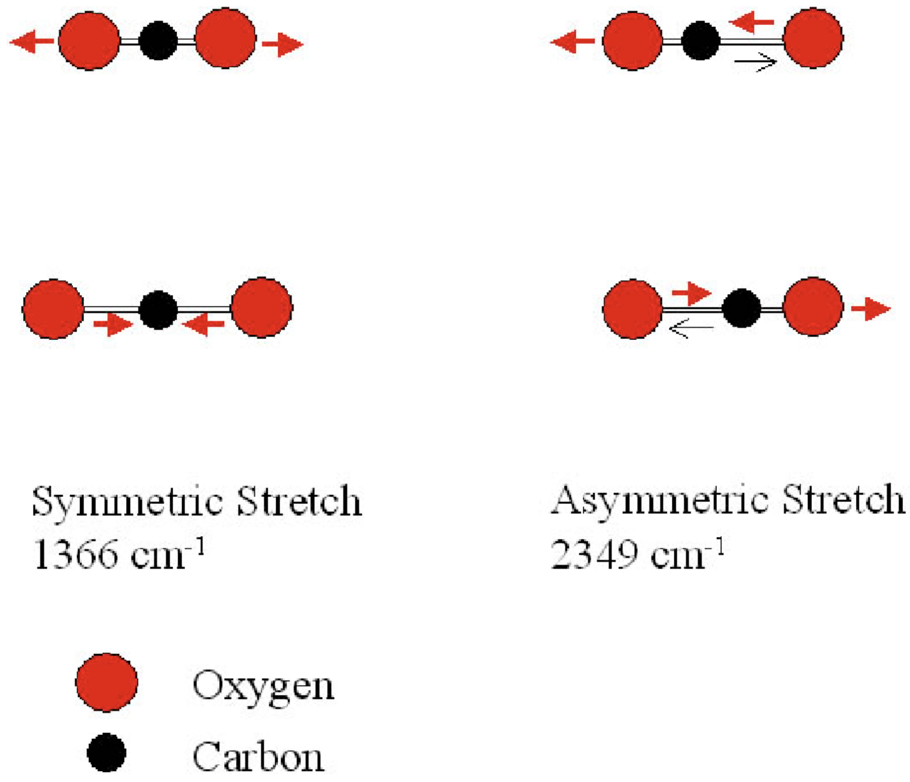
Coupled harmonic oscillators

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \frac{\kappa}{2}(u_{i+1} - u_i)^2$$



Fermi-Pasta-Ulam model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[\frac{\kappa}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3}(u_{i+1} - u_i)^3 \right]$$

$\alpha = 0$

Linear system.

