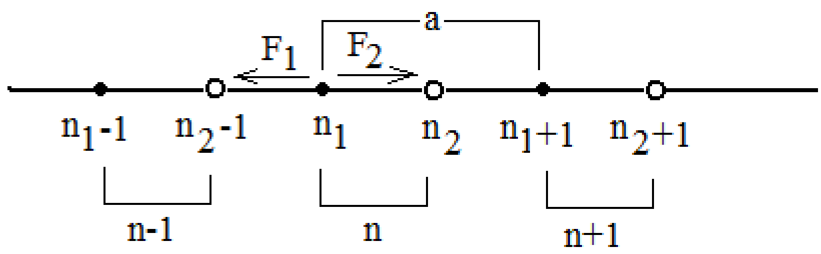
**Curs 7**

❖ **Dinamica structurii lineare cu doi atomi in baza**

- celula elementara copntine doi atomi diferiti, $M_1 \neq M_2;\ M_1 > M_2$;
- fortele de interactie sunt de natura elastica, indiferent de tipul de atomi:

$$F_1 = f\left(u_{n_1} - u_{n_2 - 1}\right)$$

$$F_2 = f\left(u_{n_1} - u_{n_2}\right)$$




Geometria problemei

- Ecuatiile de miscare:

$$M_1 \frac{d^2 u_{n_1}}{dt^2} + f\left(u_{n_1} - u_{n_2 - 1}\right) + f\left(u_{n_1} - u_{n_2}\right) = 0$$

$$M_2 \frac{d^2 u_{n_2}}{dt^2} + f\left(u_{n_2} - u_{n_1}\right) + f\left(u_{n_2} - u_{n_1 + 1}\right) = 0$$

- Cu solutii de forma:

$$u_{n_1} = A_1 e_1 e^{i[qna - \omega t]};\ u_{n_1+1} = A_1 e_1 e^{i[q(n+1)a - \omega t]}$$

$$u_{n_2} = A_2 e_2 e^{i\left[q\left(n+\frac{1}{2}\right)a - \omega t\right]};\ u_{n_2 - 1} = A_2 e_2 e^{i\left[q\left(n-\frac{1}{2}\right)a - \omega t\right]}$$

✓ In cazul particular, amplitudini egale $A_1 = A_2 = A$, aceeasi frecventa de vibratie, directii de polarizare diferite $e_1 \neq e_2$;

- Ecuatiile de miscare devin:

$$-\omega^2 M_1 e_1 + f\left(e_1 - e_2 e^{-i\frac{qa}{2}}\right) + f(e_1 - e_2) = 0$$

$$-\omega^2 M_2 e_2 + f(e_2 - e_1) + f\left(e_2 - e_1 e^{i\frac{qa}{2}}\right) = 0$$

✓ separand dupa directiile de polarizare, nenule:

$$(-\omega^2 M_1 + 2f)e_1 - f\left(1 + e^{-i\frac{qa}{2}}\right)e_2 = 0$$

$$(-\omega^2 M_2 + 2f)e_2 - f\left(1 + e^{i\frac{qa}{2}}\right)e_1 = 0$$

✓ ecuatia seculara a sitemului ecuatiilor de miscare:

$$\begin{vmatrix} (-\omega^2 M_1 + 2f) & -f\left(1 + e^{-i\frac{qa}{2}}\right) \\ -f\left(1 + e^{i\frac{qa}{2}}\right) & (-\omega^2 M_2 + 2f) \end{vmatrix} = 0$$

✓ Conduce la ecuatia bipatratica in $\omega$:

$$\omega^4 - 2f\frac{M_1 + M_2}{M_1 M_2}\omega^2 + \frac{2f^2}{M_1 M_2}2sin^2\frac{qa}{2} = 0$$

