FORMULARI ESTAT SÒLID

CS (a)	$\vec{a}_1=a\,\hat{i}\,;\,\vec{a}_2=a\,\hat{j}\,;\,\vec{a}_3=a\,\hat{k}$	$\vec{b}_1=\frac{2\pi}{a}\hat{i}\,;\vec{b}_2=\frac{2\pi}{a}\hat{j}\,;\vec{b}_3=\frac{2\pi}{a}\hat{k}$
BCC (a)	$\vec{a}_1=\frac{a}{2}\left(-\hat{i}+\hat{j}+\hat{k}\right);\vec{a}_2=\frac{a}{2}\left(\hat{i}-\hat{j}+\hat{k}\right)$ $\vec{a}_3=\frac{a}{2}\left(\hat{i}+\hat{j}-\hat{k}\right)$	$\vec{b}_1=\frac{2\pi}{a}\left(\hat{j}+\hat{k}\right);\vec{b}_2=\frac{2\pi}{a}\left(\hat{i}+\hat{k}\right);\vec{b}_3=\frac{2\pi}{a}\left(\hat{i}+\hat{j}\right)$
FCC (a)	$\vec{a}_1=\frac{a}{2}\left(\hat{j}+\hat{k}\right);\vec{a}_2=\frac{a}{2}\left(\hat{i}+\hat{k}\right);\vec{a}_3=\frac{a}{2}\left(\hat{i}+\hat{j}\right)$	$\vec{b}_1=\frac{2\pi}{a}\left(-\hat{i}+\hat{j}+\hat{k}\right);\vec{b}_2=\frac{2\pi}{a}\left(\hat{i}-\hat{j}+\hat{k}\right)$ $\vec{b}_3=\frac{2\pi}{a}\left(\hat{i}+\hat{j}-\hat{k}\right)$
Hexagonal (a,c)	$\vec{a}_1=a\,\hat{i}\,;\,\vec{a}_2=\frac{a}{2}\left(\hat{i}+\sqrt{3}\,\hat{j}\right);\vec{a}_3=c\,\hat{k}$	$\vec{b}_1=\frac{2\pi}{a}\left(\hat{i}-\frac{1}{\sqrt{3}}\hat{j}\right);\vec{b}_2=\frac{4\pi}{\sqrt{3}\,a}\hat{j}\,;\vec{b}_3=\frac{2\pi}{c}\hat{k}$

$$\vec{R}=n_i\vec{a}_i\,;\,\vec{G}=h\vec{b}_1+k\,\vec{b}_2+l\,\vec{b}_3 \qquad \vec{b}_i\cdot\vec{a}_j=2\pi\,\delta_{ij} \qquad e^{i\vec{G}\cdot\vec{R}}=1$$

Estructura cristal·lina	Xarxa Bravais	Base atòmica	Factor estructura
Diamant	FCC	$\vec{r}_1=(0,0,0)_{c.s.};\vec{r}_2=(1/4,1/4,1/4)_{c.s}$	$S_{\text{diamant}}=S_{fcc}\cdot\left[1+e^{-i\frac{\pi}{2}(h+k+l)}\right]$
CsCl	CS	$\vec{r}_{Cs^+}=(0,0,0)_{c.s}$ $\vec{r}_{Cl^-}=(1/2,1/2,1/2)_{c.s}$	$S=f_1+f_2\,e^{-i\pi(h+k+l)}$
NaCl	FCC	$\vec{r}_{Na^+}=(1/2,1/2,1/2)_{c.s}$ $\vec{r}_{Cl^-}=(0,0,0)_{c.s}$	$S=S_{fcc}\cdot\left[f_1+f_2\,e^{-i\pi(h+k+l)}\right]$
Zinc Blenda	FCC	$\vec{r}_{Zn^+}=(0,0,0)_{c.s}$ $\vec{r}_{S^-}=(1/4,1/4,1/4)_{c.s}$	$S=S_{fcc}\cdot\left[f_{Zn}+f_S\,e^{-i\frac{\pi}{2}(h+k+l)}\right]$
"FCC"	CS	$\vec{r}_1=(0,0,0)_{c.s.};\vec{r}_2=(0,1/2,1/2)_{c.s}$ $\vec{r}_3=(1/2,0,1/2)_{c.s};\vec{r}_4=(1/2,1/2,0)_{c.s}$	$S_{fcc}=f\cdot\left[1+e^{-i\pi(h+k)}+e^{-i\pi(h+l)}+e^{-i\pi(k+l)}\right]$
"BCC"	CS	$\vec{r}_1=(0,0,0)_{c.s};\vec{r}_2=(1/2,1/2,1/2)_{c.s}$	$S_{bcc}=f\left[1+e^{-i\pi(h+k+l)}\right]$

