) = 2\frac{V}{(2\pi)^3}\int d\bar{k} n_F(\beta(E(\bar{k}) - \mu))$$

Fermi energy $(E_F = \mu(T \to 0))$

$$E_F = \frac{\hbar^2 k_F^2}{2m} = k_B T_F, \quad p_F = \hbar k_F$$
$$N = 2\frac{V}{(2\pi)^3}\int_{|k|<k_F} dk \Rightarrow k_F = (3\pi^2 n)^{\frac{1}{3}}, \quad E_F = \frac{\hbar^2(3\pi^2 n)^{\frac{2}{3}}}{2m}$$

$$\bar{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}, \quad n_x, n_y, n_z \in \mathbb{Z} \Rightarrow k^2 = \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

Considerando los dos espines (multiplicamos por 2)

$$N_T = 2\cdot\left(\frac{4}{3}\pi(n_x^2 + n_y^2 + n_z^2)^{3/2}\right) \quad \Rightarrow \quad k_{max}^2 = k_F^2 = (3n\pi^2)^{\frac{2}{3}}$$

<u>Electrones casi-libres</u>

$$\psi_+ \sim \cos(\pi\frac{x}{a}), \quad \psi_- \sim \sin(\pi\frac{x}{a})$$
$$E^\pm = \frac{1}{2}(E^0_{\bar{k}-\bar{G}} + E^0_{\bar{k}}) \pm \sqrt{\frac{1}{4}(E^0_{\bar{k}-\bar{G}} - E^0_{\bar{k}})^2 + |V_{\bar{G}}|^2}$$

<u>Enlace fuerte, celda primitiva cúbica</u>

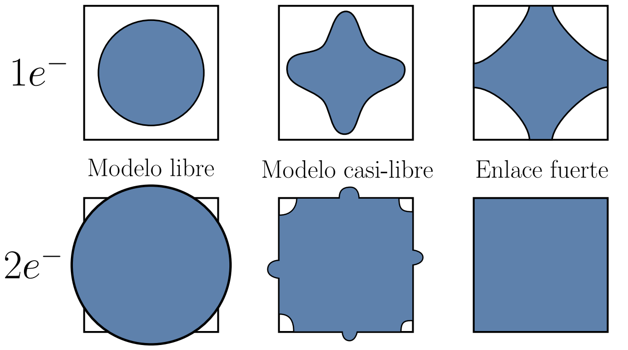
$$E(\bar{k}) \approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a)$$
$$A = -\langle\varphi_{i,n}|v|\varphi_{i,n}\rangle, \quad B = -\langle\varphi_{i,m}|v|\varphi_{i,n}\rangle$$
$$\bar{v} = \nabla_{\bar{k}}\omega(\bar{k}) = \frac{1}{\hbar}\nabla_{\bar{k}}E(\bar{k})$$

Carga de un campo $\overline{\mathcal{E}}$

$$\dot{v}_i = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 E}{\partial k_i \partial k_j}(-e\mathcal{E}_j), \quad \left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E(\overline{k})}{\partial k_i \partial k_j}$$

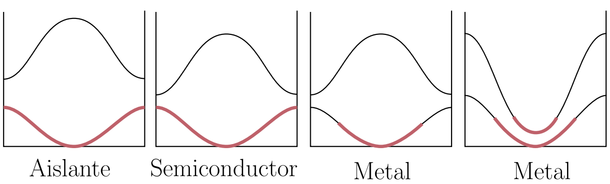
Caso totalmente degenerado

$$m^* = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}, \quad E(\overline{k}) = E_0 + \frac{\hbar^2}{2m^*}|k|^2, \quad \sigma \simeq \frac{e^2\tau(E_F)n}{m^*}$$



Tipos de materiales

Aislante: Banda llena ($2e^-$). $V_g > 4eV$
Semiconductor Banda llena ($2e^-$). $V_g < 4eV$.
Metal Banda semillena ($1e^2$ ó $2e^-$ con bandas solapantes).



4 Semiconductores

Densidad de estados

$$D_C = \frac{(2m_n^*)^{2/3}}{2\pi^2\hbar^3}\sqrt{E - E_C}, \quad D_V = \frac{(2m_p^*)^{2/3}}{2\pi^2\hbar^3}\sqrt{E_V - E}$$

$$n = 2\left(\frac{2\pi m_n^* k_B T}{h^2}\right)^{3/2} e^{\beta(E_F - E_C)} = N_{eff}^C e^{\beta(E_F - E_C)}$$

$$p = 2\left(\frac{2\pi m_p^* k_B T}{h^2}\right)^{3/2} e^{\beta(E_V - E_F)} = N_{eff}^V e^{\beta(E_V - E_F)}$$

$$np = N_{eff}^C N_{eff}^V e^{-\beta E_g} = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_n^* m_p^*)^{3/2} e^{-\beta E_g}$$

$$e^{2\beta E_F} = \frac{N_{eff}^V}{N_{eff}^C} e^{\beta(E_V + E_C)}, \quad E_F = \frac{E_C + E_V}{2} + \frac{3}{4}k_B T \ln\left(\frac{m_p^*}{m_n^*}\right)$$

$$\mu = \frac{e\tau}{m^*}, \quad \sigma = e(n\mu_n + p\mu_p), \quad E_g = E_C - E_V$$

Semiconductores dopados

$$E_n = \frac{m^* e^4}{2(4\pi\varepsilon\hbar)^2}\frac{1}{n^2}, \quad r = \varepsilon\frac{h^2}{\pi m^* e^2}$$

$$n \approx \frac{2N_D}{1 + \sqrt{1 + 4\frac{N_D}{N_{eff}^C}e^{\beta E_d}}}$$

Unión p-n

$$n_n = N_{eff}^C e^{\beta(E_F - E_C^n)}; \quad p_p = N_{eff}^V e^{\beta(E_V - E_F)}$$

$$d_n^0 = \sqrt{\frac{2\varepsilon V_D}{e}\frac{N_A/N_D}{N_A + N_D}}; \quad d_p^0 = \sqrt{\frac{2\varepsilon V_D}{e}\frac{N_D/N_A}{N_A + N_D}}$$

$$d_n(U) = d_n^0\sqrt{1 - \frac{U}{V_D}}; \quad d_p(U) = d_p^0\sqrt{1 - \frac{U}{V_D}}$$

$$eV_D = k_B T \ln\left(\frac{n_n p_p}{n_i^2}\right); \quad I(U) = (I_n^{gen} + I_p^{gen})(e^{\beta eU} - 1)$$

5 Mates

$$\sin^2\left(\frac{x}{2}\right) = \frac{1 - \cos a}{2}$$

$$\int_0^\infty \frac{1}{e^x - 1}dx = +\infty, \quad \int_0^\infty \frac{1}{e^x + 1}dx = \ln(2)$$

$$\int_0^\infty \frac{x}{e^x - 1}dx = \frac{\pi^2}{6}, \quad \int_0^\infty \frac{x}{e^x + 1}dx = \frac{\pi^2}{12}$$

$$\int_0^\infty \frac{x^2}{e^x - 1}dx = 2\zeta(3), \quad \int_0^\infty \frac{x^2}{e^x + 1}dx = \frac{3}{2}\zeta(3)$$

$$\int_0^\infty \frac{x^3}{e^x - 1}dx = \frac{\pi^4}{15}, \quad \int_0^\infty \frac{x^3}{e^x + 1}dx = \frac{7\pi^4}{120}$$