**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 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

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

## 1.2 Estructuras comunes

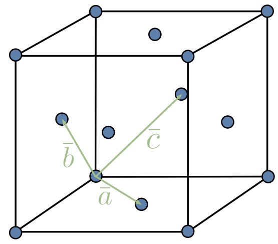
FCC

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

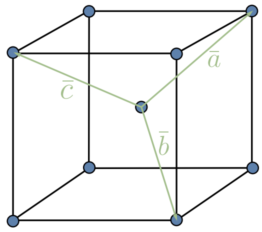
BCC

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

FCC

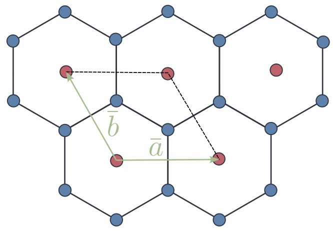


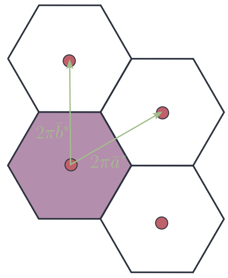

BCC




Hexagonal

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




# 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

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

Forma matricial

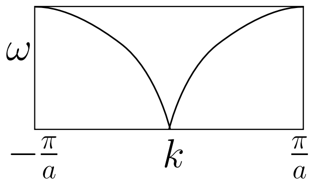
$$m\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1+k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{ika} & (k_1+k_2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = K \begin{pmatrix} A \\ B \end{pmatrix}$$

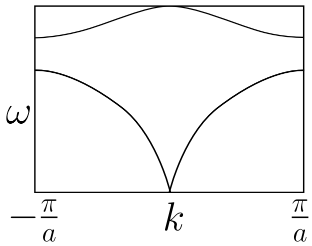
$$0 = \det(K - m\omega^2 I) = |(k_1+k_2) - m\omega^2|^2 - |k_2 + k_1 e^{ika}|^2$$

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

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

# 3 Mates

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

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

$$\int_0^\infty \frac{x^2}{e^x-1}dx = 2\zeta(3) \approx 2.40411$$

$$\int_0^\infty \frac{x^3}{e^x-1}dx = \frac{\pi^4}{15}$$