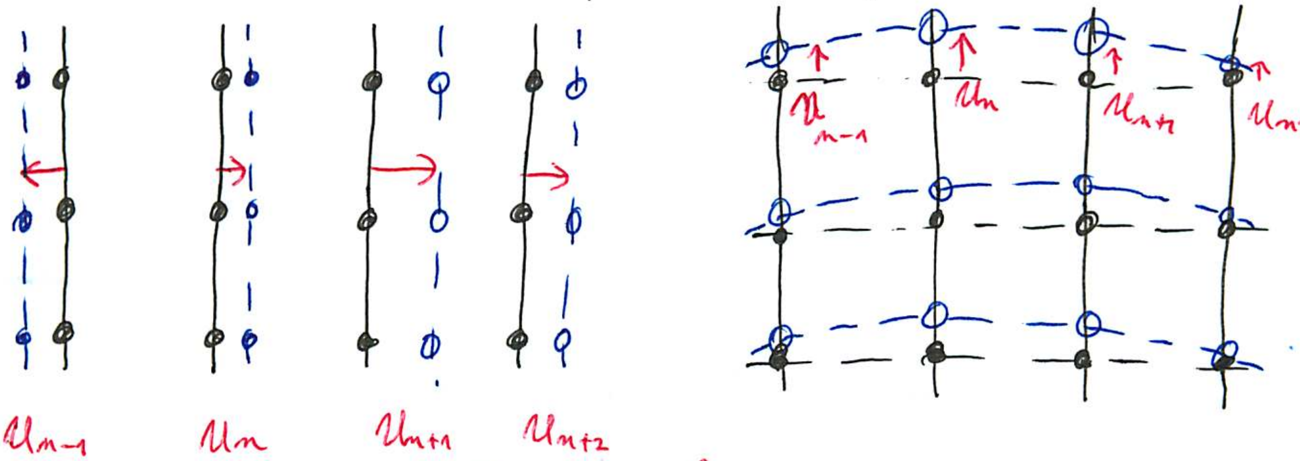
Mrežna nihanja - fononi

- Zaradi termičnih ekscitacij atomi kristalne mreže nihajo okoli ravnovesnih leg.

Predpostavke:

- Propagacija el. valov zgolj v smereh (1,0,0), (1,1,0) ter (1,1,1) kubičnega kristala. V tem primeru celotne mrežne ravnine nihajo v fazi kot togo telo:



Problem tako postane 1-D

Longitudinalni val. Transverzalni val

- Predpostavimo, da je elastični odziv kristala linearna funkcija zun. sil. Oziroma, da je elastična energija kvadratno odvisna od premenih odmikov od ravnovesnih leg.
- Upoštevamo le elastično energijo relativnih odmikov med prvimi sosedi:

$$U^{harm} = \frac{K}{2} \sum_n (u_n - u_{n-1})^2$$

K: elastična konstanta med sosednjimi mrežnimi ravninami, definirana na en atom n-te ravnine

- Sila na atom v n-ti ravnini:

$$F_n = -\frac{\partial U^{harm}}{\partial u_n} = -K\left(2u_n - u_{n-1} - u_{n+1}\right)$$

- Enačba gibanja atoma n-te ravnine:

$$M\ddot{u}_n = K\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

Časovna odvisnost $u_n(t) = e^{-i\omega t}\, u_n$

$$-M\omega^2 u_n = K\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

Nastavek za krajevno odvisnost:

$$u_n = u_0\, e^{ikna}$$

$$-\omega^2 M \cancel{u_0 e^{ikna}} = K \cancel{u_0 e^{ikna}} \left(e^{ika} + e^{-ika} - 2\right)$$

$$\omega^2 = \frac{K}{M}\, 2\left(1 - \cos ka\right) = \frac{K}{M}\, 4 \sin^2\frac{ka}{2}$$

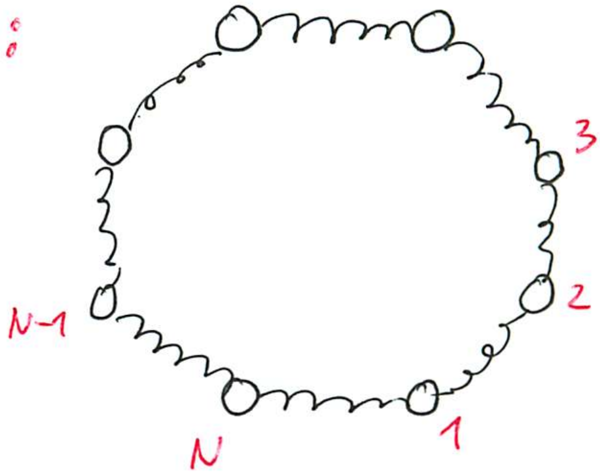
$$\omega = 2\sqrt{\frac{K}{M}}\left|\sin\frac{ka}{2}\right|$$

Model mr. nihanj: 

Veriga atomov, povezana z vzmetmi

– Periodični robni pogoji:

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



$$u_0 e^{ik(N+1)a} = u_0 e^{ika}$$

$$e^{ikNa} = 1 \Rightarrow kNa = 2\pi n \; ; \quad n \in \mathbb{Z}$$

Cela št.

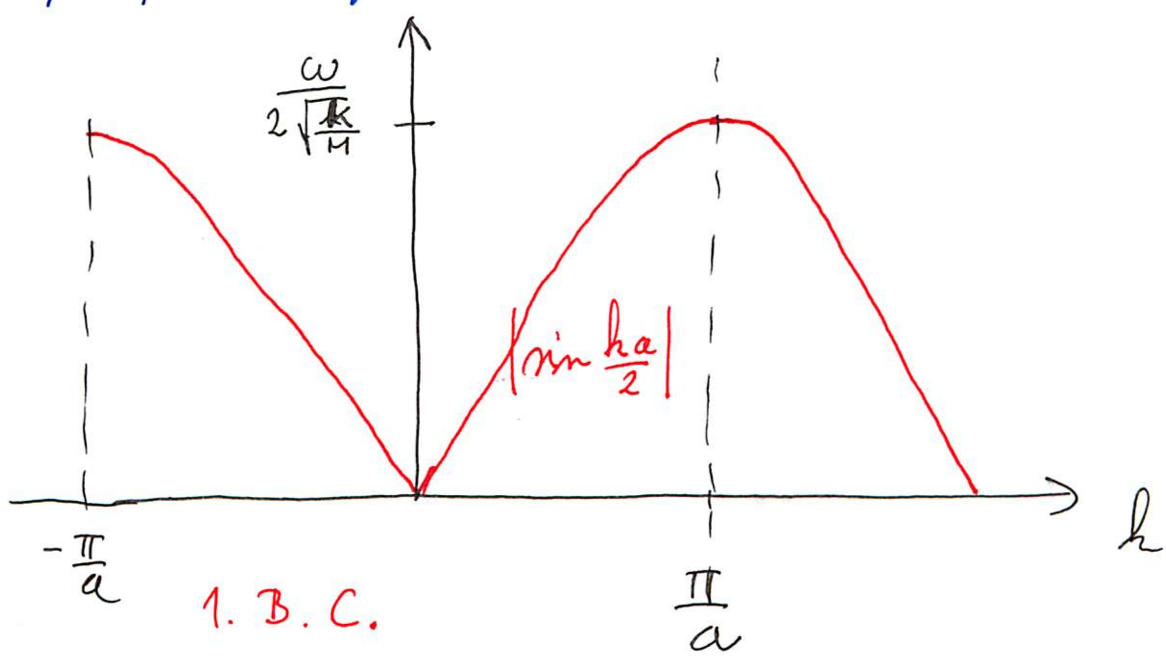
$$n = 0, 1, \dots, N-1$$

oziroma

$$-\frac{N}{2} < n < \frac{N}{2} \Rightarrow -\frac{\pi}{a} < k < \frac{\pi}{a}$$