$$\boxed{\vec{k}\cdot\left(\frac{1}{2}\vec{G}\right)=\left(\frac{1}{2}\vec{G}\right)^2\Rightarrow 2\mathrm{d}\sin\theta=n\lambda} \qquad d=\frac{2\pi}{|\vec{G}|} \qquad I=\text{degen.}\left|S^2\right|$$

$$F=N\int_{\text{cel·la}}dV\,n(\vec{r})\,e^{-i\vec{G}\cdot\vec{r}}=N\cdot S_G \qquad \boxed{S_{\vec{G}}=\sum_j f_j\,e^{-i\vec{G}\,\vec{r}_j}} \qquad f_j=\int_{\text{cel·la}}dV\,n_j(\vec{\rho})\,e^{-i\vec{G}\cdot\vec{\rho}}$$

Gas e- lliures: $\psi_{\vec{k},s}=\frac{1}{V}e^{i\vec{k}\vec{r}}\chi_{1/2\,m_s}$ $\qquad E_{\vec{k}}=\frac{\hbar^2k^2}{2m}$ $\qquad k_i=\frac{2\pi}{L}n_i$ $\qquad D(k)=\frac{1\,estat}{\left(\frac{2\pi}{L}\right)^{\text{dimensió}}}$

$$N_{1D}=k_F\cdot 2_{(\text{spin})}\cdot D(k)$$
$$N_{2D}=(\pi k_F^2)\,2_{(\text{spin})}\cdot D(k)$$
$$N_{3D}=\frac{4\pi k_F^3}{3}\,2_{(\text{spin})}\cdot D(k)$$

$$D(E)=\frac{dN}{dk}\cdot\frac{dk}{dE} \qquad D_{3D}(E)=\left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\hbar^2}\right)^{3/2}E^{1/2} \quad \text{(densitat d'estats monoparticulars)} \qquad E_F=\frac{\hbar^2}{2\mathrm{m}}\left(3\pi^2\rho\right)^{2/3}$$

$$\rho=\frac{N}{V} \qquad N=\int_0^\infty D(E)\,f(E)\,dE \qquad U=\int_0^\infty D(E)\,f(E)\,E\,dE \qquad \Delta U\approx\frac{\pi^2}{6}\left(k_BT\right)^2D(E_F) \qquad C=\frac{\pi^2}{2}\left(k_B\frac{T}{E_F}\right)N\,k_B$$

$$f_0=\frac{1}{e^{\frac{E-\mu}{k_Bt}}+1} \qquad \mu\approx E_F\left[1-\frac{1}{3}\left(\frac{\pi k_BT}{2E_F}\right)^2\right]$$

Sòlid: $\phi_{\vec{k}}(\vec{r})=\sum_{\vec{G}}C_{\vec{k}-\vec{G}}\,e^{i(\vec{k}-\vec{G})\vec{r}}$ $\qquad$ Eq. Central: $\boxed{\left[\frac{\hbar^2|\vec{k}-\vec{G}|^2}{2m}-E_{\vec{k}}\right]C_{\vec{k}-\vec{G}}+\sum_{\vec{G}''}V_{\vec{G}''-\vec{G}}\,C_{\vec{k}-\vec{G}''}=0}$

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Xarxa buida: $\boxed{E_{\vec{k}-\vec{G}}=\frac{\hbar^2}{2m}|\vec{k}-\vec{G}|^2}$ *Fortament lligats* (LCAO): $E(\vec{k})=E_0-\alpha-\gamma\sum_m e^{i\vec{l}\cdot\vec{\rho}_m}$

