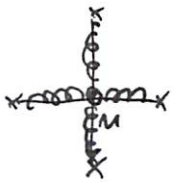
Square lattice, springs b/w nearest-neighbors only:

$10 + 10 + 10 + \cancel{10}^{10} + 10 = 10$

n.n. $\delta \in \{\pm\vec{a}_1, \pm\vec{a}_2\}$, $a_1 = a(1,0)$, $a_2 = a(0,1)$; $\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + \vec{u}_n$

Pot. energy: $$U_n = \frac{k}{2}\left\{\sum_\delta \left[\,|\vec{R}_n - \vec{R}_{n+\delta}| - |\vec{\delta}|\,\right]^2 = \frac{k}{2}\sum_\delta \left[\frac{\vec{\delta}}{\delta}\cdot\left(\vec{u}_n - \vec{u}_{n+\delta}\right)\right]^2 + \mathcal{O}(u^3) =\right.$$



$$= \frac{k}{2}\left\{\left[u_n^x - u_{n+\hat{1}}^x\right]^2 + \left[u_n^x - u_{n-\hat{1}}\right]^2 + \left[u_n^y - u_{n+\hat{2}}^y\right]^2 + \left[u_n^y - u_{n-\hat{2}}^y\right]^2\right\}$$

$$U = \frac{1}{2}\sum_n U_n = \frac{1}{2}\frac{k}{2}\sum_{n,\delta}\left[\,|\vec{R}_n - \vec{R}_{n+\delta}| - \delta\right]^2 = \frac{1}{2}\frac{k}{2}\sum_n\Big\{\left(u_n^x - u_{n+\hat{1}}^x\right)^2 + \left(u_n^x - u_{n-\hat{1}}^x\right)^2$$
$$+ \left(u_n^y - u_{n+\hat{2}}^y\right)^2 + \left(u_n^y - u_{n-\hat{2}}^y\right)^2\Big\} =$$

sum over all Bravais lattice vectors, but put factor of ½ in front since U_n is energy of a pair!

$$= \frac{1}{2}\frac{k}{2}\sum_n\Big\{\left(u_n^x\right)^2 - 2u_n^x u_{n+\hat{1}}^x + \left(u_{n+\hat{1}}^x\right)^2 + \left(u_n^x\right)^2 - 2u_n^x u_{n-\hat{1}}^x + \left(u_{n-\hat{1}}^x\right)^2$$
$$+ \left(u_n^y\right)^2 - 2u_n^y u_{n+\hat{2}}^y + \left(u_{n+\hat{2}}^y\right)^2 + \left(u_n^y\right)^2 - 2u_n^y u_{n-\hat{2}}^y + \left(u_{n-\hat{2}}^y\right)^2\Big\} =$$

$$= \frac{1}{2}\frac{k}{2}\sum_n\Big\{2\left(\left(u_n^x\right)^2 + \left(u_n^y\right)^2\right) + \left(u_{n+\hat{1}}^x\right)^2 + \left(u_{n-\hat{1}}^x\right)^2 + \left(u_{n+\hat{2}}^y\right)^2 + \left(u_{n-\hat{2}}^y\right)^2$$
$$- 2\left(u_n^x u_{n+\hat{1}}^x + u_n^x u_{n-\hat{1}}^x + u_n^y u_{n+\hat{2}}^y + u_n^y u_{n-\hat{2}}^y\right)\Big\}.$$

$$U = \frac{1}{2}\frac{k}{2}\sum_{n}\Big\{\Big[2(u_n^x)^2 + 2(u_n^y)^2 + (u_{n+\hat{1}}^x)^2 + (u_{n+\hat{2}}^y)^2 + (u_{n-\hat{1}}^x)^2 + (u_{n-\hat{2}}^y)^2\Big]$$
$$-2\Big[u_n^x u_{n+\hat{1}}^x + u_n^x u_{n-\hat{1}}^x + u_n^y u_{n+\hat{2}}^y + u_n^y u_{n-\hat{2}}^y\Big]\Big\}.$$

$\hat{1} = (1,0)$
$\hat{2} = (0,1)$.
$n = (n_1, n_2)$.