Dovoljeni k: $k = \frac{2\pi}{Na} \cdot n$

$\omega(k)$: Disperzijska relacija



Pokaži, da iz

$$M\ddot{u}_n = K\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

sledi valovna enačba če $u_n \to u(x)$

$$M\frac{\partial^2 u}{\partial t^2} = K\left(u(x+a) + u(x-a) - 2u(x)\right) \quad ; \quad x = na$$

$$M\frac{\partial^2 u}{\partial t^2} = K a^2 \lim_{a\to 0} \frac{\frac{u(x+a)-u(x)}{a} - \frac{u(x)-u(x-a)}{a}}{a}$$

$$M\frac{\partial^2 u}{\partial t^2} = K a^2 \frac{\partial^2 u}{\partial x^2} \quad ; \quad \boxed{\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2}}$$

$$c = a\sqrt{\frac{K}{M}}$$

Vektor recipročne mreže: G

$\omega(k+G)=\omega(k)$ podobno, kot pri elektronih v periodičnem potencialu

Značilnosti $\omega(k)$:

- $\left.\frac{d\omega^2(k)}{dk}\right|_{k=\frac{\pi}{a}}=0$; $\frac{d\omega^2}{dk}=2\sqrt{\frac{K}{M}}\,2\sin\frac{ka}{2}\cos\frac{ka}{2}\cdot\frac{a}{2}$

$$\left.\frac{d\omega^2}{dk}\propto\sin ka\right|_{k=\frac{\pi}{a}}=0$$

- Dolgovalovna limita:

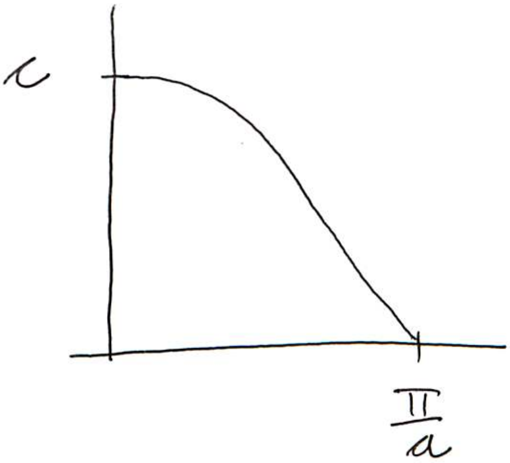
$$\omega(k)=2\sqrt{\frac{K}{M}}\sin\frac{ka}{2}\sim\sqrt{\frac{K}{M}}\,ka \quad \text{za } ka\ll 1$$

oziroma $k\ll\frac{1}{a}$ ali $\lambda\gg a$!

$\omega=c\cdot k$; $c=\sqrt{\frac{K}{M}}\cdot a$; c: zvočna hitrost

- Grupna hitrost (hitrost valovnega paketa)

$$v_g=\frac{d\omega}{dk}=c\cdot\cos\frac{ka}{2}$$

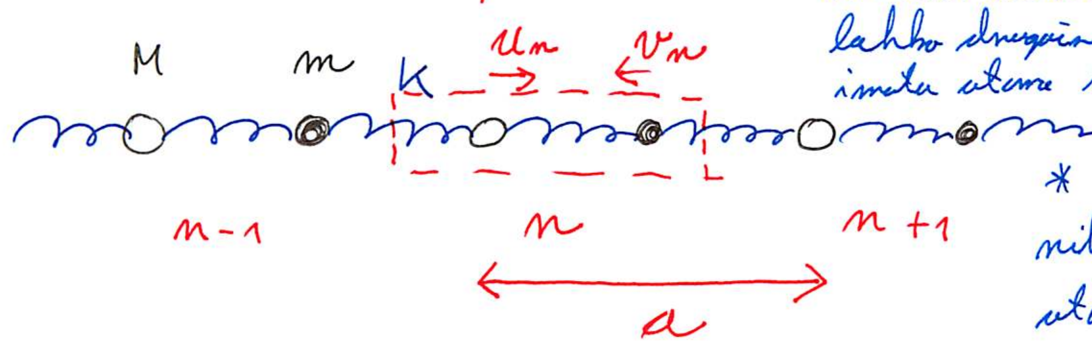


$v_g(k=\frac{\pi}{a})=0\Rightarrow$ stoječe valovanje

$u_n=u_0\,e^{i\frac{\pi}{a}na}=u_0(-1)^n$; $k=\frac{\pi}{a}$

- Dve atoma na primit. celica:

* Če ima mreža bazo z (dvema) identičnima atomoma, so lahko drugačne konstante vzmeti, saj imata atoma baze različni okolici!



* Model opiše tudi nihanje verige, ki vsebuje atome M ter m.

$$U^{harm} = \frac{K}{2} \sum_n (u_n - v_n)^2 + (v_n - u_{n+1})^2$$

Vsako vzmet opišemo z(le)enim členom!

Sili na u_n- ter v_n-ta atoma:

$$F_{u_n} = -\frac{\partial U^{harm}}{\partial u_n} = -K\left(u_n - v_n - (v_{n-1} - u_n)\right)$$

$$F_{v_n} = -\frac{\partial U^{harm}}{\partial v_n} = -K\left(v_n - u_n + v_n - u_{n+1}\right)$$

Enačbi gibanja

$$M\ddot{u}_n = -K(2u_n - v_n - v_{n-1})$$

$$m\ddot{v}_n = -K(2v_n - u_n - u_{n+1})$$

$$u_n, v_n \propto e^{-i\omega t} \Rightarrow$$

$$M\omega^2 u_n = K(2u_n - v_n - v_{n-1})$$

$$m\omega^2 v_n = K(2v_n - u_n - u_{n+1})$$

Nastavek za krajevno odvisnost:

$$u_n = u_0\, e^{ikna} \; ; \quad v_n = v_0\, e^{ikna}$$

$$M\omega^2 u_0 = K\left(2u_0 - v_0 - v_0 e^{-ika}\right)$$

$$m\omega^2 v_0 = K\left(2v_0 - u_0 - u_0 e^{ika}\right)$$

Homogen sistem:

$$\begin{bmatrix} M\omega^2 - 2K \, , & K\left(1 + e^{-ika}\right) \\ K\left(1+e^{ika}\right) , & m\omega^2 - 2K \end{bmatrix} = 0$$

$$\left(M\omega^2 - 2K\right)\left(m\omega^2 - 2K\right) - 2K^2\left(1 + \cos ka\right) = 0$$

$$mM\omega^4 - 2K(m+M)\omega^2 + 2K^2\left(1 - \cos ka\right) = 0$$

$$\omega^2 = \frac{1}{2mM}\left(2K(m+M) \pm \sqrt{4K^2(m+M)^2 - 8K^2 mM\left(1-\cos ka\right)}\right)$$

$$\omega^2 = K\left(\frac{1}{m} + \frac{1}{M}\right) \pm K\sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4}{mM}\sin^2\frac{ka}{2}}$$

- $\omega^2 > 0$ vedno!
- $\pm \Rightarrow$ dve veji

- Dolgovalovna limita $ka \to 0$

$$\omega^2 = K\left(\frac{1}{m}+\frac{1}{M}\right) \pm K\sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{k^2a^2}{mM}}$$

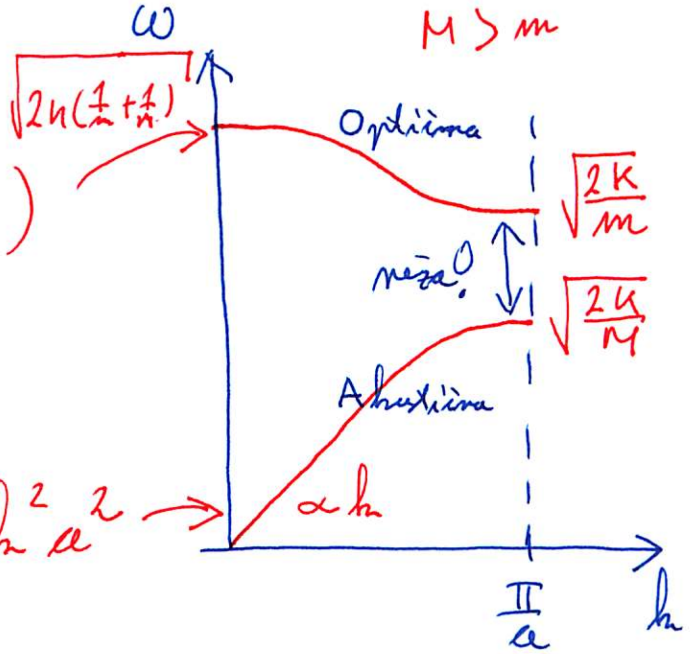
$$\omega^2 = K\left(\frac{1}{m}+\frac{1}{M}\right)\left[1 \pm \left(1 - \frac{k^2a^2}{\left(\frac{1}{m}+\frac{1}{M}\right)^2 mM}\right)^{\frac{1}{2}}\right]$$