Feblement lligats: No degen. $E_{\vec{k}-\vec{G}}=\frac{\hbar^2}{2m}|\vec{k}-\vec{G}|^2+V_0+\frac{\sum_{\vec{G}''\neq 0}|V_{\vec{G}''}|^2}{\frac{\hbar^2}{2m}|\vec{k}-\vec{G}|^2-\frac{\hbar^2}{2m}|\vec{k}-\vec{G}-\vec{G}''|^2}$

Quasi degen: $E_{\pm}=\frac{E^0_{\vec{k}-\vec{G}}+E^0_{\vec{k}-\vec{G}-\vec{G}'}}{2}\pm\sqrt{\left(\frac{E^0_{\vec{k}-\vec{G}}-E^0_{\vec{k}-\vec{G}-\vec{G}'}}{2}\right)^2+|V_{\vec{G}'}|^2}$ Degenerat: $E_{\pm}=\frac{\hbar^2}{2m}|\vec{k}-\vec{G}|^2\pm|V_{\vec{G}}'|$ (1 pla bisector, $V_0=0$)

<u>Propietats de transport:</u>

$$\left[\frac{-\hbar^2}{2\text{m}}\nabla^2+V(\vec{r})\right]\phi_{n\vec{k}}(\vec{r})=E_n(\vec{k})\phi_{n\vec{k}}(r)\quad\Rightarrow\quad\phi_n(\vec{r},t)=\sum_{\vec{k}}g(\vec{k})\phi_{n\vec{k}}(r)e^{-iE_n(\vec{k})\frac{t}{\hbar}}$$

$$\boxed{\vec{v}_n(\vec{k})=\frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E_n(\vec{k})\Big|_{\vec{k}=\vec{k}_0}}\qquad\vec{F}=\hbar\frac{d\vec{k}}{dt}\qquad\vec{F}=-e[\vec{\epsilon}+\vec{v}\times\vec{B}]\qquad\left(\frac{1}{m^*}\right)_{ij}=\frac{1}{\hbar^2}\frac{\partial^2E}{\partial k_i\partial k_j}\qquad a_i=\left(\frac{1}{m^*}\right)_{ij}F_j$$

$\frac{\partial f}{\partial t}+\vec{v}\cdot\vec{\nabla}_{\vec{r}}f+\frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_{\vec{k}}f=\left(\frac{\partial f}{\partial t}\right)_{col}$ (estacionari, t relaxació) $\approx\Rightarrow f=f_0-\tau\vec{v}\cdot\vec{\nabla}_{\vec{r}}f-\tau\frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_{\vec{k}}f$

(homogeni, linealització) $f(\vec{k})\approx f_0(\vec{k})-\tau(\vec{k})\frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_{\vec{k}}f_0(\vec{k})$ (no val per camps magnètics)

$\vec{J}=-\frac{e}{V}\sum_{\vec{k}}f(\vec{k})\vec{v}(\vec{k})\qquad\sigma_{ij}=\frac{-e^2}{V}\sum_{\vec{k}}\tau(\vec{k})\frac{\partial f_0}{\partial E}v_iv_j$, metalls: $J_x=e^2\frac{\epsilon}{3\text{V}}\tau(k_F)v^2(k_F)D(E_F)$ $\quad\sigma=\frac{e^2\tau_Fn}{m^*}$

$$\vec{F}=-e[\vec{\epsilon}+\vec{v}\times\vec{B}]\Rightarrow f(\vec{k})=f_0(\vec{k})+\frac{e\tau}{1+\omega_c^2\tau^2}\frac{\partial f_0}{\partial E}\vec{v}\cdot\left[\vec{\epsilon}-\frac{e\tau}{m^*}(\vec{\epsilon}\times\vec{B})\right]\qquad\omega_c=\frac{eB}{m^*}$$