can be described by normal modes

no energy exchange between the modes

no equipartition of the energy among the normal modes

$\alpha \neq 0$

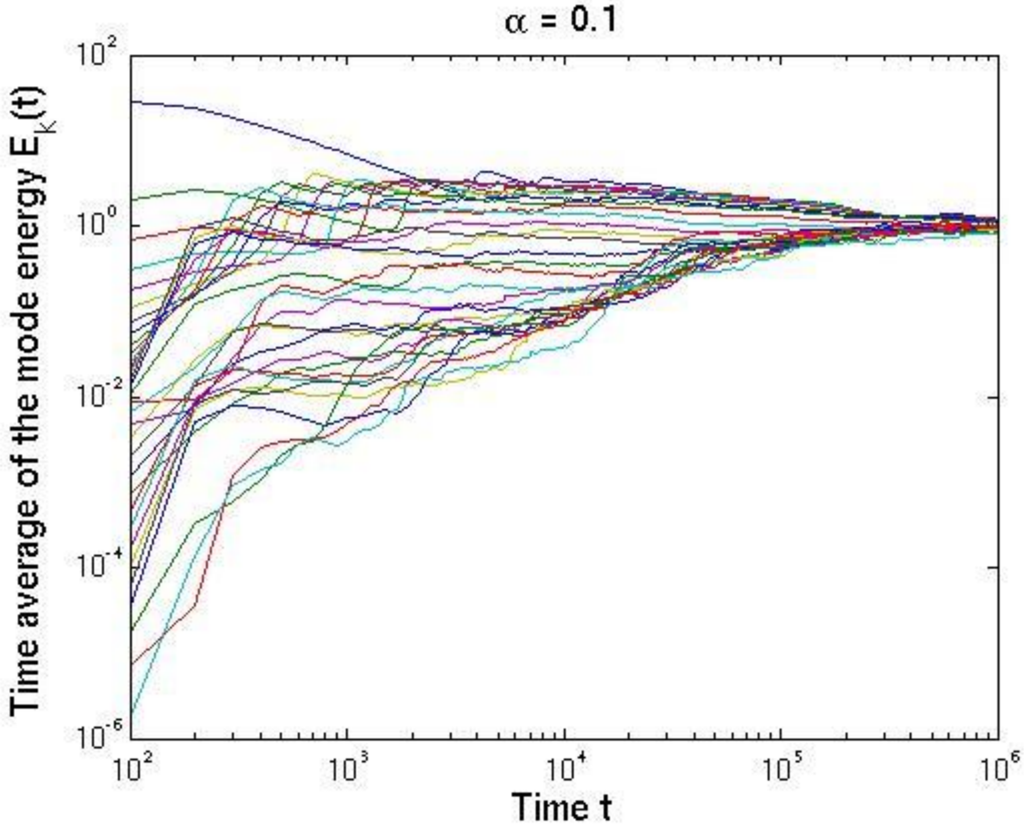
Non-linear system

can approximately be described by normal modes (weak non-linearity)

energy exchange between the modes

equipartition of the energy among the normal modes **?**

Anharmonic system – numerical result



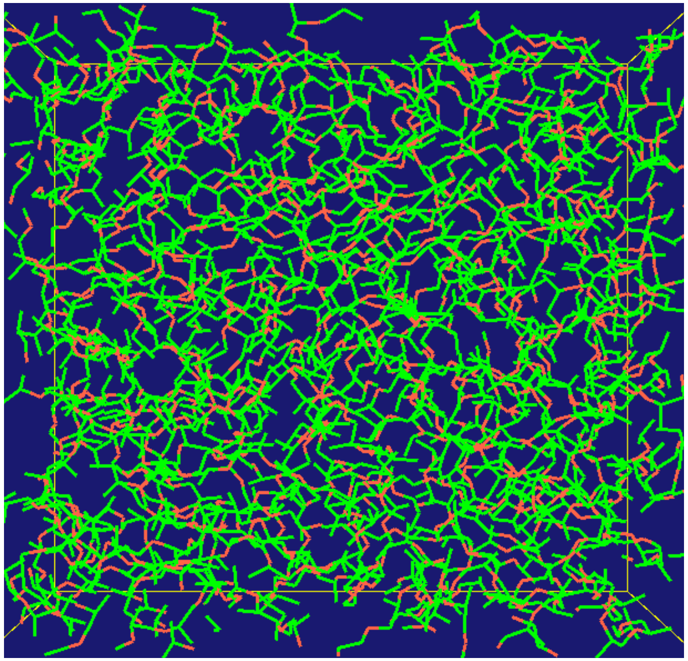
Equipartition of the energy !

