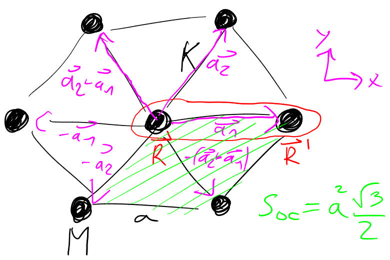
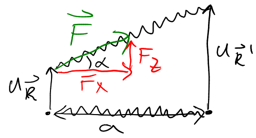
mrežna nihanja
- trikotna mreža
- odmiki naj bodo $\perp$ na ravnino kristala
- vzmeti so prednapete, samo med najbližjimi sosedi

$\vec{a}_1 = a(1,0)$

$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$





neraztegnjena vzmet je dolga $a_0 < a$

raztezek:

$$\sqrt{a^2 + (u_{\vec{R}'} - u_{\vec{R}})^2} - a_0 = \qquad |u_{\vec{R}'} - u_{\vec{R}}| \ll a$$

$$= a\sqrt{1 + \frac{(u_{\vec{R}'} - u_{\vec{R}})^2}{a^2}} - a_0 \doteq$$

$$\doteq a + \frac{1}{2}\frac{(u_{\vec{R}'} - u_{\vec{R}})^2}{a} - a_0 = a - a_0 + \frac{1}{2}\frac{(u_{\vec{R}'} - u_{\vec{R}})^2}{a}$$

velikost sile:

$$F = K\left(a - a_0 + \frac{1}{2}\frac{(u_{\vec{R}'} - u_{\vec{R}})^2}{a}\right)$$

$$F_x = F\cos\alpha \doteq F\left(1 - \frac{\alpha^2}{2}\right) = K(a - a_0) + \mathcal{O}\left((u_{\vec{R}'} - u_{\vec{R}})^2\right)$$

$$F_z = F\sin\alpha \doteq F\alpha = \underbrace{K\frac{a-a_0}{a}}_{\tilde{K}}(u_{\vec{R}'} - u_{\vec{R}}) + \mathcal{O}\left((u_{\vec{R}'} - u_{\vec{R}})^3\right)$$

$$\alpha \doteq \operatorname{tg}\alpha = \frac{u_{\vec{R}'} - u_{\vec{R}}}{a}$$

$$M\ddot{u}_{\vec{R}} = \tilde{K}\sum_{\vec{R}'=n.s.\vec{R}} (u_{\vec{R}'} - u_{\vec{R}})$$

$$u_{\vec{R}} = u_0 e^{i(\vec{q}\cdot\vec{R} - \omega t)}$$

$$e^{-i\vec{q}\cdot\vec{R}} \,/\, -M\omega^2 \cancel{u_0} e^{i(\vec{q}\cdot\vec{R} - \cancel{\omega t})} =$$

$$= \tilde{K}\sum_{\vec{R}'=n.s.\vec{R}} \cancel{u_0}\left(e^{i(\vec{q}\cdot\vec{R}' - \cancel{\omega t})} - e^{i(\vec{q}\cdot\vec{R} - \cancel{\omega t})}\right)$$

$$-M\omega^2 = \tilde{K}\sum_{\vec{R}'=n.s.\vec{R}} \left[e^{i\vec{q}\cdot(\vec{R}'-\vec{R})} - 1\right]$$

$$-M\omega^2 = \tilde{K}\left(e^{i\vec{q}\cdot\vec{a}_1} - 1 + e^{i\vec{q}\cdot\vec{a}_2} - 1 + e^{i\vec{q}\cdot(\vec{a}_2-\vec{a}_1)} - 1 + e^{-i\vec{q}\cdot\vec{a}_1} - 1 + \dots\right) =$$

$$= \tilde{K}\left(2\cos(\vec{q}\cdot\vec{a}_1) - 2 + 2\cos(\vec{q}\cdot\vec{a}_2) - 2 + 2\cos[\vec{q}\cdot(\vec{a}_2 - \vec{a}_1)] - 2\right) = \qquad \sin^2\frac{\alpha}{2} = \frac{1-\cos\alpha}{2}$$