The matrix of force constants is defined as

$$U = \frac{1}{2}\sum_{n,m}\sum_{\substack{i,k \\ \in\{x,y\}}} C_{ik}\left(\vec{R}_n^{(0)} - \vec{R}_m^{(0)}\right) u_n^i u_m^k .$$

We thus <u>read-off</u> its elements:

$$C_{xx}(\vec{0}) = 2k, \quad C_{xy}(\vec{0}) = 0, \quad C_{xx}(\vec{a}_1) = -k, \quad C_{xx}(-\vec{a}_1) = -k$$
$$C_{yx}(\vec{0}) = 0, \quad C_{yy}(\vec{0}) = 2k, \quad C_{yy}(\vec{a}_2) = -k, \quad C_{yy}(-\vec{a}_2) = -k .$$

<u>Check:</u> $\sum_{R_m} C_{ij}(R_m) = 0$ is fulfilled for all elements.

Calculate <u>elasticity tensor</u>:

$$K_{ijkl} = -\frac{1}{8 v_{EZ}} \sum_n \Big[R_{n,j} R_{n,l} C_{ik}(R_n) + R_{n,i} R_{n,l} C_{jk}(R_n) + R_{n,j} R_{n,k} C_{il}(R_n) + R_{n,i} R_{n,k} C_{jl}(R_n) \Big].$$

$v_{EZ} = 1$; only non-zero elements <u>with</u> $R_n \neq 0$ are: $C_{xx}(\pm \vec{a}_1) = -2\kappa$; $C_{yy}(\pm \vec{a}_2) = -2\kappa$.

$\Rightarrow$ only non-zero elements:

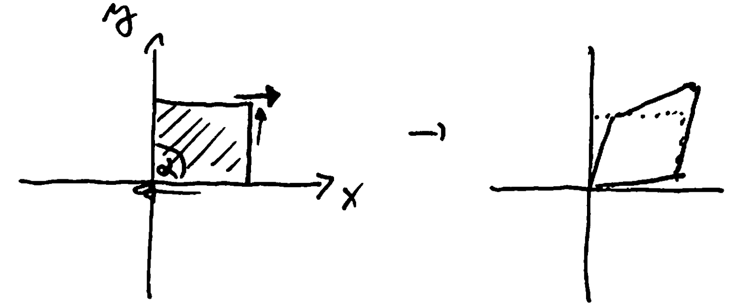
$$\boxed{K_{xxxx} = \kappa, \quad K_{yyyy} = \kappa, \quad \text{all other elements of } K_{ijkl} \text{ vanish.}}$$

Response to shear stress: general stress-strain relation:

$$\sigma_{ij} = K_{ijkl}\, u_{kl}, \quad \text{where } \sigma_{ij} = \text{force on surface } j \text{ in direction } i$$

σ_{ij}: stress tensor (Spannungstensor)
K_{ijkl}: tensor of elasticity
u_{kl}: strain tensor (Verzerrungstensor)
i: f_i
j: normal of surface.

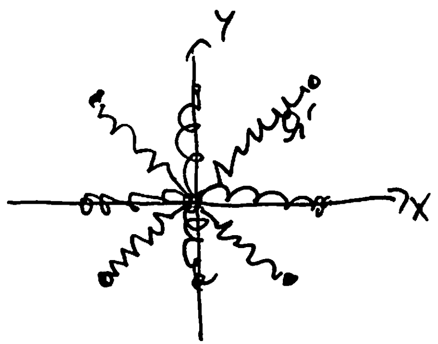
Response to shear stress: $\sigma_{xy} \neq 0$
(changing angle α):



$$\sigma_{xy} = \underbrace{K_{xy\beta l}}_{=0}\, u_{\beta l} \quad \Rightarrow \quad u_{\beta l} \Rightarrow \infty .$$

$\Rightarrow$ Response is infinite! no restoring force against shear stress in this model with $\gamma' = 0$.

