Formulari de Física de l'Estat Sòlid

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I. Cristal·lografia

Xarxa de Bravais:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \quad n_i \in \mathbb{Z}$$

Cel·la primitiva: unitària de volum mínim.

$$V_p = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$$

Xarxa recíproca: $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$

$$\mathbf{G} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3 \quad k_i \in \mathbb{Z}$$

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_p} \quad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_p} \quad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_p}$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij} \quad \exp(i\mathbf{G}\cdot\mathbf{R}) = 1$$

$$V_p^* = \frac{(2\pi)^2}{V_p}$$

Funció $n(\mathbf{r})$ amb la peridocitat de la X.D.

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \mathrm{e}^{i\mathbf{G}\cdot\mathbf{r}} \quad n_{\mathbf{G}} = \frac{1}{V_c}\int_C \mathrm{d}V n(\mathbf{r})\exp(-i\mathbf{G}\cdot\mathbf{r})$$

Plans Cristal·lins

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \quad |\mathbf{G}| = \frac{2\pi}{d}$$

Xarxes Cúbiques:

Cúbica simple (sc): 1 nus/cel·la conv. $V = a^3$, 6 1rs. v.

$$\mathbf{a}_i = a\mathbf{e}_i, \quad \mathbf{b}_j = \frac{2\pi}{a}\mathbf{e}_j$$

Cúbica centrada a l'interior (bcc): 2 nusos/cel·la conv. $V_p = a^3/2$, $|a_i| = a\sqrt{3}/2$, $\theta_{ij} = 110°$, 8 1rs. v.

$$\mathbf{a}_1 = \frac{a}{2}(-\mathbf{x}+\mathbf{y}+\mathbf{z}),\ \mathbf{a}_2 = \frac{a}{2}(\mathbf{x}-\mathbf{y}+\mathbf{z}),\ \mathbf{a}_3 = \frac{a}{2}(\mathbf{x}+\mathbf{y}-\mathbf{z})$$

$$\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}),\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{z}),\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y})$$

Cúbica centrada a les cares (fcc): 4 nusos/cel·la conv. $V_p = a^3/4$, $|a_i| = a\sqrt{2}/2$, $\theta_{ij} = 60°$, 12 1rs. v.

$$\mathbf{a}_1 = \frac{a}{2}(\mathbf{y}+\mathbf{z}),\ \mathbf{a}_2 = \frac{a}{2}(\mathbf{x}+\mathbf{z}),\ \mathbf{a}_3 = \frac{a}{2}(\mathbf{x}+\mathbf{y})$$

$$\mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x}+\mathbf{y}+\mathbf{z}),\ \mathbf{a}_2 = \frac{2\pi}{a}(\mathbf{x}-\mathbf{y}+\mathbf{z}),\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}-\mathbf{z})$$

Altres xarxes:

Hexagonal: $V_p = a^2c\sqrt{3}/2$

$$\mathbf{a}_1 = a\mathbf{x},\ \mathbf{a}_2 = \frac{a}{2}(\mathbf{x}+\sqrt{3}\mathbf{y}),\ \mathbf{a}_3 = c\mathbf{z}$$

$$\mathbf{b}_1 = \frac{2\pi}{a\sqrt{3}}(-\mathbf{y}+\sqrt{3}\mathbf{x}),\ \mathbf{b}_2 = \frac{4\pi}{a\sqrt{3}}\mathbf{y},\ \mathbf{b}_3 = \frac{2\pi}{c}\mathbf{z}$$

$$d = \frac{a}{\sqrt{\frac{3}{3}\left(h^2+k^2-4k\right)+\frac{a^2}{c^2}l^2}}$$

Base 2 àtoms:

$$\mathbf{r}_1 = \mathbf{0} \quad \mathbf{r}_2 = \frac{\mathbf{a}_1+\mathbf{a}_2}{3} + \frac{\mathbf{a}_3}{2}$$

II. Difracció Elàstica

Llei de Bragg

$$2d\sin\theta = n\lambda$$

Amplitud de dispersió:

$$F = \int_V \mathrm{d}V n(\mathbf{r})\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \sum_{\mathbf{G}}\int_V \mathrm{d}V n_{\mathbf{G}}\mathrm{e}^{i(\mathbf{G}-\Delta\mathbf{k})\cdot\mathbf{r}}$$

