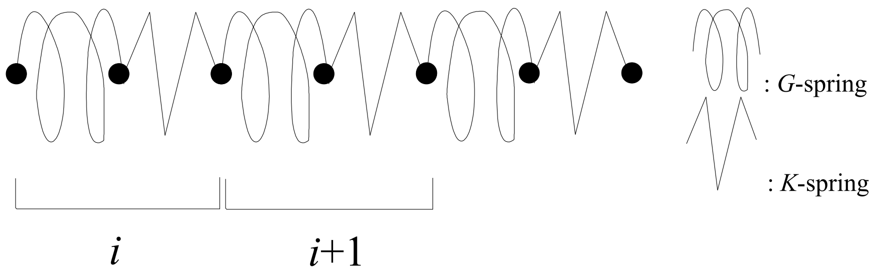
3.4 Specific heat capacitance of phonons (Bosons)

One-dimensional lattice vibrations
We investigate a chain of identical atoms which are coupled by different kinds of springs:



Always two atoms form a unit (basis) addressed by an index i.
The lattice distance shall be a.
The excursion of both atoms is denominated by u_1 and u_2:
for the potential energy we find:

$$U^{harm} = \frac{K}{2}\sum_n [u_1(na) - u_2(na)]^2 + \frac{G}{2}\sum_n [u_2(na) - u_1((n+1)a)]^2 \qquad . \tag{3.19}$$

The equations of motion are:

$$\begin{aligned} M\ddot{u}_1(na) &= -\frac{\partial U^{harm}}{\partial u_1(na)} \\ &= -K[u_1(na) - u_2(na)] - G[u_1(na) - u_2((n-1)a)] \end{aligned} \tag{3.20}$$

$$\begin{aligned} M\ddot{u}_2(na) &= -\frac{\partial U^{harm}}{\partial u_2(na)} \\ &= -K[u_2(na) - u_1(na)] - G[u_2(na) - u_1((n+1)a)] \end{aligned} \tag{3.21}$$

Due to the translational invariance we search for lattice periodic functions. Just for simplicity we use periodic boundary conditions:

$$\begin{aligned} u_1(na) &= \epsilon_1 \exp\left(i(kna - \omega t)\right) \\ u_2(na) &= \epsilon_2 \exp\left(i(kna - \omega t)\right) \end{aligned} \tag{3.22}$$

ϵ_1 and ϵ_2 are parameters which describe the relative amplitudes and phases between both atoms.
For k the following relation holds:

$$\exp(ikNa) = 1 \text{ , i.e. } \quad k = \frac{2\pi}{a}\frac{n}{N}, \qquad n = -\frac{N}{2}, \ldots., \frac{N}{2} \qquad . \tag{3.23}$$

Including this into Eq. (3.20) and Eq. (3.21) we get:

$$\begin{aligned} [M\omega^2 - (K+G)]\epsilon_1 + (K + Ge^{-ika})\epsilon_2 = 0 \\ (K + Ge^{-ika})\epsilon_1 + [M\omega^2 - (K+G)]\epsilon_2 = 0 \end{aligned} \tag{3.24}$$

This system of linear equations only has solutions if the coefficient determinant vanishes:

$$[M\omega^2 - (K+G)]^2 = \left|K + Ge^{-ika}\right|^2 = K^2 + G^2 + 2KG\cos(ka) \qquad . \tag{3.25}$$

We find

$$\omega^2(k) = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2 + G^2 + 2KG\cos(ka)} \tag{3.26}$$

and

$$\frac{\epsilon_2}{\epsilon_1} = \mp\frac{K + Ge^{ika}}{|K + Ge^{ika}|} \qquad . \tag{3.27}$$

For the N different k-values we always find two ω-values, i.e. we find $2N$ modes; this corresponds to the $2N$ degrees of freedom (2 atoms in N elementary cells).
We can choose

$$K > G \qquad . \tag{3.28}$$

The both solutions are:
1)

$$\omega(0) = \sqrt{2\frac{K+G}{M}} \text{ , and } \quad \frac{\epsilon_2}{\epsilon_1} < 0 \quad , \tag{3.29}$$

i.e. both atoms oscillate in anti-phase. If the atoms are charged, thus a dipole moment would be introduced. Light can couple at this oscillations. Therefor the solution is called the optical mode.
2) We find

$$\omega(0) = 0 \text{ , and } \quad \frac{\epsilon_2}{\epsilon_1} > 0 \quad , \tag{3.30}$$

i.e. both atoms oscillate in phase. We will find density oscillations within the crystal. A sound wave will move through the crystal. Therefor his solution is called the acoustic mode.