



Kondenzált anyagok fizikája

Rácsrezgések

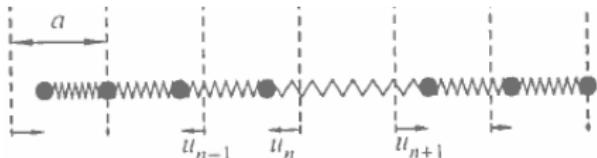
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ELTE

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Lineáris lánc



$$M\ddot{u}_n = D[u_{n+1} - u_n + u_{n-1} - u_n]$$

$$M\ddot{u}_n = -D[2u_n - u_{n+1} - u_{n-1}]$$

Keressük a megoldást

$$u_n = A_n e^{i\omega t}$$

alakban. Ekkor

$$\omega^2 A_n = \omega_0^2 [2A_n - A_{n+1} - A_{n-1}]$$

$$\omega_0^2 = \frac{D}{M}$$

Lineáris lánc

$$\omega^2 \begin{pmatrix} A_1 \\ A_2 \\ \cdot \\ \cdot \\ A_N \end{pmatrix} = \omega_0^2 \begin{pmatrix} 2 & -1 & \cdot & \cdot & ? \\ -1 & 2 & -1 & & \\ \cdot & \cdot & \cdot & & \\ ? & \cdot & \cdot & -1 & 2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \cdot \\ \cdot \\ A_N \end{pmatrix}$$

Periodikus határfeltétel

$$u_{N+1} = u_1$$

$$\omega^2 \begin{pmatrix} A_1 \\ A_2 \\ \cdot \\ \cdot \\ A_N \end{pmatrix} = \omega_0^2 \begin{pmatrix} 2 & -1 & \cdot & \cdot & -1 \\ -1 & 2 & -1 & & \\ \cdot & \cdot & \cdot & & \\ -1 & \cdot & \cdot & -1 & 2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \cdot \\ \cdot \\ A_N \end{pmatrix}$$



Lineáris lánc

$$A_n = A_q e^{jqan}$$

$$\omega^2 = \omega_0^2 \left[2 - e^{jqa} - e^{-jqa} \right]$$

$$\omega^2 = 2\omega_0^2 [1 - \cos(qa)] = 4\omega_0^2 \sin^2 \left(\frac{qa}{2} \right)$$

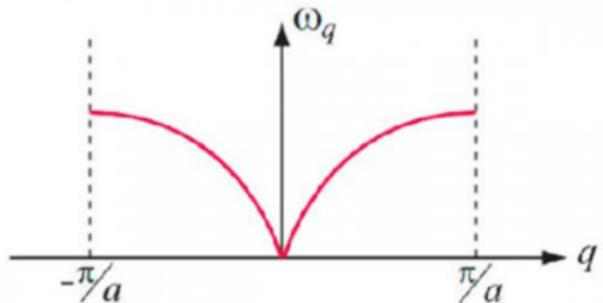
$$\omega = 2\omega_0 \left| \sin \left(\frac{qa}{2} \right) \right|$$

Periodikus határfeltétel miatt

$$1 = e^{jqaN} \longrightarrow q_m = m \frac{2\pi}{Na}$$

Lineáris lánc

Brillouen zóna

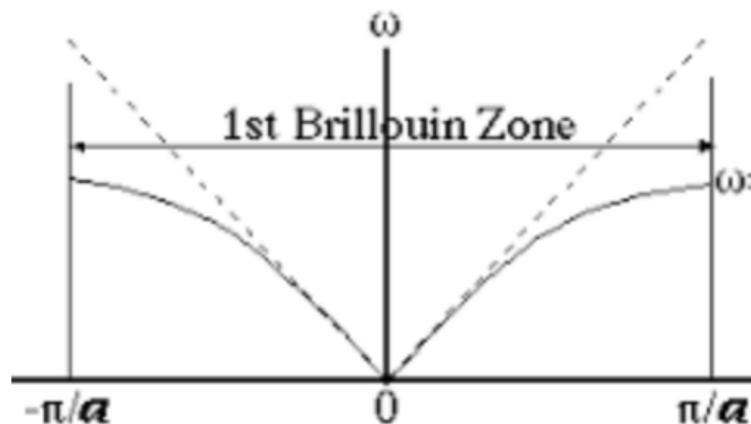


$$M\ddot{u}_n = Da^2 \frac{\frac{u_{n+1}-u_n}{a} - \frac{u_n-u_{n-1}}{a}}{a} \approx Da^2 \frac{\partial^2}{\partial x^2} u_n$$