Condició de difracció:

$$\Delta\mathbf{k} = \mathbf{G}$$

Llei de Laue:

$$2\mathbf{k}\cdot\mathbf{G} = G^2$$

Factor d'estructura i de forma atòmica

$$S_{\mathbf{G}} = \int_C \mathrm{d}V n(\mathbf{r})\exp(i\mathbf{G}\cdot\mathbf{r}) = \sum_j \mathrm{e}^{-i\mathbf{G}\cdot\mathbf{r}_j}\int_C \mathrm{d}V n_j(\boldsymbol{\rho})\mathrm{e}^{-i\mathbf{G}\cdot\boldsymbol{\rho}}$$

$$f_j = \int_C \mathrm{d}V n_j(\boldsymbol{\rho})\mathrm{e}^{-i\mathbf{G}\cdot\boldsymbol{\rho}} \qquad S_{\mathbf{G}} = \sum_j f_j \mathrm{e}^{-i\mathbf{G}\cdot\mathbf{r}_j}$$

Exemples:

S.C.

1 sola espècie: $S = f$

2 espècies diferents: $S = f_1 + f_2\exp(-i\pi l)$

2 espècies iguals: $S = f[1+\exp(-i\pi l)]$, ext. si l senar

B.C.C.

1 espècie: $S = f\{1+\exp[-i\pi(h+k+l)]\}$ cal que $h+k+l$ parell.

F.C.C.

1 espècie: cal que índex mateixa paritat

$$S = f\{1+\exp[-i\pi(h+k)]+\exp[-i\pi(h+l)]+\exp[-i\pi(k+l)]\}$$

III. Gas de Fermi. Teorema de Bloch

Gas d'electrons lliures:

$$\psi_{\mathbf{k},s}(\mathbf{r}) = \frac{1}{\sqrt{V}}\exp(i\mathbf{k}\cdot\mathbf{r})\chi_{\frac{1}{2},m_s} \qquad E_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2\mathrm{m}}$$

Dens. espais ocupats en espai **k**:

$$\frac{1 \text{ estat}}{(2\pi/L)^3} = \frac{V}{8\pi^3}$$

Estat fonamental:

$$N = 2\left(\frac{4\pi}{3}k_F^3\right)\left(\frac{V}{8\pi^3}\right) \qquad \rho = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

$$k_F = \left(3\pi^2\frac{N}{V}\right)^{1/3} = (3\pi^2\rho)^{1/3} \quad E_F = \frac{\hbar^2}{2\mathrm{m}}(3\pi^2\rho)^{2/3}$$

$$E_{tot} = 2\int_0^{k_F} E_k N_k \mathrm{d}V_k = 2\int_0^{k_F}\frac{\hbar^2k^2}{2\mathrm{m}}\frac{V}{8\pi^3}4\pi k^2\mathrm{d}k = \frac{3}{5}NE_F$$

Estats excitats:

$$f(E,T) = \frac{1}{\exp\left[\frac{E-\mu}{k_BT}\right]+1} \qquad \mu \approx E_F\left[1-\frac{1}{3}\left(\frac{\pi k_B T}{2E_F}\right)^2\right]$$

Densitat d'estats $D(E)$:

$$\mathrm{d}N = \left(\frac{V}{2\pi^2}\right)\left(\frac{2\mathrm{m}}{\hbar^2}\right)^{3/2} E^{1/2}\mathrm{d}E$$

$$D(E) = \left(\frac{V}{2\pi^2}\right)\left(\frac{2\mathrm{m}}{\hbar^2}\right) E^{1/2} = \frac{3}{2}\frac{N}{E}$$

$$D(E)\mathrm{d}E = D(k)\mathrm{d}k = \frac{V}{4\pi^3}\mathrm{d}V_k = \frac{V}{\pi^2}k^2\mathrm{d}k$$

Número de partícules:

$$N = \int_0^\infty \mathrm{d}E D(E) f(E)$$

Energia interna i capacitat calorífica:

$$U = \int_0^\infty \mathrm{d}E E D(E) f(E)$$

$$\Delta U = \int_0^\infty \mathrm{d}E E D(E) f(E) - \frac{3}{5}NE_F \approx \frac{\pi^2}{6}(k_BT)^2 D(E_F)$$

$$C = \frac{\mathrm{d}(\Delta U)}{\mathrm{d}T} = \frac{\pi^2}{3}k_B T^2 D(E_F) = \frac{\pi^2}{2}\left(\frac{k_BT}{E_F}\right)Nk_B$$