$\vec{J}=\sigma_0\vec{A}\qquad\vec{A}=\frac{e\tau}{1+\omega_c^2\tau^2}\left[\vec{\epsilon}-\frac{e\tau}{m^*}(\vec{\epsilon}\times\vec{B})\right]\qquad\frac{1}{\tau}=\frac{1}{\tau_{xarxa}}+\frac{1}{\tau_{impureses}}$ Efecte Hall: $R_H=\frac{-e\tau}{m^*\sigma_0}=-\frac{1}{ne}$

<u>Moviment dels ions:</u> $V=\sum_s\frac{C}{2}(u_{s+1}-u_s)^2\qquad m\frac{d^2u_s}{dt^2}=C[u_{s+1}+u_{s-1}-2\text{u}_s]\qquad u_s(x,t)=Ae^{i(kx-\omega t)}$

$$\omega=\sqrt{\frac{4\text{C}}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|\qquad v_g=\frac{d\omega}{dk}=a\sqrt{\frac{C}{m}}\cos\left(\frac{ka}{2}\right)\qquad\omega_{\text{màx}}=\frac{2v_{so}}{a}\qquad v_{so}=\frac{d\omega}{dk}\Big|_{\vec{k}\to\vec{0}}=a\sqrt{\frac{C}{m}}$$

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

En 3D: $F_{s,\alpha}=-\sum_r\sum_\beta\phi_{\alpha\beta}(s,r)u_{r,\beta}\qquad\phi_{\alpha\beta}=\frac{\partial^2V}{\partial u_{s,\alpha}\partial u_{r,\beta}}\qquad m_s\ddot{u}_{s,\alpha}=-\sum_r\sum_\beta\phi_{\alpha\beta}(s,r)u_{r,\beta}$

$$Det[\phi_{\alpha\beta}(s,r)-m_s\omega^2\delta_{sr}\delta_{\alpha\beta}]=0$$

<u>Fonons:</u> $H=\frac{p^2}{2\text{m}}+\frac{1}{2}kx^2=\hbar\omega(N+\frac{1}{2})\qquad\langle n_{\vec{k}s}\rangle=\frac{\sum_{n=0}^{\infty}ne^{-n\hbar\omega_s(\vec{k})/k_BT}}{\sum_{n=0}^{\infty}e^{-n\hbar\omega_s(\vec{k})/k_BT}}=\frac{1}{e^{\hbar\omega_s(\vec{k})/k_BT}-1}$

$$\langle E_{\vec{k}s}\rangle=\langle n_{\vec{k}s}\rangle\hbar\omega_s(\vec{k})=\frac{\hbar\omega_s(\vec{k})}{e^{\hbar\omega_s(\vec{k})/k_BT}-1}\qquad N=\frac{V}{6\pi^2}k^3\qquad D_s(\omega)=\frac{dN}{d\omega}=\left(\frac{Vk^2}{2\pi^2}\right)\frac{dk}{d\omega}\ -$$

$$U=\sum_{p\ branques}\int d\omega D_p(\omega)\left(\frac{1}{2}+\frac{1}{e^{\hbar\omega/k_BT}-1}\right)\hbar\omega\qquad C_{\text{xarxa}}=k_B\sum_s\int d\omega D_s(\omega)\frac{x^2e^x}{(e^x-1)^2}\qquad x=\frac{\hbar\omega}{k_BT}$$

Debye: $\omega=v_sk\qquad D(\omega)=\frac{V\omega^2}{2\pi^2v_s^3}\qquad\omega_D=\left(\frac{6\pi^2v_s^3N}{V}\right)^{1/3}\qquad\theta_D=\frac{\hbar\omega_D}{k_B}\qquad C=9\text{Nk}_B\left(\frac{T}{\theta_D}\right)^3\int_0^{x_D}\frac{x^4e^x}{(e^x-1)^2}dx$

Einstein: $\omega=\omega_E\qquad D(\omega)=3N\delta(\omega-\omega_E)\qquad\theta_E=\frac{\hbar\omega_E}{k_B}\qquad C=3\text{Nk}_B\frac{e^{\theta_E/T}}{(e^{\theta_E/T}-1)^2}\left(\frac{\theta_E}{T}\right)^2$