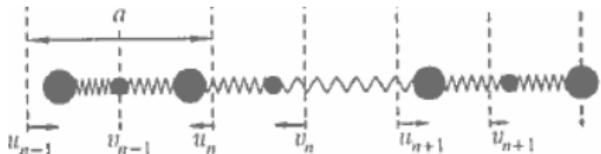
$$M = \rho a A \text{ ill. } E = Da/A$$

$$\rho \frac{\partial^2}{\partial t^2} u(x, t) = E \frac{\partial^2}{\partial x^2} u(x, t)$$

$$u(x, t) = u_0 e^{j(\omega t + qx)} \longrightarrow \omega = \left(\frac{D}{M} \right)^{1/2} a |q| = \omega_0 a |q|$$



Kétatomos lineáris lánc



$$\begin{aligned} M_1 \ddot{u}_n &= -D[2u_n - v_n - v_{n-1}] \\ M_2 \ddot{v}_n &= -D[2v_n - u_{n+1} - u_n] \end{aligned}$$

Határfeltétel

$$u_{N+1} = u_1$$

$$v_{N+1} = v_1$$

Keressük a megoldást

$$\begin{aligned} u_n &= u(q) e^{j(\omega t + qan)} \\ v_n &= v(q) e^{j(\omega t + qan)} \end{aligned}$$

alakban

Kétatomos lineáris lánc

$$\begin{aligned}-\omega^2 M_1 u(q) &= -2Du(q) + D \left(1 + e^{-jq^a}\right) v(q) \\ -\omega^2 M_2 v(q) &= -2Dv(q) + D \left(1 + e^{+jq^a}\right) u(q)\end{aligned}$$

Ekkor

$$\begin{vmatrix} 2D - \omega^2 M_1, & -2De^{-jq\frac{a}{2}} \cos\left(\frac{qa}{2}\right) \\ -2De^{+jq\frac{a}{2}} \cos\left(\frac{qa}{2}\right), & 2D - \omega^2 M_2 \end{vmatrix} = 0$$

Megoldás

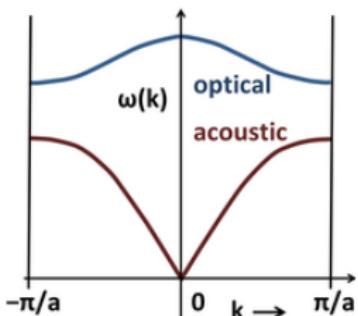
$$\omega_{\pm}^2 = \frac{D}{M_1 M_2} \left\{ (M_1 + M_2) \pm \sqrt{(M_1 + M_2)^2 - 4M_1 M_2 \sin^2\left(\frac{qa}{2}\right)} \right\}$$

Bevezetve

$$\omega_0^2 = 2D \left(\frac{1}{M_1} + \frac{1}{M_2} \right), \quad \gamma^2 = 4 \frac{M_1 M_2}{(M_1 + M_2)^2} \leq 1$$

Kétatomos lineáris lánc

$$\omega_{\pm}^2 = \frac{1}{2}\omega_0^2 \left\{ 1 \pm \sqrt{1 - \gamma^2 \sin^2 \left(\frac{qa}{2} \right)} \right\}$$



$$\omega_{-}(q \rightarrow 0) \approx \frac{1}{2}\omega_0 \gamma a |q|$$

$$\omega_{+}(q \rightarrow 0) \approx \omega_0$$

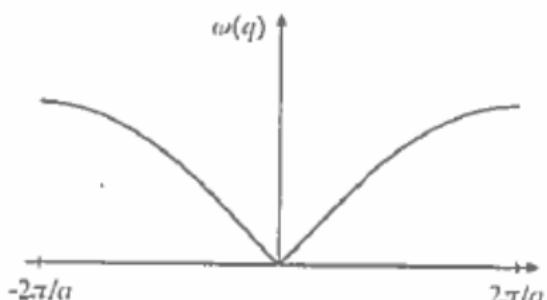
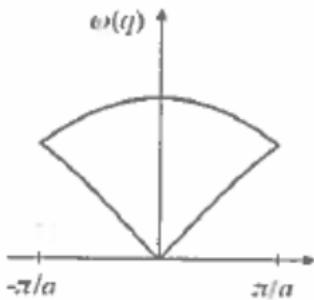
$$\omega_{\pm}^2(q = \pi/a) = \frac{1}{2}\omega_0^2 \left\{ (1 \pm \sqrt{1 - \gamma^2}) \right\}$$