$$= \tilde{K}\left(-4\sin^2\frac{\vec{q}\cdot\vec{a}_1}{2} - 4\sin^2\frac{\vec{q}\cdot\vec{a}_2}{2} - 4\sin^2\frac{\vec{q}\cdot(\vec{a}_2-\vec{a}_1)}{2}\right)$$

$$\omega^2 = \frac{4\tilde{K}}{M}\left(\sin^2\frac{\vec{q}\cdot\vec{a}_1}{2} + \sin^2\frac{\vec{q}\cdot\vec{a}_2}{2} + \sin^2\frac{\vec{q}\cdot(\vec{a}_2-\vec{a}_1)}{2}\right)$$

$\vec{a}_1 = a(1,0)$

$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

$\vec{a}_2 - \vec{a}_1 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

$$\boxed{\omega^2 = \frac{4\tilde{K}}{M}\left(\sin^2\frac{q_x a}{2} + \sin^2\frac{(q_x + \sqrt{3}q_y)a}{4} + \sin^2\frac{(-q_x + \sqrt{3}q_y)a}{4}\right)} \longrightarrow \omega(\vec{q}=0) = 0 \quad \text{akustična}$$

$\omega\left(|\vec{k}| \ll \frac{\pi}{a}\right) = c(\varphi)\,k$

↳ hitrost zvoka

$\vec{k} = (k\cos\varphi, k\sin\varphi)$

$$\omega^2 \doteq \frac{4\tilde{K}}{M}\left(\frac{q_x^2 a^2}{4} + \frac{(q_x^2 + \cancel{2\sqrt{3}q_x q_y} + 3q_y^2)a^2}{16} + \frac{(q_x^2 - \cancel{2\sqrt{3}q_x q_y} + 3q_y^2)a^2}{16}\right) =$$

$$= \frac{\tilde{K}a^2}{M}\left(\frac{3}{2}q_x^2 + \frac{3}{2}q_y^2\right) = \frac{3\tilde{K}a^2}{2M}q^2 \longrightarrow \omega = \underbrace{\sqrt{\frac{3\tilde{K}}{2M}}\,a}_{=c \neq c(\varphi)}\,k$$

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prispevek teh nihanj k specifični toploti kristala:

$$C = \frac{dE}{dT} \qquad E = \sum_{\vec{q}\in 1BC} \hbar\omega_{\vec{q}}\left(n_{\vec{q}} + \frac{1}{2}\right) = \sum_{\vec{q}\in 1BC} \hbar\omega_{\vec{q}}\left(\frac{1}{e^{\beta\hbar\omega_{\vec{q}}} - 1} + \frac{1}{2}\right) =$$

$$= \left(\frac{L}{2\pi}\right)^2 \int_{1BC} d\vec{q}\; \hbar\omega_{\vec{q}}\left(\frac{1}{e^{\beta\hbar\omega_{\vec{q}}} - 1} + \frac{1}{2}\right)$$

1.) nizke temperature (velik β)

$\beta\hbar\omega_{\vec{k}} \gg 1$ razen za $\vec{q}$ v bližini središča 1BC

↳ $n_{\vec{q}} \to 0$

$$E = \left(\frac{L}{2\pi}\right)^2 \int_{\infty} d\vec{q}\; \hbar c q \frac{1}{e^{\beta\hbar c k} - 1} + \text{konst.}$$

$$E = \left(\frac{L}{2\pi}\right)^2 \int_0^\infty 2\pi q\, dq\, \frac{\hbar c q}{e^{\beta\hbar c k} - 1} + \text{konst.}$$

$u = \beta\hbar c k$

$$E = \left(\frac{L}{2\pi}\right)^2 \int_0^\infty 2\pi \frac{u}{\beta\hbar c}\frac{du}{\beta\hbar c}\frac{\frac{u}{\beta}}{e^u-1} + \text{konst} =$$

$$= \frac{L^2}{2\pi\cdot\beta^3\hbar^2c^2}\int_0^\infty \frac{u^2\,du}{e^u-1} + \text{konst}$$

$$\frac{u^2}{e^u-1} = \begin{cases} u\,; & u \ll 1 \\ u^2 e^{-u}\,; & u \gg 1\end{cases}$$

$$E = \frac{L^2 (k_B T)^3}{\hbar^2 c^2}\cdot\frac{1}{2\pi}\int_0^\infty \frac{u^2\,du}{e^u-1} + \text{konst}$$

specifična toplota na atom

površina kristala

$$C = \frac{1}{N}\frac{dE}{dT} = \frac{S\,k_B^3T^2}{N\hbar^2c^2}\cdot\frac{3}{2\pi}\int\frac{u^2\,du}{e^u-1}$$