✓ se introduc notatiile:

$$\omega_0^2 = 2f\frac{M_1 + M_2}{M_1 M_2};\ \gamma^2 = 4\frac{M_1 M_2}{(M_1 + M_2)^2};\ \frac{2f^2}{M_1 M_2}2 = \frac{\omega_0^4\gamma^2}{4}$$

✓ se obtine ecuatia:

$$\omega^4 - \omega_0^2\omega^2 + \frac{\omega_0^4\gamma^2}{4}sin^2\frac{qa}{2} = 0$$

✓ Cu solutiile $\omega(q)$, reprezentand legile de dispersie ale oscilatiilor:

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

- **Domeniul valorilor lui q:**

✓ din conditia de invarianta la translatie,

$$U(x) = U(x + a)$$

$$1 = e^{iqa};\ qa \in [0,2\pi];\ -\frac{\pi}{a} \le q < \frac{\pi}{a};$$

- ✓ din conditiile de ciclicitate in structura cu $N$celule elementare,

$u_0(t) = u_N(t)$

$1 = e^{iqNa}; \; q = \frac{1}{N}\frac{2\pi}{a}$

***Comentariu asupra dispersiei***

- **la marginile IZB**
- ✓ pentru $q = 0, sin\frac{qa}{2} = 0$,

$\omega_+^2 = \omega_0^2; \; \omega_+ = \omega_0; \; \omega_+ = \omega_{op}(0)$

$\omega_-^2 = 0; \; \omega_- = 0; \; \omega_- = \omega_{ac}(0)$

- ✓ pentru $q = \frac{\pi}{a}, sin\frac{qa}{2} = 1$,

$\omega_+^2 = \frac{\omega_0^2}{2}\left[1 + \sqrt{1-\gamma^2}\right]; \; \omega_+ = \frac{\omega_0}{\sqrt{2}}\sqrt{1 + \sqrt{1-\gamma^2}}; \; \omega_+ = \omega_{op}(\frac{\pi}{a})$

$\omega_-^2 = \frac{\omega_0^2}{2}\left[1 - \sqrt{1-\gamma^2}\right]; \; \omega_- = \frac{\omega_0}{\sqrt{2}}\sqrt{1 - \sqrt{1-\gamma^2}}; \; \omega_- = \omega_{ac}(\frac{\pi}{a})$

- ✓ ***De remarcat ordonarea*** $\boldsymbol{\omega_{op}(0) > \omega_{op}\left(\frac{\pi}{a}\right) > \omega_{ac}\left(\frac{\pi}{a}\right) > \omega_{ac}(0)}$

***Justificarea definitiilor*** $\boldsymbol{\omega_+ = \omega_{op}}$ ***(oscilatii optice) si*** $\boldsymbol{\omega_- = \omega_{ac}}$ ***(oscilatii acustice): particularitatile miscarii de oscilatie:***

§ **oscilatii optice (fononi optici)**

- ✓ $q = 0, q = \frac{2\pi}{\lambda_{oscilatie}}; \; \lambda_{oscilatie} \to \infty$; substituim $\omega = \omega_0 = \omega_{op}(0)$ in una din ecuatiile de miscare care contin directiile de polarizare (de oscilatie):