Molecular dynamics simulation

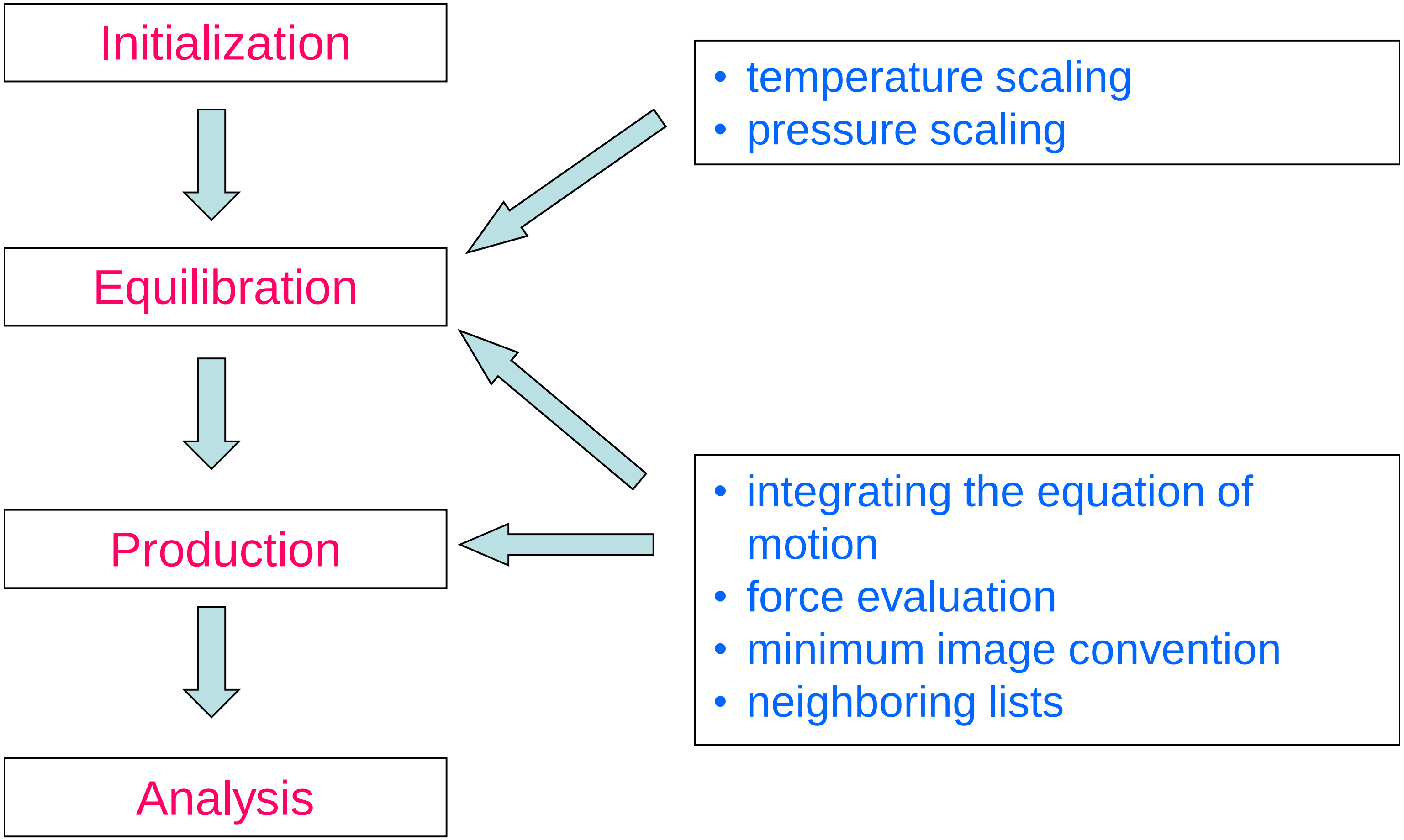
A numerical technique to compute
the equilibrium and transport properties
of classical many-particle systems
by solving Newton's equation of motion.