št. atomov

$$c^2 = \frac{3}{2}\frac{\tilde{K}}{M}a^2$$

površina osnovne celice: $S_{oc} = \frac{a^2\sqrt{3}}{2}$

$$S = N S_{oc}$$

$$\frac{S}{N} = S_{oc} = \frac{a^2\sqrt{3}}{2}$$

$$C = \frac{\cancel{a^2}\sqrt{3}}{2}\,\frac{k_B^3T^2}{\hbar^2\cdot\frac{\cancel{3}}{\cancel{2}}\frac{\tilde{K}}{M}\cancel{a^2}}\cdot\frac{\cancel{3}}{\cancel{2}\pi}\int_0^\infty\frac{u^2\,du}{e^u-1}$$

$$C = k_B\cdot\frac{(k_BT)^2}{\left(\hbar\sqrt{\frac{\tilde{K}}{M}}\right)^2}\cdot\frac{\sqrt{3}}{2\pi}\int_0^\infty\frac{u^2\,du}{e^u-1}$$

$\omega_0 = \sqrt{\frac{\tilde{K}}{M}}$ $\qquad \omega(\text{na robu 1BC}) \approx \omega_0$

$$\boxed{C = k_B\cdot\left(\frac{k_BT}{\hbar\omega_0}\right)^2\cdot\frac{\sqrt{3}}{2\pi}\int_0^\infty\frac{u^2\,du}{e^u-1}}$$

$\rightarrow C \propto T^2 \rightarrow$ **2D** kristal

2.) <u>visoke temperature</u> (majhen β) $\longrightarrow \beta\hbar\omega_0 \ll 1$

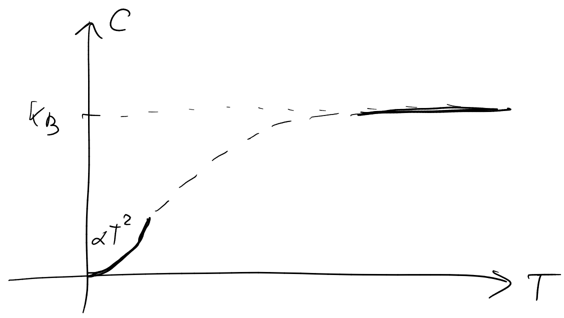
$\beta\hbar\omega(\vec{q}) \ll 1$ za $\forall\vec{q}$

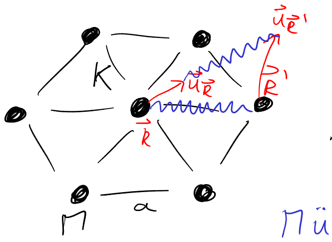
$$E = \sum_{\vec{q}\in 1BC}\hbar\omega_{\vec{q}}\left(\frac{1}{e^{\beta\hbar\omega_{\vec{q}}}-1}+\frac{1}{2}\right) \doteq$$

$$\doteq \sum_{\vec{q}\in 1BC}\hbar\omega_{\vec{q}}\left(\frac{1}{\cancel{1}+\beta\hbar\omega_{\vec{q}}-\cancel{1}}+\frac{1}{2}\right) = \sum_{\vec{q}\in 1BC}\frac{1}{\beta} + \text{konst} =$$

$$= k_BT\left(\sum_{\vec{q}\in 1BC}1\right) + \text{konst} = k_BTN + \text{konst}$$

$$C = \frac{1}{N}\frac{dE}{dT} = k_B$$





odmiki v ravnini kristalne mreže (v 2D)