$(-\omega_0^2 M_1 + 2f)e_1 - 2fe_2 = 0$

$(-\omega_0^2 M_2 + 2f)e_2 - fe_1 = 0$

$\left(-2f\frac{M_1 + M_2}{M_1 M_2}M_1 + 2f\right)e_1 = 2fe_2$

$$\frac{M_1}{M_2} = -\frac{e_2}{e_1} < 0$$

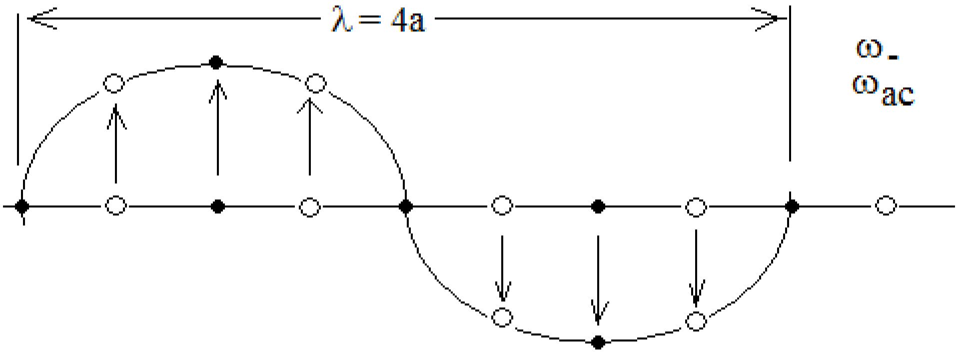
- in cadrul oscilatiilor optice, atomii de tip diferit oscileaza in opozitie de faza in unda cu $\lambda_{oscilatie} \to \infty$;
- frecventa oscilatiilor optice nu depinde de vectorul de unda, ci doar de proprietatile elastice ale structurii;

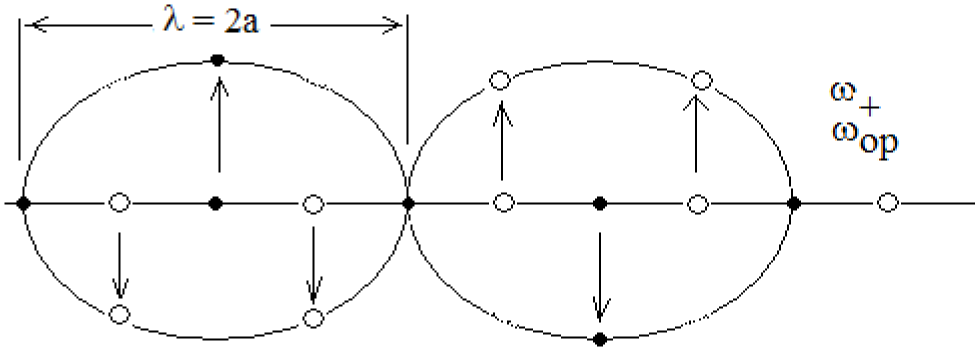
§ **oscilatii acustice (fononi acustici)**

✓ $q = 0, q = \frac{2\pi}{\lambda_{oscilatie}}$; $\lambda_{oscilatie} \to \infty$, substituim $\omega = 0 = \omega_{ac}(0)$ in una din ecuatiile de miscare care contin directiile de polarizare (de oscilatie):

$$+2f)e_1 - 2fe_2 = 0; \frac{e_2}{e_1} = 1 > 0$$

✓ in cadrul oscilatiiloracustice, atomii de tip diferit oscileaza in faza in unda cu $\lambda_{oscilatie} \to \infty$;




oscilatiile acustice au lungimi de unda mari, de la 4a > dimensiunea celulei elementare, la $\lambda_{ac} \in (4a, \infty)$;

oscilatiile optice au lungime de unda scurta, dictata de distantele interatomice, comparabile cu dimensiunea celulei elementare

*Comentariu asupra dispersiei*

- **in IZB**

✓ pentru $q \to 0$ $(q \neq 0)$, $sin\frac{qa}{2} \approx \frac{qa}{2}$

$$\omega_{+} = \frac{\omega_0}{\sqrt{2}}\sqrt{1 + \sqrt{1 - \frac{\gamma^2 (qa)^2}{4}}} \approx \frac{\omega_0}{\sqrt{2}}\sqrt{1 + (1 - \frac{1}{2}\frac{\gamma^2 (qa)^2}{4})}$$

$$= \omega_0 \sqrt{1 - \frac{1}{4}\frac{\gamma^2 (qa)^2}{4}} \approx \omega_0 (1 - \frac{1}{8}\frac{\gamma^2 (qa)^2}{4}) \approx \omega_0$$