$(+) \Rightarrow$ Optična veja:

$$\omega^2 \cong 2K\left(\frac{1}{m}+\frac{1}{M}\right)$$

$(-) \Rightarrow$ Akustična veja:

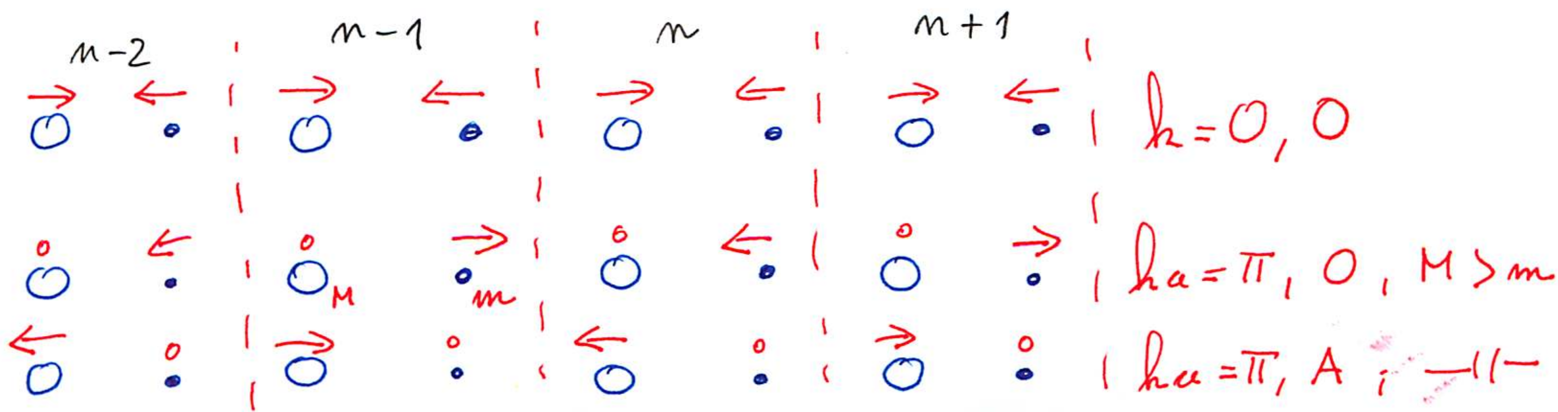
$$\omega^2 = \frac{\frac{1}{2}K}{(m+M)}k^2a^2$$



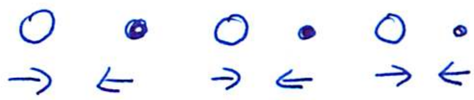
- Dol. I. B. C.; $ka = \pi \Rightarrow$

$$\omega^2 = K\left(\frac{1}{m}+\frac{1}{M}\right) \pm K\sqrt{\underbrace{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4}{mM}}_{\left(\frac{1}{m}-\frac{1}{M}\right)^2}}$$

$$\omega_1 = \sqrt{\frac{2K}{m}}\,; \quad \omega_2 = \sqrt{\frac{2K}{M}}$$



- $k=0$, <u>Optično nihanje:</u>



Pri $k=0 \Rightarrow$
$\omega = 2K\left(\frac{1}{m}+\frac{1}{M}\right)$

$$\begin{bmatrix} 2K\left(\frac{M}{m}+1\right)-2K \;, & 2K \\ 2K & ,\; 2K\left(\frac{m}{M}+1\right)-2K \end{bmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = 0$$

$$\begin{bmatrix} \frac{M}{m} \;, & 1 \\ 1 \;, & \frac{m}{M} \end{bmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = 0 \Rightarrow \boxed{\frac{v_0}{u_0} = -\frac{M}{m}}$$

✓

- $ka = \pi$
$\omega^2 = \frac{2K}{m}$

$$\begin{bmatrix} \frac{M}{m}-1 \;, & 0 \\ 0 \;, & 0 \end{bmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = 0 \Rightarrow \boxed{\begin{matrix} u_0 = 0 \\ v_0 \neq 0 \end{matrix}}$$

Nihajo le m-atomi!

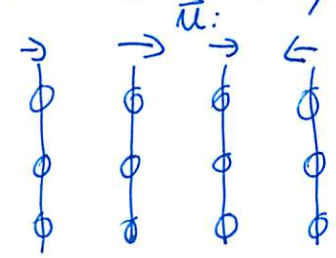
Obratno velja pri $\omega^2 = \frac{2K}{M}$; Nihajo le M-atomi!

- Zdaj se dogaja za ω: $\sqrt{\frac{2K}{M}} < \omega < \sqrt{\frac{2K}{m}}$

Valovna rešitev ne obstaja, $k \in \mathrm{Im}$ valovanje je ~~zd~~ zadušeno, v kraju eksponentno pada!

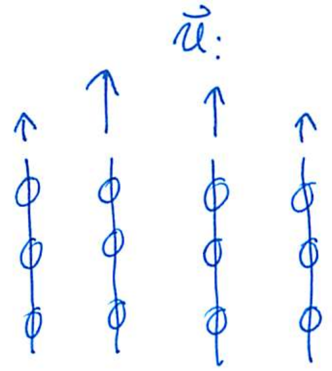
Približek togih ravnin:

a.)



Longitudinalno

b.)

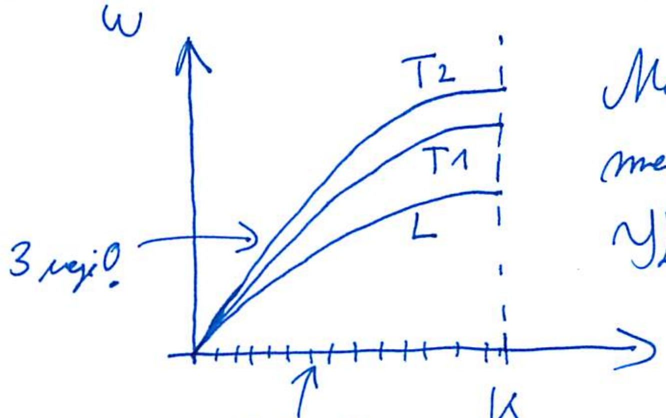


Transverzalno

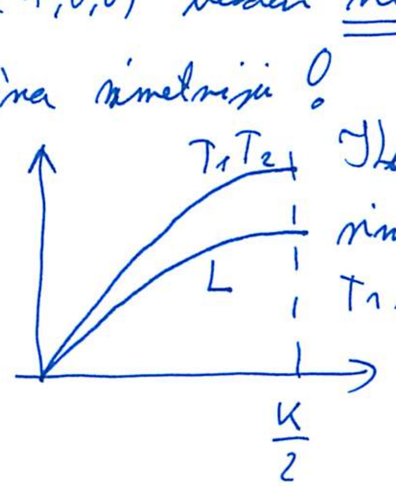
Model: $U^{harm} = \frac{K}{2} \sum_n (u_n - u_{n-1})^2$

Relaksacija modela togih ravnin:

1.) 1 at na osn. celico, N atomov (celic), 3 dimenzije $\Rightarrow$ 3N prostostnih stopenj – 3N lastnih nihanj, vendar le N različnih vel. vektorjev k! $\Rightarrow$ 3 veje!