(v 3D so odmiki v poljubni smeri)

vzameti nižo predpogoste

$$M\ddot{\vec u}_{\vec R} = \sum_{\text{na } \vec R} \vec F$$

Lagrange: $L = T - V \longrightarrow \dfrac{\partial L}{\partial \vec u_{\vec R}} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{\vec u}_{\vec R}} = 0$

$$T = \sum_{\vec R} \frac{1}{2} M \left(\dot{\vec u}_{\vec R}\right)^2$$

$$V = \frac{1}{2}\sum_{\vec R' \neq \vec R} \frac{1}{2} K_{\vec R' - \vec R}\left[\underbrace{\left|\vec R' + \vec u_{\vec R'} - (\vec R + \vec u_{\vec R})\right|} - \cancel{|\vec R' - \vec R|}\right]^2$$

$$\left|\vec R' - \vec R + (\vec u_{\vec R'} - \vec u_{\vec R})\right| = \sqrt{(\vec R' - \vec R + \vec u_{\vec R'} - \vec u_{\vec R})^2} =$$

$$= \sqrt{(\vec R' - \vec R)^2 + 2(\vec R' - \vec R)\cdot(\vec u_{\vec R'} - \vec u_{\vec R}) + \dots} =$$

$$= |\vec R' - \vec R|\sqrt{1 + 2\frac{(\vec R' - \vec R)\cdot(\vec u_{\vec R'} - \vec u_{\vec R})}{|\vec R' - \vec R|^2} + \dots} \doteq$$

$$\doteq |\vec R' - \vec R|\left(1 + \frac{(\vec R' - \vec R)\cdot(\vec u_{\vec R'} - \vec u_{\vec R})}{|\vec R' - \vec R|^2}\right) =$$

$$= \cancel{|\vec R' - \vec R|} + \frac{(\vec R' - \vec R)\cdot(\vec u_{\vec R'} - \vec u_{\vec R})}{|\vec R' - \vec R|}, \qquad \frac{\vec R' - \vec R}{|\vec R' - \vec R|} = \hat e_{\vec R' - \vec R}$$

$$V = \frac{1}{4}\sum_{\vec R' \neq \vec R} K_{\vec R' - \vec R}\left[(\vec u_{\vec R'} - \vec u_{\vec R})\cdot \hat e_{\vec R' - \vec R}\right]^2$$

$\forall \vec R_0$:

$$\boxed{\frac{\partial L}{\partial \vec u_{\vec R_0}}} = -\frac{\partial V}{\partial \vec u_{\vec R_0}} = -\frac{1}{4}\sum_{\vec R' \neq \vec R} K_{\vec R' - \vec R}\, 2\left[(\vec u_{\vec R'} - \vec u_{\vec R})\cdot \hat e_{\vec R' - \vec R}\right]\left(\underbrace{\delta_{\vec R', \vec R_0}}_{= \frac{\partial \vec u_{\vec R'}}{\partial \vec u_{\vec R_0}}} - \delta_{\vec R, \vec R_0}\right)\cdot \hat e_{\vec R' - \vec R} =$$

$$= -\frac{1}{2}\sum_{\vec R \neq \vec R_0} K_{\vec R_0 - \vec R}\left[(\vec u_{\vec R_0} - \vec u_{\vec R})\cdot \hat e_{\vec R_0 - \vec R}\right]\hat e_{\vec R_0 - \vec R} + \frac{1}{2}\sum_{\vec R \neq \vec R_0} \underbrace{K_{\vec R - \vec R_0}}_{= K_{\vec R_0 - \vec R}}\left[\underbrace{(\vec u_{\vec R} - \vec u_{\vec R_0})}_{= -(\vec u_{\vec R_0} - \vec u_{\vec R})}\cdot \underbrace{\hat e_{\vec R - \vec R_0}}_{= -\hat e_{\vec R_0 - \vec R}}\right]\underbrace{\hat e_{\vec R - \vec R_0}}_{= -\hat e_{\vec R_0 - \vec R}} =$$

$$= \boxed{-\sum_{\vec R \neq \vec R_0} K_{\vec R_0 - \vec R}\left[(\vec u_{\vec R_0} - \vec u_{\vec R})\cdot \hat e_{\vec R_0 - \vec R}\right]\hat e_{\vec R_0 - \vec R}}$$