Teorema de Bloch

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}}\exp(i\mathbf{G}\cdot\mathbf{r}) \quad V_{\mathbf{G}} = \frac{1}{V_c}\int_C \mathrm{d}\mathbf{r} V(\mathbf{r})\exp(-i\mathbf{G}\cdot\mathbf{r})$$

$$\phi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}}\mathrm{e}^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}}$$

$$\left[\frac{\hbar^2|\mathbf{k}-\mathbf{G}|^2}{2\mathrm{m}} - E_{\mathbf{k}}\right]C_{\mathbf{k}-\mathbf{G}} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}}C_{\mathbf{k}-\mathbf{G}} = 0$$

IV. Conseqüències del Teorema de Bloch

Model de Xarxa Buida:

$$V_{\mathbf{G}} = 0 \qquad \phi_{\mathbf{k}}(\mathbf{r}) = C_{\mathbf{k}-\mathbf{G}}\mathrm{e}^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} \quad E_{\mathbf{k}-\mathbf{G}} = \frac{\hbar^2}{2\mathrm{m}}|\mathbf{k}-\mathbf{G}|^2$$

Electrons quasilliures:

$$\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}}\mathrm{e}^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} \qquad k^2 \approx |\mathbf{k}-\mathbf{G}|^2$$

No degenerat:

$$\phi_{\mathbf{k}}(\mathbf{r}) = C_{\mathbf{k}-\mathbf{G}}\mathrm{e}^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}}$$

$$E(\mathbf{k}-\mathbf{G}) = \frac{\hbar^2}{2\mathrm{m}}|\mathbf{k}-\mathbf{G}|^2 + V_0 + \sum_{\mathbf{G}''\neq 0}\frac{|V_{\mathbf{G}''}|^2}{\frac{\hbar^2}{2\mathrm{m}}|\mathbf{k}-\mathbf{G}|^2 - \frac{\hbar^2}{2\mathrm{m}}|\mathbf{k}-\mathbf{G}-\mathbf{G}''|^2}$$

Degenerat (x2):

$$E_\pm = \frac{\hbar^2}{2\mathrm{m}}|\mathbf{k}-\mathbf{G}|^2 \pm |V_{\mathbf{G}'}|$$

Electrons fortament lligats:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_j \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_j}\Omega(\mathbf{r}-\mathbf{r}_j)$$

Bandes:

$$E(\mathbf{k}) = E_0 - \alpha - \gamma\sum_m \mathrm{e}^{i\mathbf{k}\cdot\boldsymbol{\rho}_m}$$

Superfície de Fermi:

$$E_n(\mathbf{k}) = E_F$$

2n orbitals per banda.

VI. Dinàmica dels Electrons de Bloch

Model semiclàssic
Velocitat de grup

$$\mathbf{v}_n(\mathbf{k}) = \left.\frac{1}{\hbar}\boldsymbol{\nabla}_{\mathbf{k}}E_n(\mathbf{k})\right|_{\mathbf{k}=\mathbf{k}_0}$$

Eq. moviment espai de vectors d'ona:

$$\mathbf{F} = \hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}$$

Evolució temporal en presència de camps:

$$\hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = -e[\boldsymbol{\mathcal{E}} + \mathbf{v}_n(\mathbf{k})\times\boldsymbol{\mathcal{B}}]$$

Corrent elèctric

$$\mathbf{j}_e = -e\mathbf{v}_e(\mathbf{k}_e)$$

Massa efectiva

$$a_i = \frac{1}{\hbar^2}\sum_{j=1}^{3}\frac{\partial^2 E}{\partial k_i \partial k_j}F_j \qquad \left(\frac{1}{\mathrm{m}^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

$$\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \left(\frac{\mathbf{1}}{\mathrm{m}^*}\right)\mathbf{F}$$

VII. Moviment dels ions. Fonons

1D; base monoatòmica

$$V = \sum_s \frac{C}{2}(u_{s+1}-u_s)^2 \quad F_s = -\frac{\partial V}{\partial u_s} = C[u_{s+1}+u_{s-1}-2u_s]$$

$$u_s(x,t) = u\mathrm{e}^{i(kx-\omega t)} = u\mathrm{e}^{i(ksa-\omega t)} \qquad \omega = \sqrt{\frac{4C}{\mathrm{m}}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Solució general i velocitat de grup:

$$u_s(x,t) = \sum_k A_k\mathrm{e}^{i(ksa-\omega_k t)} \quad v_g = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} = a\sqrt{\frac{C}{\mathrm{m}}}\cos\left(\frac{ka}{2}\right)$$

Velocitat de fase, velocitat del sol i $\omega_{\max}$:

$$v_f = \left.\frac{\omega}{k}\right|_{k\to 0} a\sqrt{\frac{C}{\mathrm{m}}}, \quad v_{\mathrm{so}} = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k\to 0} = a\sqrt{\frac{C}{\mathrm{m}}}, \quad \omega_{\max} = \sqrt{\frac{4C}{\mathrm{m}}} = \frac{2v_{\mathrm{so}}}{a}$$

D branques acústiques, $Dp - D$ branques òptiques.