Monoatomni kristal, simetrijska smer (1,0,0) vendar ni Najvišja simetrija!



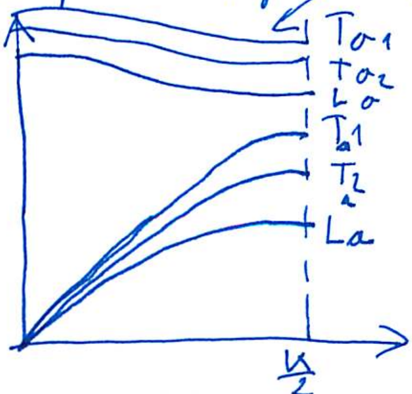
Najvišja simet. T1 in T2 degenerirani!

2.) 2 at na osn. celico (NaCl, Diamant!)

$p = 2$; $3pN$ prost. stopenj

$(p-1)\cdot 3$ optičnih vej

3 akustične veje



Degeneracija s T-vej je odvisna od smeri in tem simetriji B.R.!

Kvantizacija mrežnih nihanj

$$\hat{H} = \sum_n \left[\frac{\hat{p}_n^2}{2M} + \frac{K}{2} (\hat{u}_n - \hat{u}_{n+1})^2 \right]$$

$$[u_n, p_{n'}] = i\hbar \delta_{n,n'}$$

Transformacija: $$u_n = \frac{1}{\sqrt{N}} \sum_k Q_k e^{ikna}$$

Inv. transf. $$Q_k = \frac{1}{\sqrt{N}} \sum_n u_n e^{-ikna}$$

Robni pogoj: PRP: $u_{N+1} = u_1$ ter

$$k = \frac{2\pi}{Na} j \, ; \quad j = 0, \pm 1, \dots, \pm \left(\frac{N}{2} - 1\right), + \frac{N}{2}$$

k - diskretni zaradi PRP!

Podobna veza za impulze: $$p_n = \frac{1}{\sqrt{N}} \sum_k P_k e^{-ikna}$$

$$P_k = \frac{1}{\sqrt{N}} \sum_n p_n e^{+ikna}$$

Preverimo komutator:

$$[Q_k, P_{k'}] = \frac{1}{N} \sum_{n,m} \underbrace{[u_n, p_m]}_{i\hbar \delta_{n,m}} e^{-i(kn - k'm)a} =$$

$$= i\hbar \frac{1}{N} \sum_n e^{-i(k-k')na} =$$

$$= i\hbar \frac{1}{N} \sum_n e^{-i2\pi(j-j')\frac{n}{N}} = i\hbar \delta_{j,j'} = i\hbar \delta_{k,k'} \checkmark$$

$$[Q_k, P_{k'}] = i\hbar \delta_{k,k'} \,!$$

Tranformacija ohranja komutacijska pravila!

Transformacija na H:

$$\sum_n p_n^2 = \frac{1}{N} \sum_{nkk'} P_k P_{k'} \underbrace{e^{-i(k+k')na}}_{\delta_{k,-k'}} = \sum_k P_k P_{-k}$$

$$\sum_n (u_n - u_{n+1})^2 = \frac{1}{N} \sum_{nkk'} Q_k Q_{k'} e^{i(k+k')na} \quad (1-e^{+ika})(1-e^{+ik'a})$$

$$= \sum_k Q_k Q_{-k} \, 2(1-\cos ka)$$

$$H = \sum_k \left[\frac{P_k P_{-k}}{2M} + K Q_k Q_{-k} (1-\cos ka) \right]$$

$$H = \sum_k \left[\frac{P_k P_{-k}}{2M} + \frac{1}{2} M \omega_k^2 Q_k Q_{-k} \right] \quad (1)$$

$$\omega_k = \sqrt{\frac{2K}{M}(1-\cos ka)}$$

Harmonski oscilator? $\quad i\hbar \dot{A} = [A, H]$

$$i\hbar \dot{Q}_k = [Q_k, H] = \frac{\cancel{i\hbar}\, 1}{2M}\left[Q_k, \sum_{k'} P_{k'} P_{-k'}\right] =$$

$k' = k$ ter $-k' = k \Rightarrow 2\times$

$$= \frac{i\hbar}{M} P_{-k} \Rightarrow \dot{Q}_k = \frac{1}{M} P_{-k}$$

$$i\hbar \ddot{Q}_k = [\dot{Q}_k, H] = \frac{1}{M}\left[P_{-k}, \sum_{k'} \frac{M}{2} \omega_{k'}^2 Q_k Q_{-k}\right] =$$

$$= -i\hbar \omega_k^2 Q_k \Rightarrow \ddot{Q}_k + \omega_k^2 Q_k = 0$$

Enačba harmonskega oscilatorja

$$\varepsilon_k = (\langle n_k \rangle + \tfrac{1}{2})\hbar \omega_k \; : \text{energija posameznega nihanja}$$

$$H = \sum_k (\hat{n}_k + \tfrac{1}{2})\hbar\omega_k \quad (2)$$

Kako iz $(1) \rightarrow (2)$?

Vpeljimo bozonske kreacijske in anihilacijske operatorje:

$$Q_k = \sqrt{\frac{\hbar}{2M\omega_k}}\left(a_k + a^+_{-k}\right)$$

$$P_k = i\sqrt{\frac{\hbar M\omega_k}{2}}\left(a^+_k - a_{-k}\right) \qquad (3)$$

Za a_k in a^+_k velja: $[a_{k}, a^+_{k'}] = a_k a^+_{k'} - a^+_{k'} a_k = \delta_{kk'}$

Test komutacijskih pravil:

$$[Q_k, P_{k'}] = i\frac{\hbar}{2}\left[a_k + a^+_{-k},\, a^+_{k'} - a_{-k'}\right] = i\hbar\,\delta_{k,k'} \checkmark$$

(3) $\Rightarrow$ (1):

$$H = \sum_k -\frac{\hbar \cancel{M}\omega_k}{2\cdot 2\cancel{M}}\left(a^+_k - a_{-k}\right)\left(a^+_{-k} - a_k\right) +$$

$$\frac{\cancel{M}\omega_k^{\cancel{2}}}{2}\frac{\hbar}{2\cancel{M\omega_k}}\left(a_k + a^+_{-k}\right)\left(a_{-k} + a^+_k\right)$$

$$= \frac{\hbar}{4}\sum_k \omega_k\left(\cancel{a_k a_{-k}} + a_k a^+_k + a^+_{-k}a_{-k} + \cancel{a^+_{-k}a^+_k}\right.$$

$$\left. - \cancel{a^+_k a^+_{-k}} - \cancel{a_k a_{-k}} + a^+_k a_k + a_{-k}a^+_{-k}\right)$$

$$= \frac{\hbar}{4}\sum_k \omega_k\left(4a^+_k a_k + 2\right) = \sum_k \hbar\omega_k\left(a^+_k a_k + \frac{1}{2}\right)$$

$$H = \sum_k \hbar\omega_k\left(a^+_k a_k + \frac{1}{2}\right) = \sum_k \hbar\omega_k\left(\hat{n}_k + \frac{1}{2}\right)$$

Fononski prispevek k specifični toploti

$$f = \frac{1}{V} \ln \sum_i e^{-\beta E_i} \; ; \qquad u = -\frac{\partial f}{\partial \beta}$$