$$\omega_{ac} = \frac{\omega_0}{\sqrt{2}}\sqrt{1 - \sqrt{1 - \frac{\gamma^2 (qa)^2}{4}}} \approx \frac{\omega_0}{\sqrt{2}}\sqrt{1 - (1 - \frac{1}{2}\frac{\gamma^2 (qa)^2}{4})} = \frac{\omega_0}{4}\gamma qa = v_s q$$

$$v_s = \frac{\omega_0}{4}\gamma a \; [\sim 10^3 ms^{-1}]$$

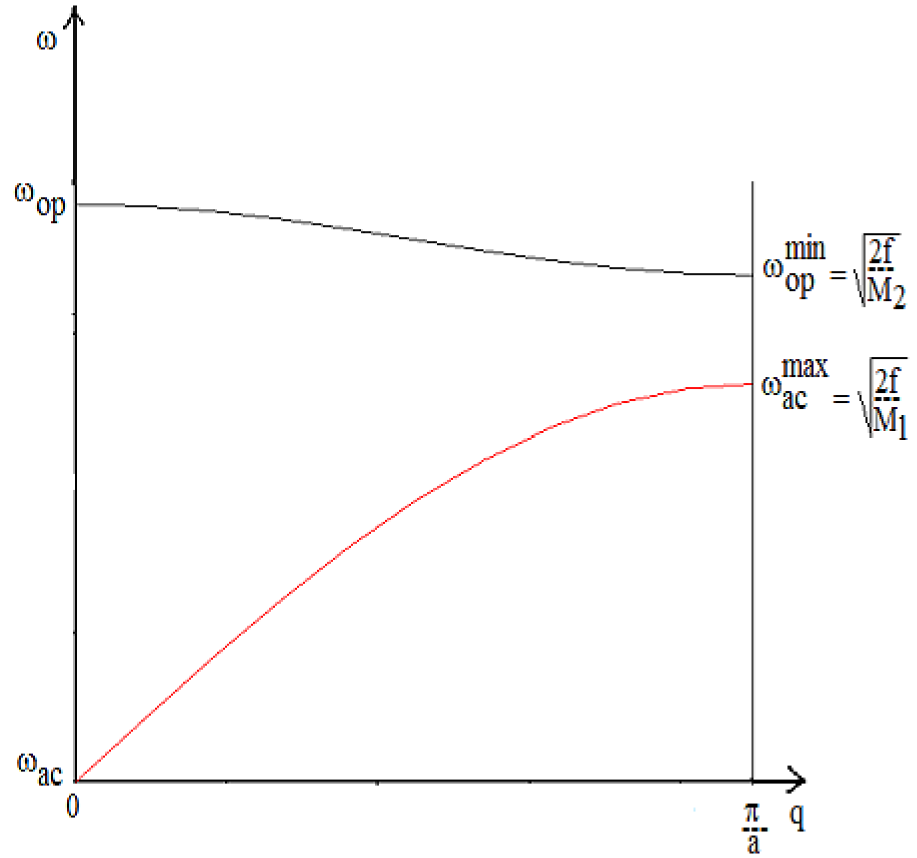
✓ pentru $q = \frac{\pi}{a}$, $sin\frac{qa}{2} = 1$,

$$\omega_{+} = \frac{\omega_0}{\sqrt{2}}\sqrt{1 + \sqrt{1 - \gamma^2}} = \frac{\omega_0}{\sqrt{2}}\sqrt{1 + \sqrt{1 - 4\frac{M_1 M_2}{(M_1 + M_2)^2}}} = \frac{\omega_0}{\sqrt{2}}\sqrt{\frac{2M_1}{M_1 + M_2}}$$

$$\omega_{+} = \sqrt{f\frac{M_1 + M_2}{M_1 M_2}\frac{2M_1}{M_1 + M_2}} = \sqrt{\frac{2f}{M_2}} = \omega_{op}(\frac{\pi}{a})$$

$$\omega_- = \frac{\omega_0}{\sqrt{2}}\sqrt{1-\sqrt{1-\gamma^2}} = \frac{\omega_0}{\sqrt{2}}\sqrt{1-\sqrt{1-4\frac{M_1M_2}{(M_1+M_2)^2}}} = \frac{\omega_0}{\sqrt{2}}\sqrt{\frac{2M_2}{M_1+M_2}}$$