1D; base diatòmica

$$F_{us} = C[v_s + v_{s-1} - 2u_s] \quad F_{vs} = C[u_s + u_{s-1} - 2v_s]$$

$$\omega^2 = C\left(\frac{\mathrm{m}+M}{\mathrm{m}M} \pm \left[\left(\frac{\mathrm{m}+M}{\mathrm{m}M}\right)^2 - \frac{2(2-\cos ka)}{\mathrm{m}M}\right]^{1/2}\right)$$

ω_+ : branca òptica, ω_- : branca acústica
$k \to 0$

$$\omega_+(k) \approx \sqrt{2C}\left(\frac{\mathrm{m}+M}{\mathrm{m}M}\right)^{1/2} \qquad \omega_-(k) \approx \left(\frac{C/2}{\mathrm{m}+M}\right)^{1/2} ka$$

$k \to \pm\pi/a$

$$\omega_+ = \sqrt{\frac{2C}{\mathrm{m}}} \qquad \omega_- = \sqrt{\frac{2C}{M}}$$

3D, base monoatòmica

$$F_{s,\alpha} = -\sum_r \sum_\beta \phi_{\alpha\beta}(s,r) u_{r,\beta} \quad \alpha, \beta \in \{x, y, z\}$$

$$\phi_{\alpha,\beta} = \frac{\partial^2 V}{\partial u_{s,\alpha} \partial u_{r,\beta}} \quad m_s \frac{\mathrm{d}^2 u_{s,\alpha}}{\mathrm{d}t^2} = -\sum_r \sum_\beta \phi_{\alpha\beta}(s,r) u_{r,\beta}$$

$$\det[\phi_{\alpha\beta}(s,r) - m_r \omega^2 \delta_{sr} \delta_{\alpha\beta}] = 0 \quad \mathbf{u}_s(t) = \mathbf{A}\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{R}_s - \omega t)}$$

A. Relacions Útils

$$\sin(x) \approx x - \frac{x^3}{3!} \qquad \cos(x) \approx 1 - \frac{x^2}{2}$$

$$\sin\left(\frac{\pi}{2} + x\right) = \cos(x) \quad \cos\left(\frac{\pi}{2} + x\right) = -\sin(x)$$

$$\sin(\alpha + \beta) = \sin\alpha\cos\beta + \cos\alpha\sin\beta$$

$$\cos(\alpha + \beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta$$

$$\sin(\alpha - \beta) = \sin\alpha\cos\beta - \cos\alpha\sin\beta$$

$$\cos(\alpha - \beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$$

$$\sin(2\alpha) = 2\sin\alpha\cos\alpha \quad \cos(2\alpha) = \cos^2\alpha - \sin^2\alpha$$

$$\sin^2(\alpha) = \frac{1}{2}[1 - \cos(2\alpha)] \quad \cos^2(\alpha) = \frac{1}{2}[1 + \cos(2\alpha)]$$

$$\sin\alpha + \sin\beta = 2\sin\frac{\alpha+\beta}{2}\cos\frac{\alpha-\beta}{2}$$

$$\sin\alpha - \sin\beta = 2\cos\frac{\alpha+\beta}{2}\sin\frac{\alpha-\beta}{2}$$

$$\cos\alpha + \cos\beta = 2\cos\frac{\alpha+\beta}{2}\cos\frac{\alpha-\beta}{2}$$

$$\cos\alpha - \cos\beta = 2\sin\frac{\alpha+\beta}{2}\sin\frac{\alpha-\beta}{2}$$

$$\sin\alpha\sin\beta = \frac{1}{2}[\cos(\alpha-\beta) - \cos(\alpha+\beta)]$$

$$\cos\alpha\cos\beta = \frac{1}{2}[\cos(\alpha-\beta) + \cos(\alpha+\beta)]$$

$$\sin\alpha\cos\beta = \frac{1}{2}[\sin(\alpha-\beta) + \sin(\alpha+\beta)]$$

$$\frac{\hbar^2}{2\mathrm{m_e}} 4\pi^2 \approx 150 \text{ eVÅ}^2$$

$$x^2 - 2jx + c^2 = 0 \quad \to \quad x_\pm \approx j\left[1 \pm \sqrt{1 - \frac{c}{j^2}}\right]$$