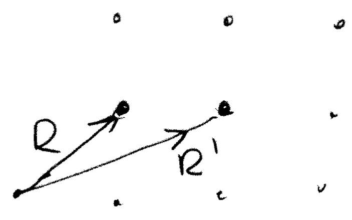
Elasticity of classical harmonic lattice

Consider lattice of atoms, that interact with pair potential $V(R-R')$

The total energy is

$$E_{int} = \frac{1}{2}\sum_{RR'} V(\vec{R}-\vec{R}')$$



- If atoms are displaced then the energy is

$$E_{int} = \frac{1}{2}\sum_{RR'} V(\vec{R}-\vec{R}'+\vec{u}(R)-\vec{u}(R')) =$$

$$= E_0 + \frac{1}{2}\sum_{R,R'} \frac{\partial V}{\partial R_i}\left[u_i(R)-u_i(R')\right] +$$

$$+ \frac{1}{4}\sum_{R,R'} \frac{\partial^2 V(R-R')}{\partial R_i \partial R_j}\left[u_i(R)-u_i(R')\right]\left[u_j(R)-u_j(R')\right]$$

- Because initial positions $(u=0)$ were equilibrium positions the linear in $u(R)$ term vanishes. As a result we obtain

$$\delta E_{int} = \frac{1}{4} \sum_{R,R',i,j} C_{ij}(R-R')[u_i(R)-u_i(R')][u_j(R)-u_j(R')]$$

with $C_{ij} = \dfrac{\partial^2 V(R)}{\partial R_i \partial R_j}$

Expanding $u_i(R) = u_i(R') + \dfrac{\partial u_i}{\partial R_j}(R-R')_j$

and shifting $R-R' \to R$ we rewrite

- $$\delta E_{int} = \frac{N}{4} \sum_R C_{ik}(R) R_j R_l \frac{\partial u_i}{\partial R_j} \frac{\partial u_k}{\partial R_l}$$

N is the total number of atoms

Since energy does not change under rotation we can replace

- $$\frac{\partial u_i}{\partial r_j} = \frac{1}{2}\left(\frac{\partial u_i}{\partial R_j} + \frac{\partial u_j}{\partial R_i}\right) + \cancel{\frac{1}{2}\left(\frac{\partial u_i}{\partial R_j} - \frac{\partial u_j}{\partial R_i}\right)} \to u_{ij}$$

Then

$$\delta E_{int} = \frac{N}{4} \sum_R C_{ik} R_j R_l u_{ij} u_{kl}$$

To write it in symmetrized form let us interchage indices and $i \leftrightarrow j$, $k \leftrightarrow l$ and add

$$\delta E_{int} = \frac{N}{16} \sum \left[C_{ik} R_j R_l u_{ij} u_{kl} + C_{jk} R_i R_l u_{ji} u_{ki} + C_{il} R_j R_k u_{ij} u_{lk} + C_{jl} R_i R_k u_{ji} u_{lk} \right.$$

Since $u_{ij} = u_{ji}$, $u_{kl} = u_{lk}$

all $u_{\sqcup} u_{\sqcup}$ are the same and we obtain

$$\delta E_{int} = \frac{N}{16} \sum_R \left[C_{ik} R_j R_l + C_{jk} R_i R_l + C_{il} R_j R_k + C_{jl} R_i R_k \right] u_{ij} u_{kl}$$

Elastic tensor is defined as

$$\delta E_{el} = \frac{1}{2} \int dV \lambda_{ijkl} u_{ij} u_{kl} \quad \Rightarrow$$

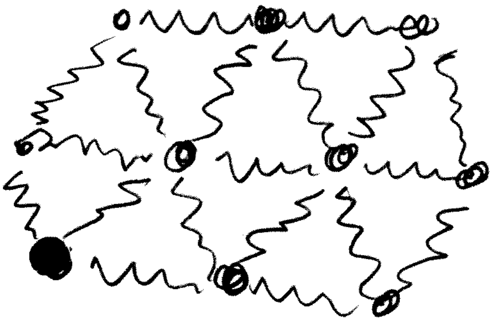
$$\lambda_{ijkl} = \frac{1}{8V_0} \sum_R \left[C_{ik}(R) R_j R_l + C_{jk}(R) R_i R_l + C_{il}(R) R_j R_k + C_{jl}(R) R_i R_k \right]$$

where V_0 is the unit cell volume

$V = N V_0$

Example

Consider hexagonal lattice of mass points connected by harmonic springs between nearest neighbors.



