

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

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

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

Cambio de base

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

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

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

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

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

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

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

Factor de estructura

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

1.3 Estructuras comunes

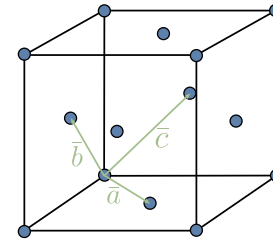
FCC

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

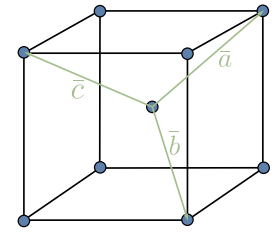
BCC

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

FCC



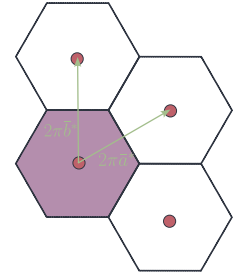
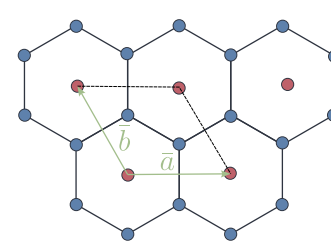
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Hexagonal

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

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



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 $\mathcal{B} = \{\bar{u}, \bar{v}, \bar{w}\}$

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

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

$R =$

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

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

2 Dinámica de cristales

2.1 Densidad de estados

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

Número de estados hasta k

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

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

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

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

$$x_n = A e^{i(kna - \omega t)} \quad y_n = B e^{i(kna - \omega t)}$$

Ecuaciones

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

Forma matricial

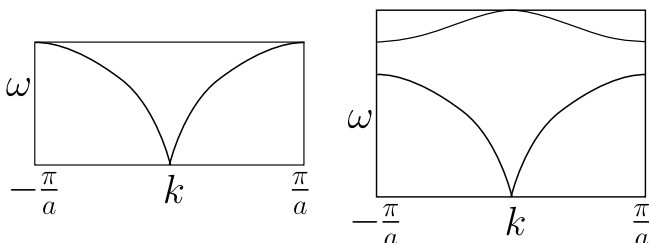
$$m\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1 + k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{ika} & (k_1 + k_2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = K \begin{pmatrix} A \\ B \end{pmatrix}$$

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

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

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

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



2.3 Modelo de Einstein

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

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

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

$$\bullet \text{ Si } T \gg T_E \Rightarrow C_v = 3Nk_B$$

$$\bullet \text{ Si } T \ll T_E \Rightarrow C_v = 3Nk_B \left(\frac{T_E}{T}\right)^2 \frac{1}{\sinh^2\left(\frac{T_E}{2T}\right)}$$

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

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

La energía y la capacidad calorífica

$$\begin{aligned} \langle E \rangle &= \int_0^{\omega_D} \hbar\omega 3g(\omega) \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right) d\omega = \\ &= E_0 + \frac{3V\hbar}{2\pi^2 \nu^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} d\omega \quad \left(x = \frac{\hbar\omega}{k_B T} \right) \end{aligned}$$

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

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

$$\bullet \text{ Si } T \gg T_D \Rightarrow \langle E \rangle \sim 3Nk_B T \Rightarrow C_v \sim 3Nk_B$$

$$\bullet \text{ Si } T \ll T_D \Rightarrow \langle E \rangle \sim \frac{3\pi^4 N k_B T^4}{5 T_D^3} \Rightarrow C_v \sim \frac{12\pi^4}{5} N k_B \left(\frac{T}{T_D}\right)^3$$

3 No se, cuanticocosas

3.1 Gas de electrones libre

$$\bar{k} = \frac{2\pi}{L}(n_1, n_2, n_3), \quad E(\bar{k}) = \frac{\hbar^2}{2m}|\bar{k}|^2, \quad n_F(x) = \frac{1}{e^x + 1}$$

$$N = 2 \sum_{\bar{k}} n_F(\beta(E(\bar{k}) - \mu)) = 2 \frac{V}{(2\pi)^3} \int d\bar{k} n_F(\beta(E(\bar{k}) - \mu))$$

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

$$E_F = \frac{\hbar^2 k_F^2}{2m} = k_B T_F, \quad p_F = \hbar k_F$$

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

3.2 Capacidad calorífica

g densidad de estados / V

$$g(\varepsilon) = \frac{3n}{2(E_F)^{\frac{3}{2}}} \varepsilon^{\frac{1}{2}} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \varepsilon^{\frac{1}{2}}, \quad k = \sqrt{\frac{2\varepsilon m}{\hbar^2}}$$

$$N = \int_0^\infty d\varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu)), \quad E_T = \int_0^\infty d\varepsilon \varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu))$$

$$C = \frac{\pi^2}{3} \left(\frac{3Nk_B}{2} \right) \left(\frac{T}{T_F} \right)$$

Teorema de Bloch

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

Electrones casi-libres

$$\psi_+ \sim \cos(\pi \frac{x}{a}), \quad \psi_- \sim \sin(\pi \frac{x}{a})$$

$$E^\pm = \frac{1}{2}(E_{\bar{k}-\bar{G}}^0 + E_{\bar{k}}^0) \pm \sqrt{\frac{1}{4}(E_{\bar{k}-\bar{G}}^0 - E_{\bar{k}}^0)^2 + |V_{\bar{G}}|^2}$$

Enlace fuerte, celda primitiva cúbica

$$E(\bar{k}) \approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a)$$

$$A = -\langle \varphi_{i,n} | v | \varphi_{i,n} \rangle, \quad B = -\langle \varphi_{i,m} | v | \varphi_{i,n} \rangle$$

$$\bar{v} = \nabla_{\bar{k}} \omega(\bar{k}) = \frac{1}{\hbar} \nabla_{\bar{k}} E(\bar{k})$$

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

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

Caso totalmente degenerado

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

4 Semiconductores

5 Mates

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

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

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

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

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