Po vseh stanjih — Gostota notranje energije

r: polarizacije, veje

$$E = \sum_{k,r} \hbar \omega_r(k) \left(n_{k,r} + \tfrac{1}{2} \right)$$

$$f = \frac{1}{V} \ln \prod_{k,r} \sum_{n_{k,r}=0,1,2,\dots} e^{-\beta \hbar \omega_r(k) \left(n_{k,r} + \frac{1}{2} \right)}$$

$$f = \frac{1}{V} \sum_{k,r} \ln \left(e^{-\beta \hbar \omega_r(k)/2} + e^{-\beta \hbar \omega_r(k)\, 3/2} + \dots \right)$$

$$= \frac{1}{V} \sum_{k,r} \ln e^{-\frac{x}{2}} \left(1 + e^{-x} + e^{-2x} + \dots \right) \; ; \quad x = \beta \hbar \omega_r(k)$$

$$= \frac{1}{V} \sum_{k,r} \ln \frac{e^{-\hbar \omega_r(k) \beta/2}}{1 - e^{-\beta \hbar \omega_r(k)}} = \frac{1}{V} \sum_{k,r} \left[-\beta \hbar \frac{\omega_r(k)}{2} - \ln \left(1 - e^{-\beta \hbar \omega_r(k)} \right) \right]$$

$$u = \frac{1}{V} \sum_{k,r} \hbar \omega_r(k) \left[\frac{1}{2} + \frac{-e^{-\beta \hbar \omega_r(k)} \; \cancel{(-\hbar \omega_r(k))} \; -1}{1 - e^{-\beta \hbar \omega_r(k)}} \right]$$

$$u = \frac{1}{V} \sum_{k,r} \hbar \omega_r(k) \left(n_r(k) + \frac{1}{2} \right)$$

$$n_r(k) = \frac{1}{e^{\beta \hbar \omega_r(k)} - 1}$$

Celotna ~~prosta~~ notranja energija:

$$u = u^{eq} + \frac{1}{V}\sum_{k,r}\left[\frac{\hbar\omega_r(k)}{2} + \frac{\hbar\omega_r(k)}{e^{\beta\hbar\omega_r(k)} - 1}\right]$$

$$c_V = \frac{1}{V}\sum_{k,r}\frac{\partial}{\partial T}\frac{\hbar\omega_r(k)}{e^{\beta\hbar\omega_r(k)} - 1}$$

a) $\underline{T \to \infty}$ Visoko-temperaturna limita ali $\beta \to 0$

$$\frac{1}{e^x - 1} = \frac{1}{x + \frac{x^2}{2} + \frac{x^3}{3!}} = \frac{1}{x}\left[1 - \frac{x}{2} + \frac{x^2}{12} + \cdots\right]$$

$$x = \frac{\hbar\omega}{k_B T}$$

$$c_V = \frac{1}{V}\sum_{k,r}\frac{\partial}{\partial T}\left[\frac{\cancel{\hbar\omega_r(k)}}{\cancel{\hbar\omega_r(k)}}k_B T - \cdots + \frac{(\hbar\omega_r(k))^2}{k_B T \cdot 12}\right]$$

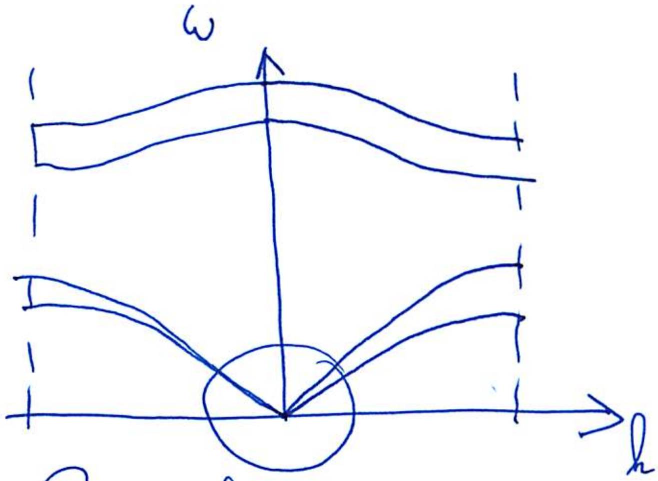
$$c_V = \frac{k_B}{V}\sum_{\substack{k,r \\ \downarrow \\ 1.\,B.\,C.}} 1 - \frac{(\hbar\omega_r(k))^2}{(k_B T)^2 \cdot 12} = c_{V0} + \Delta c_V$$

$$c_{V0} = \underbrace{k_B \frac{3pN}{V}}_{\text{DULONG-PETIT}} - \Delta c_V \; ; \quad p \cdot N: \text{št. atomov}$$

$$\Delta c_V = + \frac{k_B}{12V(k_BT)^2}\sum_{k,r}\left(\hbar\,\omega_r(k)\right)^2$$

b.) $T \to 0$; velik k!

$$\boxed{\omega_r(k) = c_r \cdot k}$$



Pri nizkih T pride v upoštev le linearni del disperzije

$$c_V = \frac{1}{V}\frac{V}{(2\pi)^3}\frac{\partial}{\partial T}\sum_r \underbrace{\int dk}_{\text{1. B. C.}} \frac{\hbar c_r k}{\left(e^{\beta\hbar c_r k} - 1\right)} \qquad \boxed{\frac{1}{c^3} = \frac{1}{3}\sum_r \int \frac{d\Omega}{4\pi}\frac{1}{c_r(\Omega)^3}}$$

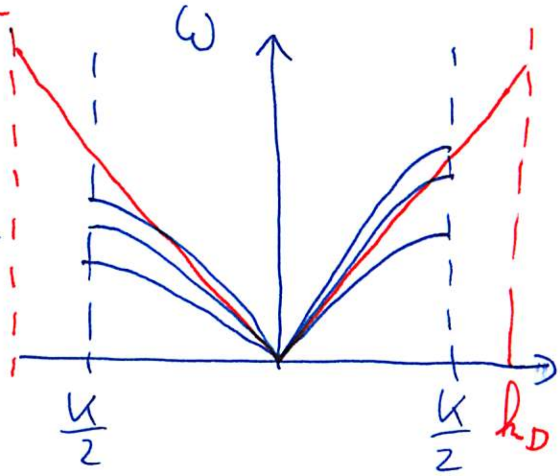
$$dk = 4\pi k^2\, dk \; ; \quad \beta\hbar c_r k = x \qquad \boxed{\frac{1}{c^3} = \frac{1}{3}\sum_{r=1}^{3}\frac{1}{c_r^3}}$$

zgornja meja → ∞

$$c_V = \frac{3}{2\pi^2}\frac{\partial}{\partial T}\frac{(k_BT)^4}{(\hbar c)^3}\underbrace{\int_0^{\infty}\frac{x^3\,dx}{e^x - 1}}_{\frac{\pi^4}{15}} = \frac{\pi^2}{10}\frac{\partial}{\partial T}\frac{(k_BT)^4}{(\hbar c)^3}$$

$$c_V = \frac{2\pi^2}{5} k_B \frac{(k_B T)^3}{(\hbar c)^3}$$

Debyjev približek



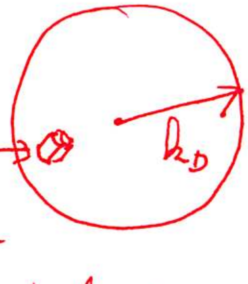
- Nadomesti vse veje $\omega_s(k)$ s tremi vejami, ki imajo vse enako linearno disperzijo $\omega = c \cdot k$

- Integral po 1. B. C. nadomesti z integralom po sferi v k-prostoru:

$$N = \frac{4\pi k_D^3}{3 \cdot \frac{(2\pi)^3}{V}}$$

Število ionov kristala !