Interaction potential

$$V = \frac{\alpha}{2}\left(\sqrt{x^2+y^2} - a\right)^2 =$$

$$= \frac{\alpha}{2}\left(x^2+y^2+a^2-2a\sqrt{x^2+y^2}\right)$$

$$C_{xx} = V''_{xx} = \alpha\left(1 - \frac{a\,y^2}{(x^2+y^2)^{3/2}}\right) = \alpha\left(1 - \frac{y^2}{a^2}\right)$$

$$C_{yy} = V''_{yy} = \alpha\left(1 - \frac{x^2}{a^2}\right)$$

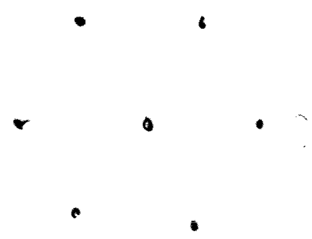
$$C_{xy} = V''_{xy} = \alpha\,\frac{xy}{a^2}$$

$$\lambda_{ijkl} = \frac{1}{8S_0}\sum_R \Big[C_{ik}(R)\,R_j R_l + C_{jk}(R)\,R_i R_l +$$

$$+ C_{il}(R)\,R_j R_k + C_{jl}(R)\,R_i R_k\Big]$$

$$S_0 = \square = a^2\frac{\sqrt{3}}{2}$$

We should sum over 6 neighbors



$$\lambda_{xxxx} = \frac{1}{8S_0} 4 \sum_R C_{xx}(R)\, X^2 = \frac{\alpha a^2}{8S_0} 4 \cdot \left[2 + 4 \cdot \frac{1}{4} \cdot \frac{1}{4}\right) = \frac{9\alpha}{8S_0}$$

$$\lambda_{xxyy} = \frac{1}{8S_0} 4 \sum_R C_{xy}(R)\, xy = \frac{\alpha}{8S_0} 4 \sum \frac{x^2 y^2}{a^4} = \frac{3\alpha a^2}{8S_0}$$

$$\lambda_{xyxy} = \frac{1}{8S_0} \sum_R \left[C_{xx}(R)\, y^2 + 2C_{xy}\, xy + C_{yy}\, x^2\right] =$$

$$= \frac{\alpha}{8S_0}\left[\frac{3}{4} + 2 \cdot \frac{3}{4} + \frac{3}{4}\right] = \frac{3\alpha a^2}{8S_0}$$

Thus $E_{el} = \frac{\lambda_{xxxx}}{2}\left(u_{xx}^2 + u_{yy}^2\right) + \lambda_{xxyy}\, u_{xx} u_{yy} +$

$$+ 2\lambda_{xyxy}\, u_{xy}^2 =$$

$$= \frac{3\alpha a^2}{16S_0}\left[3\left(u_{xx}^2 + u_{yy}^2\right) + 2u_{xx}u_{yy} + 4u_{xy}^2\right] =$$

$$= \frac{3\alpha a^2}{8S_0}\Big[\underbrace{\frac{(u_{xx}+u_{yy})^2}{2}}_{\frac{\lambda}{2} u_{ll}^2} + \underbrace{\left(u_{xx}^2 + u_{yy}^2 + 2u_{xy}^2\right)}_{\mu\, u_{ik}^2}$$

$$\Rightarrow \mu = 2\lambda = \frac{3\alpha a^2}{8S_0}$$

$$K = \lambda + \mu = \frac{3}{2}\mu$$