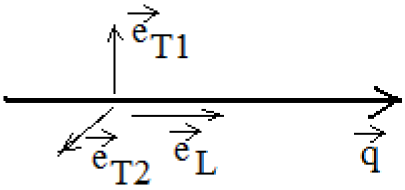
$$\omega_- = \sqrt{f\frac{M_1+M_2}{M_1M_2}\frac{2M_2}{M_1+M_2}} = \sqrt{\frac{2f}{M_1}} = \omega_{ac}(\frac{\pi}{a})$$




Legile de dispersie ale oscilatiilor optice si acustice

- **Directii de oscilatie**

✓ pentru fiecare directie de propagare $\vec{q}$, exista 3 directii de oscilatie: 2 perpendiculare pe directia de propagare $\vec{q}$ (oscilatii transversale), si 1 in lungul directiei de propagare (oscilatie longitudinala).




$\vec{e}_{T1}, \vec{e}_{T2}$ sunt versorii directiilor de oscilatie transversale, iar $\vec{e}_L$ este versorul directiei oscilatiei longitudinale.

✓ o directie de propagare $\vec{q}$ caracterizeaza 3 stari de vibratie.

❖ **Numarul de stari de vibratie. Densitatea de stari de vibratie**

$$(\vec{q}\vec{a}) \rightarrow (\vec{q}N\vec{a})$$

$$N = \begin{cases} nr.\, de\ baze\ din\ cristal \\ nr.\, de\ celule\ elementare\ in\ RD \\ nr.\, de\ celule\ elementare\ in\ RR \end{cases}$$

$$e^{i(\vec{q}N\vec{a})} = 1;\ \vec{q}N\vec{a} = 2\pi m; m \in Z$$

$$q_i = \frac{2\pi}{N_i a_i} m_i;\ m_i \in Z$$

$$q_i \in \left[ -\frac{\pi}{\frac{N_i}{2} a} m_i ; \frac{\pi}{\frac{N_i}{2} a} m_i \right]$$

$$-\frac{N_i}{2} \leq m_i < \frac{N_i}{2}$$

- $q$ are valori discrete; numarul valorilor distincte ale lui $q$ este egal cu numarul celulelor unitate din cristal; numarul starilor de vibratie este egal cu numarul celulelor unitate din cristal.
- volumul unei stari, $\Delta\vec{q}$ corespunde unei variatii $\Delta m = 1$;

$$\Delta\vec{q} = \Delta q_1 \cdot \Delta q_2 \cdot \Delta q_3 = \frac{(2\pi)^3}{V_{crist}}$$

- densitatea de stari:

$$\frac{dn}{d\vec{q}} = \frac{1}{\Delta\vec{q}} = \frac{V_{crist}}{(2\pi)^3} = \frac{Nv_{cel\ elem}}{(2\pi)^3} = \frac{N}{\Omega}$$

- $\Omega = \frac{(2\pi)^3}{v_{cel\ elem}}$ este volumul celulei elementare in RR.
- $N = \Omega\frac{dn}{d\vec{q}}$ numarul total de oscilatii din cristal este produsul volumului celulei elementare in RR cu densitatea de stari de vibratie.
- in cristal, $N$ este foarte mare, starile $\vec{q}$ sunt distribuite cvasicontinuu, astfel incat, in evaluarea unei functii $f(\vec{q})$ care descrie o proprietate a cristalului, se poate trece de la suma dupa toate starile, la integrarea pe volulul tuturor starilor, $\sum_{\vec{q}}^{N} f(\vec{q}) = \frac{V_{crist}}{(2\pi)^3}\sum_{\vec{q}}^{N} f(\vec{q})\Delta\vec{q} \to \frac{V_{crist}}{(2\pi)^3}\int f(\vec{q})d\,\vec{q}$.
- **Densitatea de stari de vibratie**
- tipuri de oscilatii**:**

$$oscilatii\ (dupa\ legea\ de\ dispersie) \to \begin{cases} ramuri\ acustice \to \begin{cases} 2T \\ L \end{cases} \\ ramuri\ optice \quad \to \begin{cases} 2T \\ L \end{cases} \end{cases}$$