Kétatomos lineáris lánc

Ha $M_1 = M_2$ akkor $\gamma = 1$

$$\omega_{\pm}^2 = \frac{2D}{M} \left[1 \pm \sqrt{1 - \sin^2 \left(\frac{qa}{2} \right)} \right] = \frac{2D}{M} \left[1 \pm \cos \left(\frac{qa}{2} \right) \right]$$

$$\omega_{\pm} = \begin{cases} 2 \left(\frac{D}{M} \right)^{1/2} |\cos(\frac{qa}{4})| \\ 2 \left(\frac{D}{M} \right)^{1/2} |\sin(\frac{qa}{4})| \end{cases}$$



Általános eset

Az atomok koordinátája

$$\underline{r}^\mu(\underline{R}_m, t) = \underline{R}_m + \underline{r}_\mu + \underline{u}^\mu(\underline{R}_m, t)$$

$\mu = 1..p$ ahol p az atomok száma az elemi cellában

A rendszer energiája

$$\Phi = \Phi_0 + \sum_{\substack{m, n \\ \alpha, \beta \\ \mu, \nu}} \frac{1}{2} D_{\alpha, \beta}^{\mu, \nu}(\underline{R}_m, \underline{R}_n) u_\alpha^\mu(\underline{R}_m) u_\beta^\nu(\underline{R}_n)$$

ahol $\alpha, \beta = 1, 2, 3$

Átírható

$$\Phi = \Phi_0 - \sum_{\substack{m, n \\ \alpha, \beta \\ \mu, \nu}} \frac{1}{4} D_{\alpha, \beta}^{\mu, \nu}(\underline{R}_m, \underline{R}_n) [u_\alpha^\mu(\underline{R}_m) - u_\alpha^\nu(\underline{R}_n)][u_\beta^\mu(\underline{R}_m) - u_\beta^\nu(\underline{R}_n)]$$

Általános eset

Az erő

$$F_\alpha^\mu(\underline{R}_m) = - \sum_{n,\nu,\beta} D_{\alpha,\beta}^{\mu,\nu}(\underline{R}_m, \underline{R}_n) u_\beta^\nu(\underline{R}_n)$$

Ha $\underline{u} = \text{const}$, akkor $F = 0$ (merev test szerű eltolás), így

$$\sum_{n,\nu} D_{\alpha,\beta}^{\mu,\nu}(\underline{R}_m, \underline{R}_n) = 0$$

Mozgás egyenlet a periodikus rendszerre

$$M_\mu \ddot{u}_\alpha^\mu(\underline{R}_m) = - \sum_{n,\nu,\beta} D_{\alpha,\beta}^{\mu\nu}(\underline{R}_m - \underline{R}_n) u_\beta^\nu(\underline{R}_n)$$

Keressük a megoldást

$$u_\alpha^\mu(\underline{R}_m) = \frac{1}{\sqrt{M_\mu}} e^{j\omega t} e^{jq\underline{R}_m} u_\alpha^\mu(\underline{q})$$

alakban

Általános eset

Behelyettesítve

$$\omega^2 \sqrt{M_\mu} e^{j\omega t} e^{j\underline{q}\underline{R}_m} u_\alpha^\mu(\underline{q}) = \sum_{n,\nu,\beta} D_{\alpha,\beta}^{\mu\nu} (\underline{R}_m - \underline{R}_n) \frac{1}{\sqrt{M_\beta}} e^{j\omega t} e^{j\underline{q}\underline{R}_n} u_\beta^\nu(\underline{q})$$

ahonnan

$$\omega^2 u_\alpha^\mu(\underline{q}) = \sum_{\nu,\beta} \bar{D}_{\alpha,\beta}^{\mu\nu}(\underline{q}) u_\beta^\nu(\underline{q})$$

ahol

$$\bar{D}_{\alpha,\beta}^{\mu\nu}(\underline{q}) = \frac{1}{\sqrt{M_\beta M_\alpha}} \sum_n D_{\alpha,\beta}^{\mu\nu}(\underline{R}_n) e^{j\underline{q}\underline{R}_n}$$