Volumen v k prostoru, ki pripada enemu izbranemu k !



$$\boxed{n = \frac{k_D^3}{6\pi^2}}$$

Izračun c_V :

$$c_V = \frac{1}{V}\frac{\partial}{\partial T}\sum_{s,k}\frac{\hbar\omega_s(k)}{e^{\beta\hbar\omega_s(k)}-1} \quad ; \quad \omega_s(k) = c \cdot k$$

$$c_V = \frac{1}{(2\pi)^3} 4\pi \cdot 3 \frac{\partial}{\partial T}\int_0^{k_D} \frac{k^2 \hbar c k \, dk}{(e^{\beta\hbar c k}-1)}$$

$$c_V = \frac{3k_B}{2\pi^2}\frac{(\hbar c)^2}{(k_BT)^2}\int_0^{k_D}\frac{k^4\, e^{\beta\hbar c k}}{(e^{\beta\hbar c k}-1)^2}\,dk \qquad x=\beta\hbar c k$$

$$\omega_D = k_D\cdot c\ ; \quad k_B\Theta_D = \hbar\omega_D = \hbar c k_D$$

$$c_V = \frac{3k_B}{2\pi^2}\frac{(\hbar c)^2}{(k_BT)^2}\left(\frac{k_BT}{\hbar c}\right)^5\int_0^{\Theta_D/T}\frac{x^4 e^x\,dx}{(e^x-1)^2}$$

$$c_V = \frac{3k_B \overbrace{k_D^3}^{=6\pi^2 n}}{2\pi^2}\left(\frac{k_BT}{\hbar c k_D}\right)^3\int_0^{\Theta_D/T}\frac{x^4 e^x\,dx}{(e^x-1)^2}$$

$$c_V = 9nk_B\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T}\frac{x^4 e^x}{(e^x-1)^2}\,dx$$

V limiti $T\Rightarrow 0$ se mora rezultat ujemati z $T\sim 0$ razvojem $\Rightarrow$

$$c_V = \frac{12\pi^4}{5}nk_B\left(\frac{T}{\Theta_D}\right)^3 = \frac{2\pi^2}{5}k_B\left(\frac{k_BT}{\hbar c}\right)^3,$$

glej str. (96)

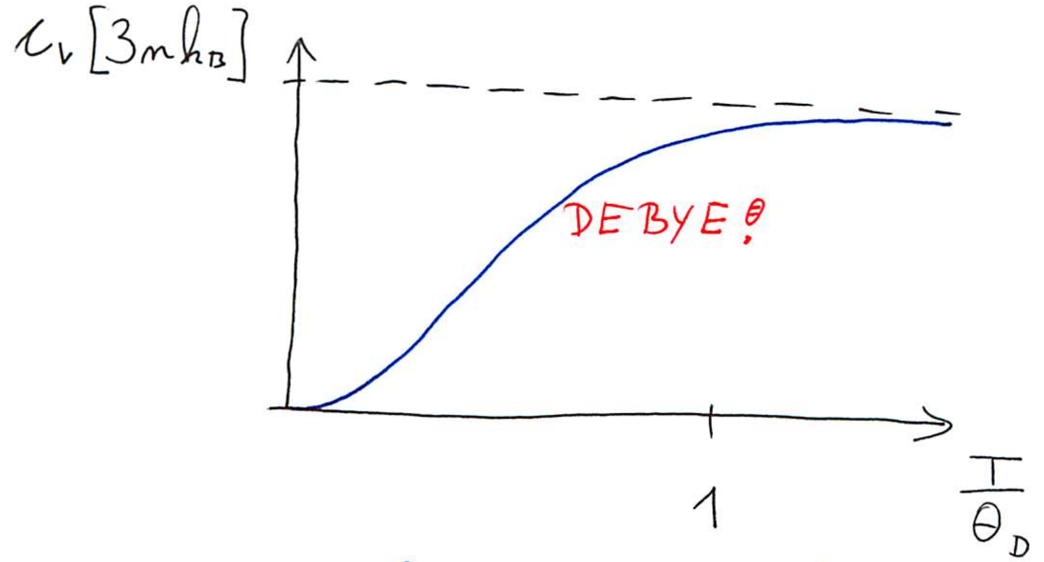
pri čemer $\Theta_D = \frac{\hbar c}{k_B}$ ter $c \Rightarrow$

$$\boxed{\frac{1}{c^3} = \frac{1}{3}\sum_s\int\frac{d\Omega}{4\pi}\frac{1}{c_s(\hat{k})^3}}$$

$$c_V = 9 n k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x}{(e^x-1)^2}\, dx$$

$$\lim_{T\to\infty} c_V(T) = \lim_{T\to 0} 9 n k_B \left(\frac{T}{\Theta_D}\right)^3 \underbrace{\int_0^{\frac{\Theta_D}{T}} \frac{x^4}{x^2}\, dx}_{\frac{1}{3}\left(\frac{\Theta_D}{T}\right)^3} = \boxed{3 n k_B}$$

DULONG-PETIT!



Θ_D igra podobno vlogo pri mrežnih nihanjih, kot T_F (Fermijeva T) pri elektronih. $\frac{T}{\Theta_D} \gg 1$ pomeni klasično obnašanje! Tipično: $\Theta_D \sim 10^2\,K$; $\Theta_D \ll T_F$!

	Θ_D [K]
NaCl	321
KCl	231
Li	400
Na	150
K	100
Cu	315
Fe	420
diamant! C	1860

Primerjava el. ter fononske c_V

$$c_V^{el} = \frac{\pi^2}{2}\left(\frac{T}{T_F}\right) n_e k_B$$

št. el.

valenca?

$$\frac{c_V^{el}}{c_V^{mr}} = \frac{5}{24\pi^2}\,\frac{Z\,\Theta_D^3}{T^2\,T_F} \Rightarrow T_0 \;(c_V^{el} = c_V^{mr})$$

$$T_0 = 0{,}145\sqrt{\frac{Z\Theta_D}{T_F}}\;\Theta_D$$

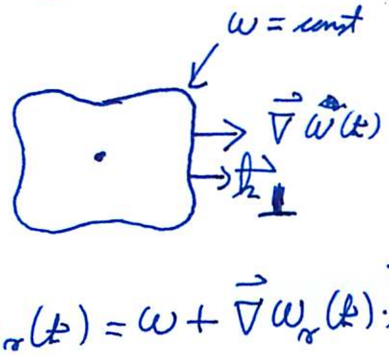
Gostota fononskih stanj

$$\frac{1}{V}\sum_{r,k} H(\omega_{r,k}) = \sum_r \int \frac{dk}{(2\pi)^3} H(\omega_r(k)) =$$

$$= \int d\omega\, g(\omega)\, H(\omega) \Rightarrow \text{gostota fononskih stanj}$$

$$g(\omega) = \sum_r \int \frac{d\vec{k}}{(2\pi)^3}\,\delta(\omega - \omega_r(k)) =$$

$$= \boxed{\sum_r \int_{\omega=\omega_r(k)} \frac{dS}{(2\pi)^3\,|\vec{\nabla}_k \omega_r(k)|}}$$



$$\omega_r(k) = \omega + \vec{\nabla}\omega_r(k)\cdot\vec{k}$$

$$= \omega + |\vec{\nabla}\omega_r(k)|\cdot k_\perp$$

$$\int \delta(x)\,dx = 1 \qquad \int dk_\perp\,\delta(|\vec{\nabla}\omega_r(k)|\,k_\perp) = \frac{1}{|\nabla\omega|}$$

Primer: Debyeva aproksimacija

$$\omega_s(k) = c \cdot k \;;\; s = 1, \dots, 3$$

$$g_D(\omega) = 3\,\frac{4\pi}{8\pi^3} \int_0^{k_D} k^2\, dk\, \delta(\omega - ck) =$$

$$= \begin{cases} \dfrac{3}{2\pi^2}\,\dfrac{\omega^2}{c^3} & ; \quad \omega < \omega_D = k_D \cdot c \\ 0 & ; \quad \omega > \omega_D \end{cases}$$

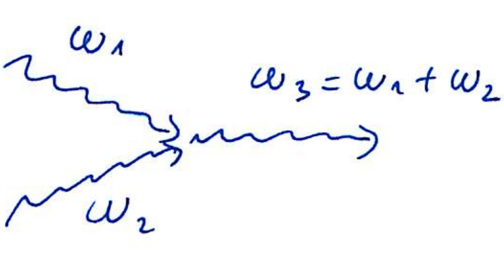
Pomen anharmonskih členov

Posledice "idealiziranega" harmonskega približka:

- Ni interakcije med fononi. Fononi imajo neskončni življenjski čas.
- Ni termičnega raztezanja
- Elastične konstante so neodvisne od p in T
- $c_V(T \to \infty) \sim 3 n k_B$: postane konstantna

V realnih kristalih moramo upoštevati tudi anharmonske člene!