$$\boldsymbol{F}_i = m_i \boldsymbol{a}_i$$

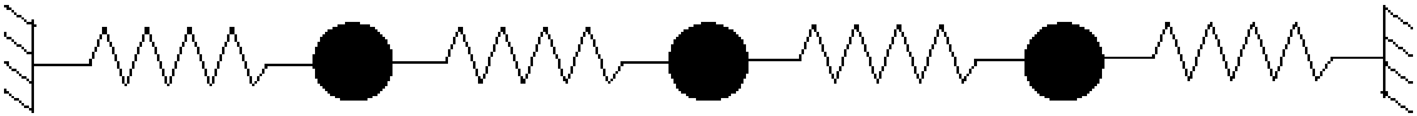
$$i = 1, \ldots, N$$

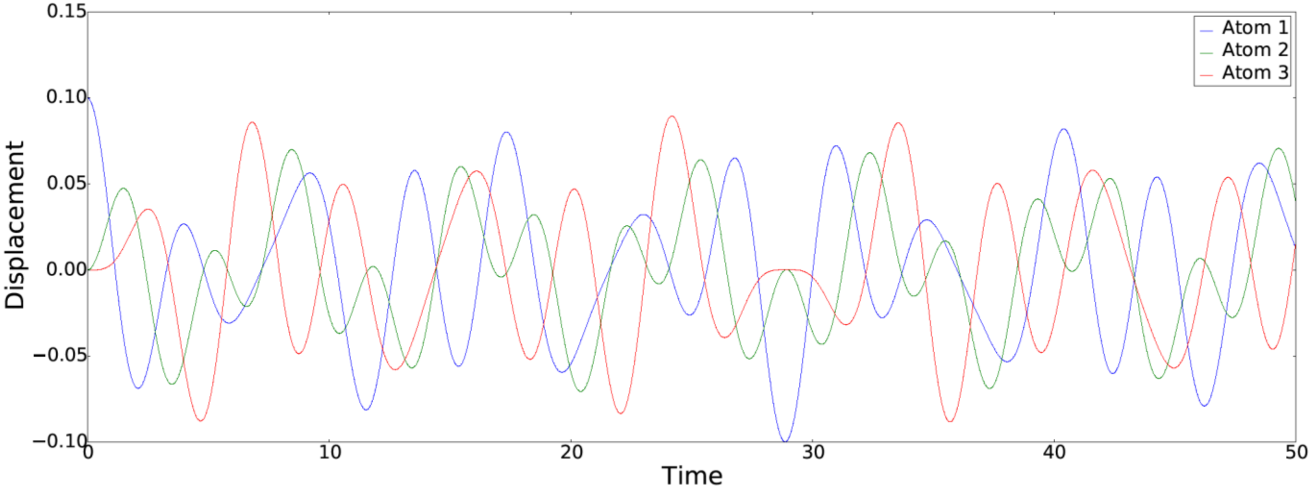


A typical program

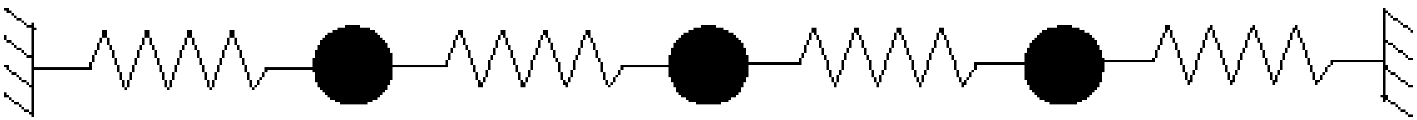


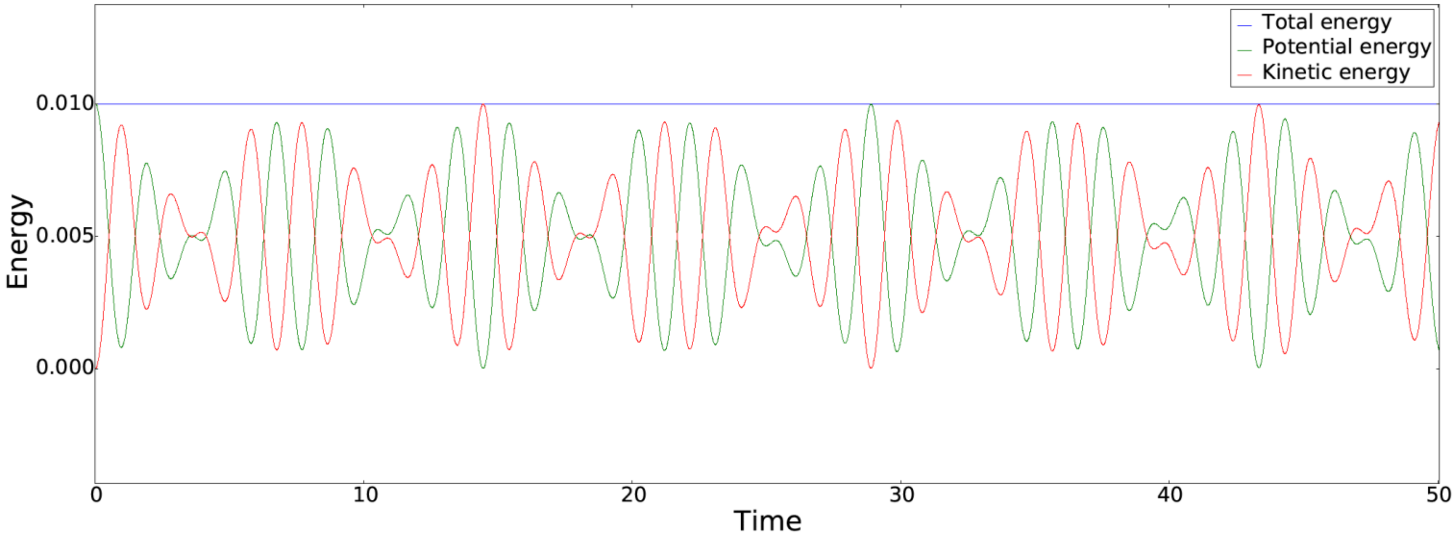
Coupled harmonic oscillators