Innen

$$\det \left[\bar{D}_{\alpha,\beta}^{\mu\nu}(\underline{q}) - \omega^2 \delta_{\alpha,\beta} \delta_{\mu,\nu} \right] = 0, \quad 3p \times 3p$$

Általános eset

3p sajátérték $\omega_\lambda^2(\underline{q})$, a $e_{\mu,\alpha}^{(\lambda)}(\underline{q})$ 3p dimenziós sajátvektorok

$$\omega_\lambda^2(\underline{q}) = \omega_\lambda^2(-\underline{q})$$

\underline{q} a Brilluen zónában van.

Normál módusok

$$u_\alpha^\mu(\underline{R}_m) = \frac{1}{\sqrt{M_\mu}} \sum_{\underline{q}, \lambda} e_{\mu,\alpha}^{(\lambda)}(\underline{q}) e^{j\underline{q}\underline{R}_m} Q_\lambda(\underline{q}, t)$$

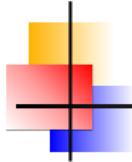
$$\ddot{Q}_\lambda(\underline{q}, t) = -\omega_\lambda^2(\underline{q}) Q_\lambda(\underline{q}, t)$$

Elemi gerjesztés = fonon

$$E = \hbar\omega$$



Kristály fajhője



$$\langle E \rangle = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}, \quad \beta = \frac{1}{k_B T}$$

Állapotösszeg

$$Z = \sum_n e^{-\beta E_n}$$

$$-\frac{d}{d\beta} \ln Z(\beta) = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

Harmonikus oszcillátorra

$$E_n = n\hbar\omega + \frac{\hbar\omega}{2}$$

$$Z = \sum_{n=0}^{\infty} e^{-\beta(n\hbar\omega + \frac{\hbar\omega}{2})} = \frac{e^{-\beta \frac{\hbar\omega}{2}}}{1 - e^{-\beta \hbar\omega}}$$



Kristály fajhője

$$-\frac{d}{d\beta} \ln \left(\frac{e^{-\beta \frac{\hbar\omega}{2}}}{1 - e^{-\beta \hbar\omega}} \right) = \frac{\hbar\omega}{2} + \frac{d}{d\beta} \ln \left(1 - e^{-\beta \hbar\omega} \right)$$

Innen

$$\langle E \rangle = \frac{\hbar\omega}{2} + \hbar\omega \frac{e^{-\beta \hbar\omega}}{1 - e^{-\beta \hbar\omega}}$$

Zéruspont energia elhagyásával

$$\langle E \rangle = \frac{\hbar\omega}{e^{\beta \hbar\omega} - 1}$$

Bose-Einstein eloszlás oszcillátorra

$$n = \frac{1}{e^{\beta \hbar\omega} - 1}$$

Kristály fajhője

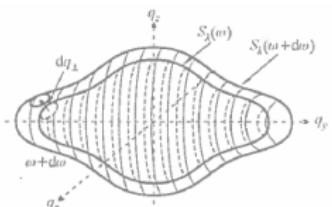
Periodikus határfeltétel $u(\underline{R}_n) = u(\underline{R}_{n+N})$

Állapotsűrűség

$$\triangle^3 q = \left| \frac{\underline{b}_1}{N_1}, \frac{\underline{b}_2}{N_2}, \frac{\underline{b}_3}{N_3} \right| = \frac{v_r}{N} = \frac{(2\pi)^3}{vN} = \frac{(2\pi)^3}{V}$$

$$\frac{1}{V} \sum_{q,\lambda} f(\omega_\lambda(\underline{q})) \approx \sum_\lambda \int \frac{dq^3}{(2\pi)^3} f(\omega_\lambda(\underline{q}))$$

$\omega_\lambda(\underline{q}) = \text{const}$ felületek



$$\Delta V_\omega = g(\omega) d\omega$$

Debye közelítés

$$\frac{1}{V} \sum_{\underline{q}, \lambda} f(\omega_\lambda(\underline{q})) \approx \sum_{\lambda} \int g(\omega_\lambda) f(\omega_\lambda(\underline{q})) d\omega_\lambda$$