Now, we add springs with spring constants γ' along next-nearest-neighbor diagonals.



$$\vec{\delta}' \in \{ a_1 + a_2,\ a_1 - a_2,\ -a_1 + a_2,\ -a_1 - a_2 \}.$$

$$|\vec{\delta}'| = \sqrt{2}.$$

New terms in the potential energy:

$$U_n = U_n(\gamma) + U_n(\gamma') : \quad U_n(\gamma') = \frac{\gamma'}{2} \sum_{\delta'} \left[\frac{\vec{\delta}'}{\delta'} \cdot \left(\vec{u}_n - \vec{u}_{n+\vec{\delta}'} \right) \right]^2 =$$

$$= \frac{\gamma'}{2} \Big\{ \frac{1}{2} \left[u_n^x - u_{n+1+2}^x + u_n^y - u_{n+1+2}^y \right]^2 + \frac{1}{2} \left[u_n^x - u_{n+1-2}^x - u_n^y + u_{n+1-2}^y \right]^2$$
$$+ \frac{1}{2} \left[-u_n^x + u_{n-1+2}^x + u_n^y - u_{n-1+2}^y \right]^2 + \frac{1}{2} \left[-u_n^x + u_{n-1-2}^x - u_n^y + u_{n-1-2}^y \right]^2 \Big\} =$$

$(C_{ij}(R_n - R_m))$ $(R_n = R_m)$

Diagonal elements do not matter for elastic tensor. Consider only $R_n \neq R_m$:

$$U_M(\vartheta') = \text{diagonal elements}\left(u_n^i u_m^k \delta_{nm}\right) + \frac{\vartheta'}{2}\Big\{\Big[u_n^x u_{n+1+2}^x - u_n^x u_{n+1+2}^y - u_{n+1+2}^x u_n^y - u_n^y u_{n+1+2}^y\Big] + \Big[-u_n^x u_{n+1-2}^x + u_n^x u_{n+1-2}^y \quad \ldots$$

Read-off matrix of force constants: $U = \frac{1}{2} \sum_n \left[U_n(k) + U_n(k') \right]$

$$C_{xx}(\vec{a}_1 + \vec{a}_2) = -k'/2$$
$$C_{xy}(a_1 + a_2) = -k'/2$$
$$C_{yx}(a_1 + a_2) = -k'/2$$
$$C_{yy}(a_1 + a_2) = -k'/2$$

$$C_{xx}(+a_1 - a_2) = -k'/2$$
$$C_{xy}(+a_1 - a_2) = k'/2$$
$$C_{yx}(a_1 - a_2) = k'/2$$
$$C_{yy}(a_1 - a_2) = -k'/2$$

$$C_{xx}(-a_1 + a_2) = -k'/2$$
$$C_{xy}(-a_1 + a_2) = k'/2$$
$$C_{yx}(-a_1 + a_2) = k'/2$$
$$C_{yy}(-a_1 + a_2) = -k'/2$$

$$C_{xx}(-a_1 - a_2) = -k'/2$$
$$C_{xy}(-a_1 - a_2) = -k'/2$$
$$C_{yx}(-a_1 - a_2) = -k'/2$$
$$C_{yy}(-a_1 - a_2) = -k'/2$$

$$K_{xxxx} = -\frac{1}{8}\left[-2k' - 2k' - 2k' - 2k' \right] = k'$$
$$K_{xxyy} =$$

It follows:

$$K_{xxxx} = k + k' \qquad K_{xyxy} = k'$$
$$K_{yyyy} = k + k' \qquad K_{yxyx} = k'$$
$$K_{xxyy} = k' \qquad K_{xyyx} = k'$$
$$K_{yyxx} = k' \qquad K_{yxxy} = k'$$

Response to shear stress now <u>finite</u>.

$$\sigma_{xy} = K_{xykl}\, u_{kl} = K_{xyxy}\, u_{xy} + K_{xyyx}\, u_{yx} =$$

$$= k'(u_{xy} + u_{yx}) = 2k'\, u_{xy} \Rightarrow$$

$$\sigma_{yx} = k'(u_{yx} + u_{xy}) \Rightarrow \quad \Rightarrow \boxed{u_{xy} = \frac{1}{2k'}\,\sigma_{xy}}$$