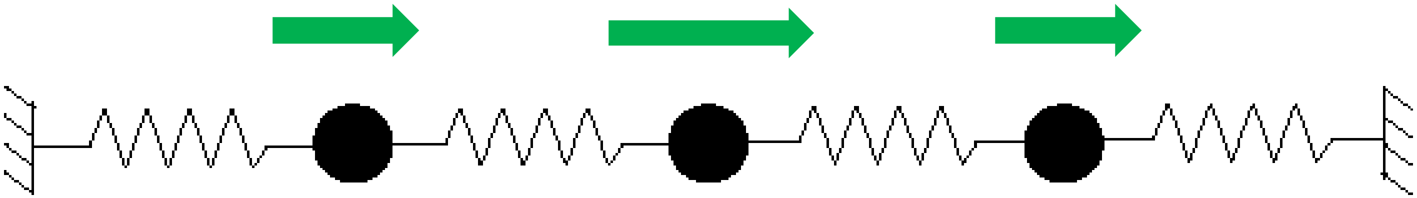


Coupled harmonic oscillators

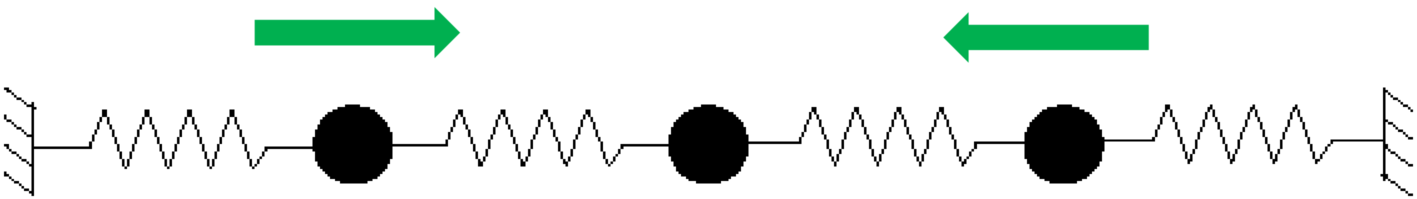




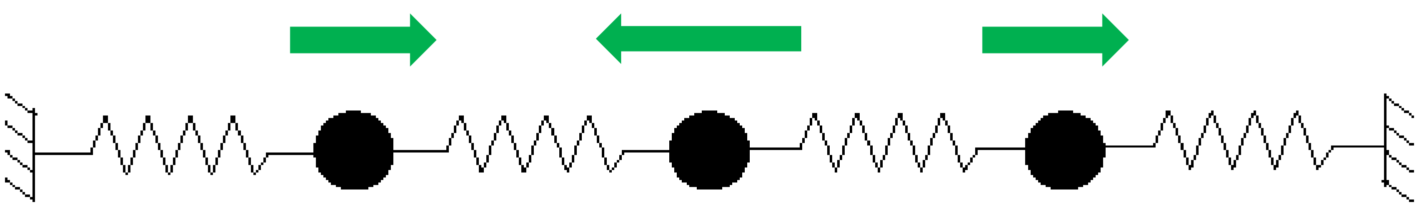
Normal modes



$$\omega_1 = \sqrt{2 - \sqrt{2}}\,\omega_0$$



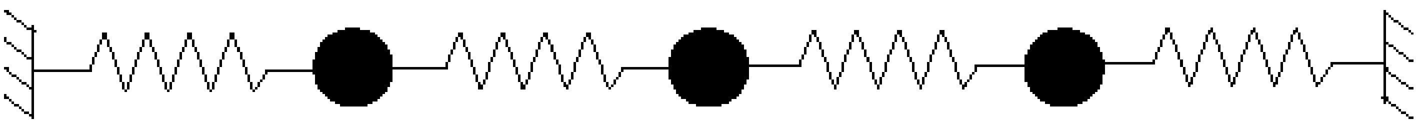
$$\omega_2 = \sqrt{2}\,\omega_0$$