Debye feltette, hogy

$$\omega_\lambda(\underline{q}) = c_\lambda |\underline{q}|$$



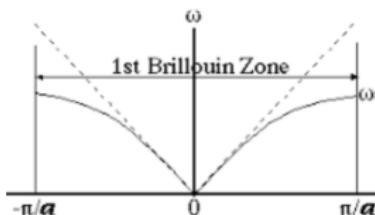
$$\frac{4\pi q^2 dq}{(2\pi)^3}$$

$$g(\omega_\lambda) = \frac{1}{2\pi^2} \frac{1}{c_\lambda^3} \omega_\lambda^2$$

Debye közelítés

3 ág van

$$g(\omega) = \frac{1}{2\pi^2} \left[\frac{1}{c_L^3} + \frac{2}{c_T^3} \right] \omega^2 = \frac{3}{2\pi^2} \frac{\omega^2}{c_D^3}$$



$$\text{Debye frekvencia } \omega_D = c_D q_D$$

ahol

$$\frac{4\pi}{3} q_D^3 = \frac{(2\pi)^3}{v}$$



Debye fajhő



$$\langle E \rangle = V \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} \frac{3}{2\pi^2 c_D^3} d\omega$$

Változó cserével $x = \beta\hbar\omega$

$$\langle E \rangle = V \frac{(k_B T)^4}{\hbar^3} \frac{3}{2\pi^2 c_D^3} \int_0^{\frac{\hbar\omega_D}{k_B T}} \frac{x^3}{e^x - 1} dx$$

Ha $T \rightarrow 0$

$$\langle E \rangle \propto T^4$$

így

$$c_V \propto T^3$$



Debye fajhő

$$T \rightarrow \infty$$

$$\langle E \rangle = V \frac{(k_B T)^4}{\hbar^3} \frac{3}{2\pi^2 c_D^3} \int_0^{\frac{\hbar\omega_D}{k_B T}} x^2 dx = V \frac{(k_B T)^4}{\hbar^3} \frac{1}{2\pi^2 c_D^3} \left(\frac{\hbar\omega_D}{k_B T} \right)^3$$

$$\langle E \rangle = V k_B T \frac{1}{2\pi^2} q_D^3 = V k_B T \frac{1}{2\pi^2} \frac{3}{4\pi} \frac{(2\pi)^3}{v} = 3k_B N T$$

Klasszikus fajhő (Dulong-Petit)

$$c_V = 3k_B N$$

Hőtágulás

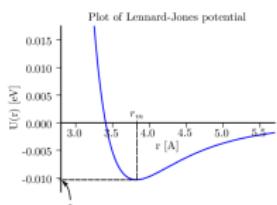
$$\langle u \rangle = \frac{\int_{-\infty}^{\infty} ue^{-\beta\Phi(u)} du}{\int_{-\infty}^{\infty} e^{-\beta\Phi(u)} du}$$

Ha

$$\Phi(u) = \Phi_0 + \frac{D}{2}u^2$$

akkor $\langle u \rangle = 0$

Anharmonicitás



$$\Phi(u) = \Phi_0 + \frac{D}{2}u^2 - \gamma u^3 + \dots$$

Hőtágulás



$$\langle u \rangle = \frac{\int_{-\infty}^{\infty} ue^{-\beta \frac{D}{2} u^2} (1 + \beta \gamma u^3) du}{\int_{-\infty}^{\infty} e^{-\beta \frac{D}{2} u^2} (1 + \beta \gamma u^3) du}$$

Amely

$$\langle u \rangle = \frac{\int_{-\infty}^{\infty} \beta \gamma u^4 e^{-\beta \frac{D}{2} u^2} du}{\int_{-\infty}^{\infty} e^{-\beta \frac{D}{2} u^2} du}$$

Bevezetve

$$x = \sqrt{\beta D / 2} u$$

új változót

$$\langle u \rangle = \frac{\beta \gamma}{(\beta D / 2)^2} \frac{\int_{-\infty}^{\infty} x^4 e^{-x^2} dx}{\int_{-\infty}^{\infty} e^{-x^2} dx} = \frac{\gamma}{D^2} C k_B T$$

$$\alpha = \frac{d \langle u \rangle}{dT} = \gamma C k_B / D^2 = \text{const}$$