② ⓐ Energy unit $\mathcal{E}$ ~ $\frac{me^4}{\hbar^2}$ (Rydberg) ~10eV

Length unit a ~ $\frac{\hbar^2}{me^2}$ (Bohr radius) ~ 1-10 nm
Distance between the atoms

$$\mathcal{E} \sim \delta a^3 \longrightarrow \delta \sim \frac{\mathcal{E}}{a^3}$$

$$\mathcal{E} \sim \gamma a^4 \longrightarrow \gamma \sim \frac{\mathcal{E}}{a^4}, \beta \sim \frac{\mathcal{E}}{a^2}$$

The crystal exists when the amplitude of the fluctuations is sufficiently small, $\langle x^2 \rangle \ll a^2$

Under these ~~assumptions~~ assumptions the expansion of U in x is the expansion in the small parameter $\frac{\langle |x| \rangle}{a}$

ⓑ according to 2a, δx^3 and γx^4 will cause only small corrections

The condition of the smallness of the oscillations:

$$\beta a^2 \gg T$$

The frequency of the harmonic oscillations: $\omega = \left(\frac{\beta}{m}\right)^{\frac{1}{2}}$

$\omega \ll T \longleftrightarrow$ Classical oscillations

$$\bar{x} = \frac{\int_{-\infty}^{+\infty} x e^{-\frac{U(x)}{T}} dx}{\int_{-\infty}^{+\infty} e^{-\frac{U(x)}{T}} dx}$$

Only the correction from the 3rd term matters

$$\int x e^{-\frac{U(x)}{T}} dx \longrightarrow \int x e^{-\frac{\gamma x^2}{T}} \left(1 - \frac{\delta x^3}{T}\right) dx =$$

$$= -\frac{\delta}{T} \int_{-\infty}^{+\infty} x^4 e^{-\frac{\beta x^2}{T}} dx = -\frac{\delta}{T} \left(\frac{T}{\beta}\right)^{\frac{5}{2}} \underbrace{\Gamma\left(\frac{5}{2}\right)}_{= \frac{3\sqrt{\pi}}{4}} = \boxed{-\frac{3\sqrt{\pi}}{4} \frac{\delta T^{\frac{3}{2}}}{\beta^{\frac{5}{2}}} = \bar{x}}$$

$$e^{-\frac{\beta x^2}{T}}\,dx = \sqrt{\frac{\pi T}{\beta}}$$

$$\overline{x} = \frac{\frac{3\sqrt{\pi}}{4}\,\frac{\delta T^{\frac{3}{2}}}{\beta^{\frac{5}{2}}}}{\sqrt{\frac{\pi T}{\beta}}} = -\frac{3}{4}\frac{\delta}{\beta^2}T \qquad (*)$$

Average distance $\quad l = a + \overline{x}$

$$\alpha = \frac{1}{l}\frac{dl}{dT} = \boxed{\frac{-3}{4}\frac{\delta}{\beta^2 a} = \alpha}$$

$$\alpha \sim \frac{1}{\varepsilon} \sim 10^{-5}\,K^{-1} \quad \checkmark$$

cf. 2a

2c

$$\mu\ddot{x} = -2\beta x - 3\delta x^2 - 4\gamma x^3 \qquad (1)$$

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass

(The centre of mass is moving under its own inertia)

Average (1) over 1 period

$$\langle\ddot{x}\rangle \equiv \frac{\langle\dot{x}(T)\rangle - \langle\dot{x}(0)\rangle}{T} = 0$$

Then (1) $\rightarrow \quad 2\beta\overline{x} = -3\delta\langle x^2\rangle \rightarrow$

$$\rightarrow \quad \overline{x} = -\frac{3\delta}{2\beta}\langle x^2\rangle = \boxed{-\frac{3\delta}{4\beta^2}T = x}$$

In agreement with $(*)$