✓ densitatea de stari de vibratie, se defineste ca numarul de stari din unitatea de volum, pe unitatea de interval de frecventa de oscilatie:

$$G(\omega_\lambda) = \frac{dn}{d\omega_\lambda} = \frac{dn}{d\vec{q}}\frac{d\vec{q}}{d\omega_\lambda}$$

✓ in formalismul suprafetelor de frecventa constanta:

$$d\vec{q} = dS_\lambda(\omega) \cdot dq_\perp$$

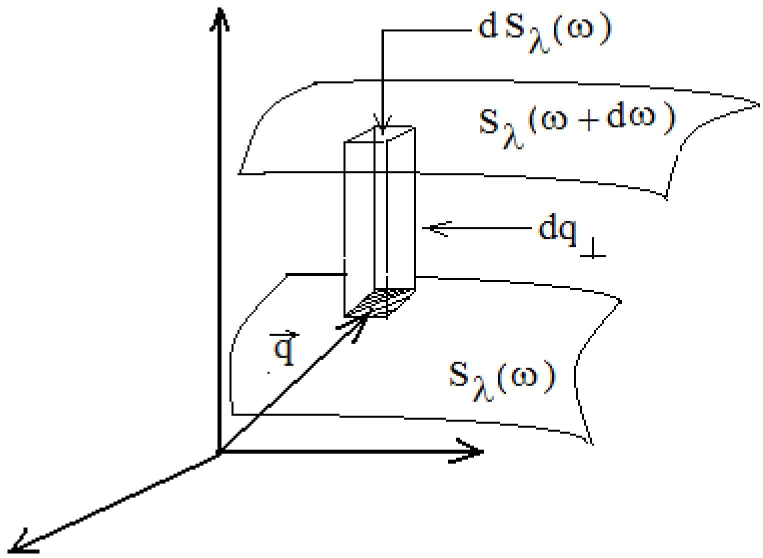
$$dn = \frac{V_{crist}}{(2\pi)^3}\int d\vec{q} = \frac{V_{crist}}{(2\pi)^3}\int dS_\lambda(\omega) \cdot dq_\perp$$

$$G(\omega_\lambda) = \frac{V_{crist}}{(2\pi)^3}\int dS_\lambda(\omega) \cdot \frac{dq_\perp}{d\omega_\lambda} = \frac{V_{crist}}{(2\pi)^3}\int \frac{dS_\lambda(\omega)}{v_{g,\lambda}}$$

Unde $\frac{d\omega_\lambda}{dq_\perp} = \nabla_{\vec{q}}\omega_\lambda = v_{g,\lambda}$ reprezinta viteza de grup pe ramura de vibratie $\lambda$.

***Aplicatii:*** in evaluarea unei functii $f((\omega_\lambda(\vec{q}))$ care descrie o proprietate a cristalului, se poate trece de la suma dupa toate starile, la integrarea pe volumul tuturor starilor,

$$\sum_{\vec{q},\lambda}^{N} f(\omega_\lambda(\vec{q})) = \sum_{\vec{q}} \int f(\omega_\lambda) G(\omega_\lambda) d\omega_\lambda$$




Elementul de volum $d\vec{q} = dS_\lambda(\omega) \cdot dq_\perp$, situat intre suprafetele de frecventa constanta $S_\lambda(\omega)$ si $S_\lambda(\omega + d\omega)$.