Posledice anharmonskih členov:

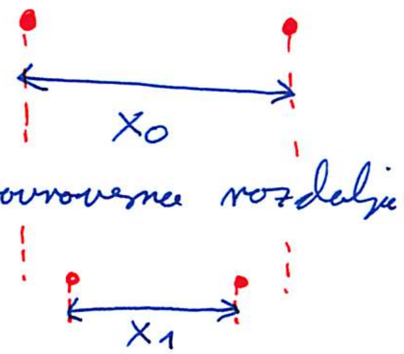


$$g\, a^{+}_{k_3}\, a_{k_2}\, a_{k_1}$$

– Termično raztezanje:

$$U(x) = cx^2 - gx^3 - fx^4$$

x: odmik od povprečne separacije (razdalje) med ionoma



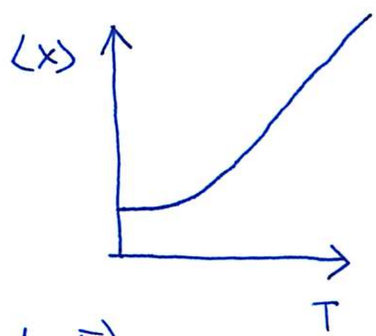
$$x = x_1 - x_0$$

$g>0$: popravek zaradi asimetrije, ki je posledica medsebojnega odboja med ionoma

$f>0$: posledica "mehčanja" nihanj pri velikih odmikih.

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} dx\, x\, e^{-\beta U(x)}}{\int_{-\infty}^{\infty} dx\, e^{-\beta U(x)}}$$

Pogoj: $g\langle x^3 \rangle$ ter $f x^4 < k_B T$: anharmonski členi morajo biti manjši od $k_B T$!



$$e^{-\beta U(x)} \cong e^{-\beta c x^2}\left(1 + \beta g x^3 + \beta f x^4\right)$$

$$\langle x \rangle \cong \frac{\int_{-\infty}^{\infty} dx\, e^{-\beta c x^2}\left(x + \beta g x^4 + \beta f x^5\right)}{\int_{-\infty}^{\infty} dx\, e^{-\beta c x^2}}$$

Linearni raztezek!

$$\langle x \rangle = \frac{3g}{4c^2} k_B T$$

Kinetična teorija mrežne topl. prevodnosti

Predpostavke:

a.) Privzamemo Debyev model

$$\omega = c \cdot k$$

Vsi fononi enako hitrost

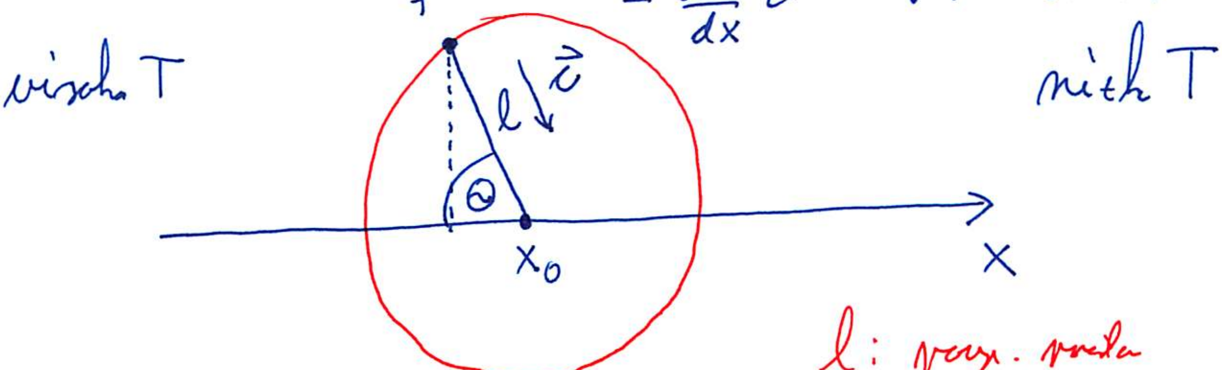
b.) Sipanje (trki) vzpostavljajo lokalno termodinamsko ravnovesje:

Po trku ima fonon pri $T(x)$ ravnovesno gostoto energije $w(x) = w^{eq}(T(x))$

c.) Doprinos fonona k toplotnem toku v smeri x: $c_x \cdot w(x)$; c_x: hitrost v smeri x

d.) Za izračun j_{θ} moramo povprečiti $c_x w(x)$ po vseh smereh (mestih) kjer je lahko prišlo do zadnjega trka (termalizacija)

$\xrightarrow{P}$ $-\frac{dT}{dx}$ gradient T le v x-smeri $\vec{\nabla} T = (\vec{\nabla} T)_x$



l: povp. vrednost ?

$$j_{\theta} = \langle c_x \, w(x_0 - l \cos\Theta) \rangle_{\Omega l}$$ povprečimo po celem prost. kotu

$$j_\Theta = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\Theta)\, \underbrace{c\cos\Theta}_{c_x}\, w(x_0 - l\cos\Theta)$$

$$= \frac{1}{2}\int_{-1}^{1} dy\, c\, y \left[w(x_0) - l y \frac{dw}{dx}\right]$$

c_V : specifična toplota!

$$\cancel{dd} \quad \frac{dw}{dx} = \frac{dw}{dT}\,\frac{dT}{dx}$$

$$j_\Theta = \underbrace{\frac{1}{3}\, c\, l\, c_V}_{K}\left(-\frac{dT}{dx}\right)$$

$$K = \frac{1}{3}\, c\, l\, c_V = \frac{1}{3}\, c^2\, \tau\, c_V$$

življenski čas (med trki)

Povprečna prosta pot l oz. življ. čas τ:

Na l, (τ) vpliva:

a.) sipanje fononov na nečistočah

b.) sipanje fononov na drugih fononih

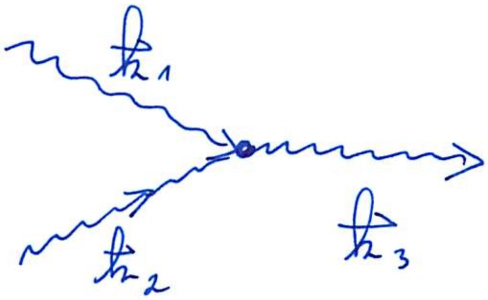
c.) sipanje na površini (surface el

Pomembno: obstajati mora mehanizem, ki vodi do lokalnega termičnega ravnovesja!

Kateri mehanizmi so možni kandidati za vzpostavitev termičnega ravnovesja?

a.) Sipanja na nečistočah (statičnih) ne spremenijo energije sipanega fonona – elastično sipanje $\Rightarrow$ ne vodijo do termičnega ravnovesja

b.) Tri – fononski členi:



– Normalni ~~pr~~ sipalni proces:

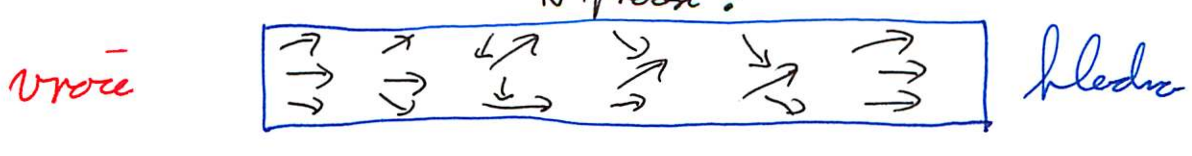
$$\vec{k}_1 + \vec{k}_2 = \vec{k}_3$$

Normalni sipalni proces ohranja celotno gibalno količino fononskega "plina"!

$$\vec{\mathcal{J}} = \underbrace{\sum_{\vec{k}} n_{\vec{k}} \hbar \vec{k}}_{\text{pred sip.}} = \underbrace{\sum_{\vec{k}} n_{\vec{k}} \hbar \vec{k}}_{\text{po sipanju}}$$