$$\omega_3 = \sqrt{2 + \sqrt{2}}\,\omega_0$$

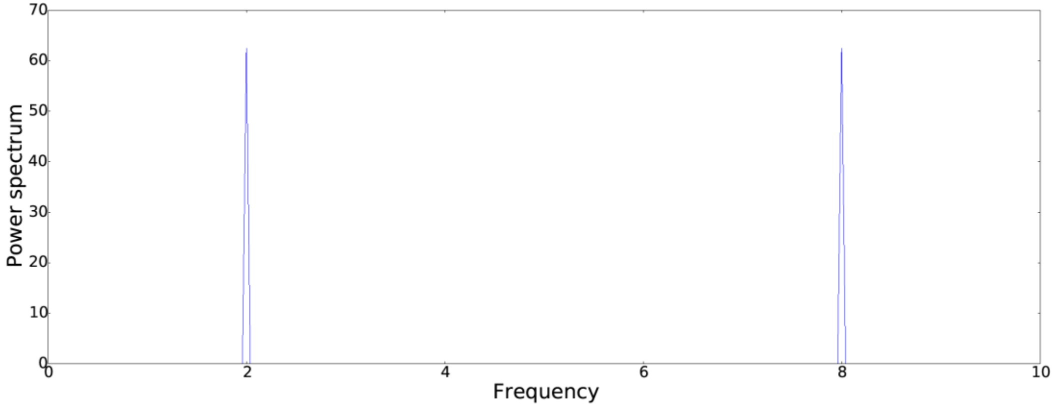
Coupled harmonic oscillators and normal modes

$$H = \sum_{i=1}^{3} \frac{p_i^2}{2m} + \sum_{i=0}^{3} \frac{\kappa}{2}(q_{i+1} - q_i)^2 \quad \Rightarrow \quad H = \frac{1}{2}\sum_{k=1}^{3} [P_k^2 + \omega^2 Q_k^2]$$