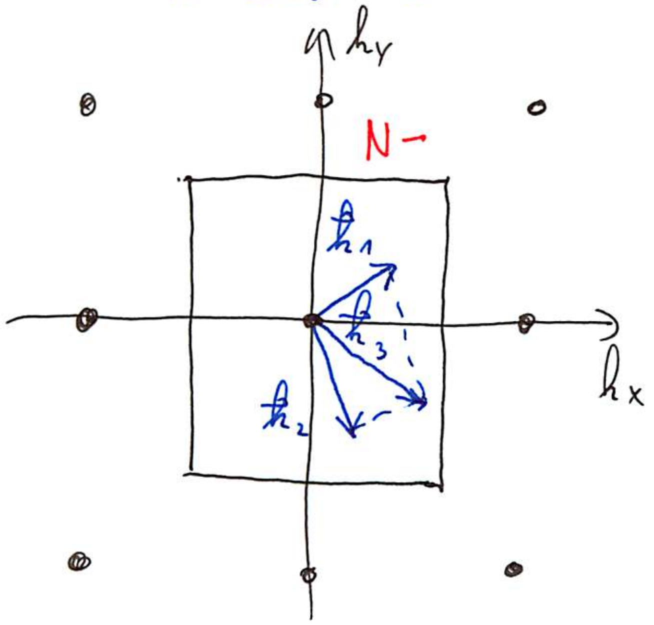
Če vzpostavimo porazdelitev, ki ima nek $\vec{\mathcal{J}} \neq 0$ na eni strani materiala, se le ta porazdelitev ohranja. $\Rightarrow$ Takšni procesi ne morejo prispevati k vzpostavitvi termičnega ravnovesja $\Rightarrow$ neskončna toplotna prevodnost

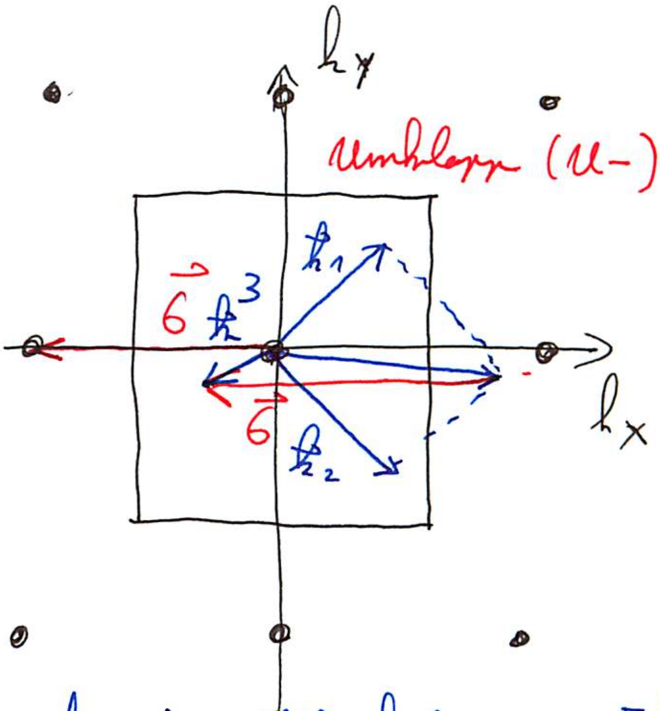
– Podobno kot plin v cevi s stenami, ki so idealno gladke:



- Umklapp procesi:

$$\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{G}$$





- Dovoljen proces, energija se ohranja, gibalna količina NE!

$$\hbar\omega(\vec{k}_1) + \hbar\omega(\vec{k}_2) = \hbar\omega(\vec{k}_3 + \vec{G}) = \hbar\omega(\vec{k}_3)$$

Ti procesi vodijo do termalizacije $\Rightarrow \vec{j}$ se ne ohranja.

Energija fononov, ki vodijo za nizanje do teh procesov mora biti dovolj velika $\sim \hbar\omega \sim \frac{k_B \Theta_D}{2}$

$K(T) = ?$

a.) $T \gg \Theta_D$ $\quad \tau \propto \frac{1}{n}$; $\quad n_{r,k} = \frac{1}{e^{\frac{\hbar\omega_{r,k}}{k_B T}} - 1} \cong \frac{k_B T}{\hbar\omega_{r,k}}$

$c_v \sim 3 n k_B \Rightarrow$

$$K \propto \frac{1}{T^x} \; ; \quad x \in [1, 2]$$

Vplivajo lahko tudi kvartični členi!

b.) $T \ll \Theta_D$

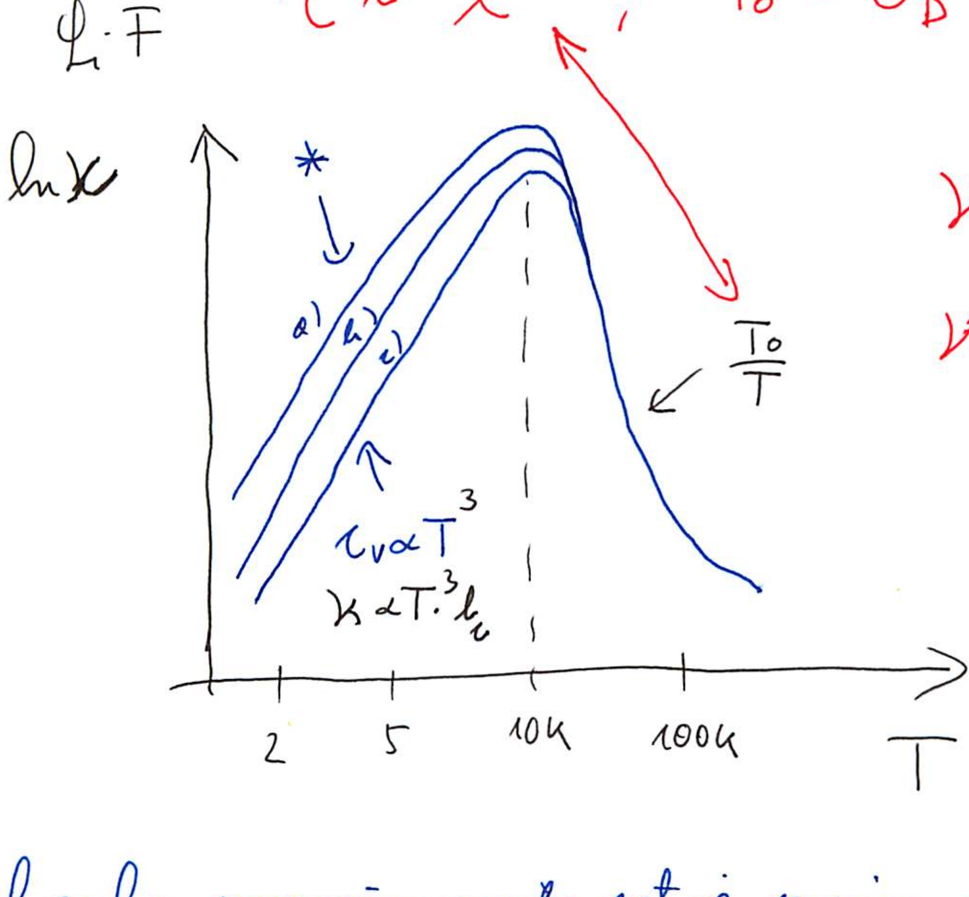
Pri nizkih T so zasedeni le fononi z $\hbar\omega_{q,t} \ll \hbar\omega_D$!

ter $k \ll k_D$

$$n_q(t) \cong \frac{1}{e^{\frac{\Theta_D}{T}}-1} \sim e^{-\frac{\Theta_D}{T}}$$

Zasedenost stanj, ki so okoli ω_D. Le ta stanja lahko vodijo do U-procesov!

$$\tau \sim e^{\frac{T_0}{T}} \; ; \; T_0 \sim \Theta_D$$



$$\kappa = \frac{1}{3} c^2 \tau \cdot c_V$$

$$\kappa = \frac{1}{3} c^2 \tau(T)\, c_V(T)!$$

* $l \sim l_c$ povprečna prosta pot je omejena z velikostjo kristala. a), b), c) ... * kristali različnih dimenzij!