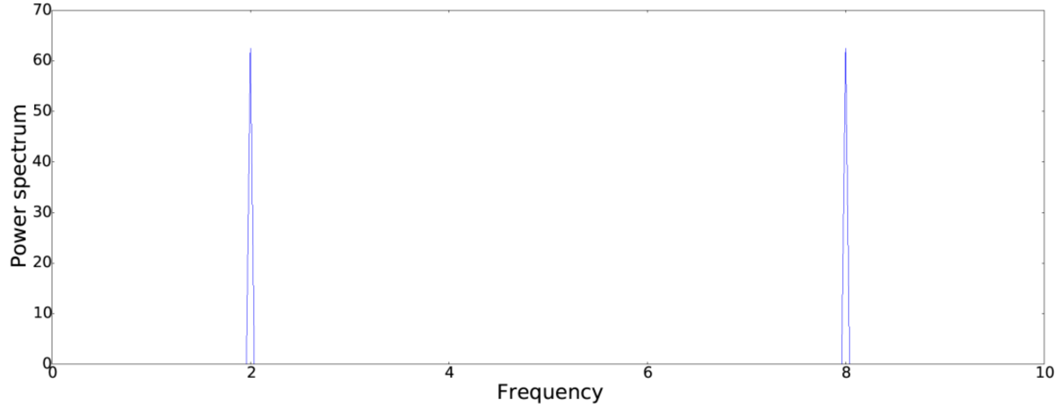
Discrete Fourier transformation

$$h(t) = cos(2\pi f t) \qquad \text{with} \quad f = 2$$

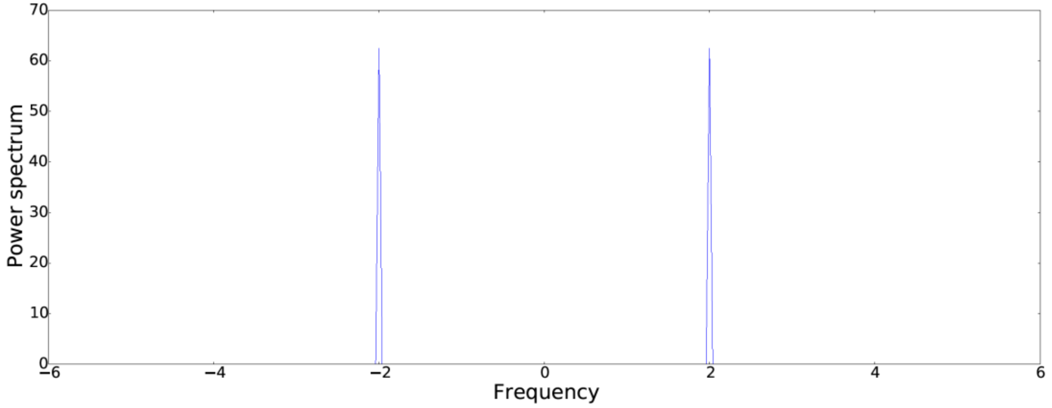


Discrete Fourier transformation

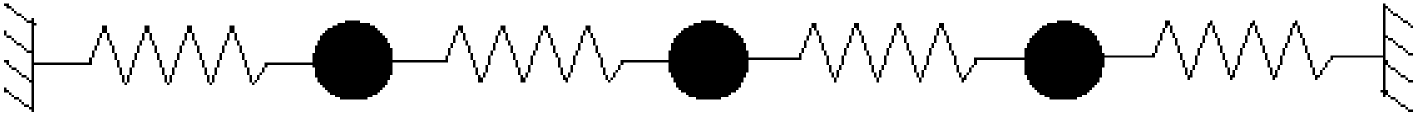
$$h(t) = cos(2\pi ft) \qquad \text{with} \quad f = 2$$

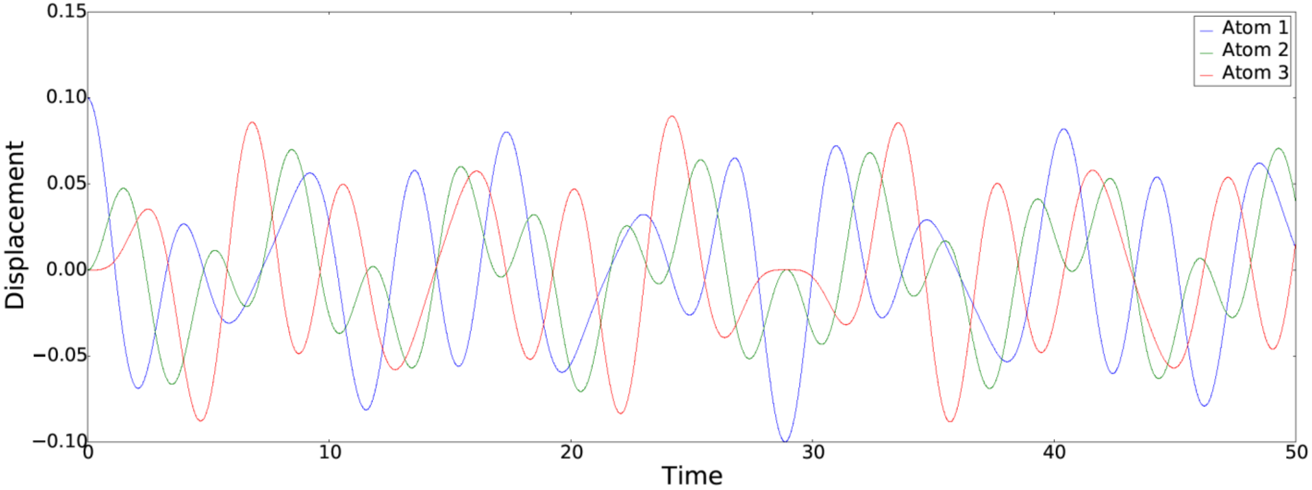


with shift

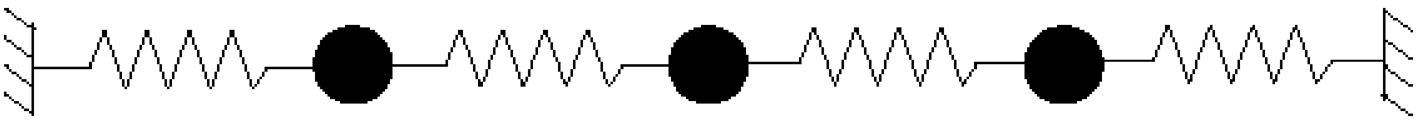


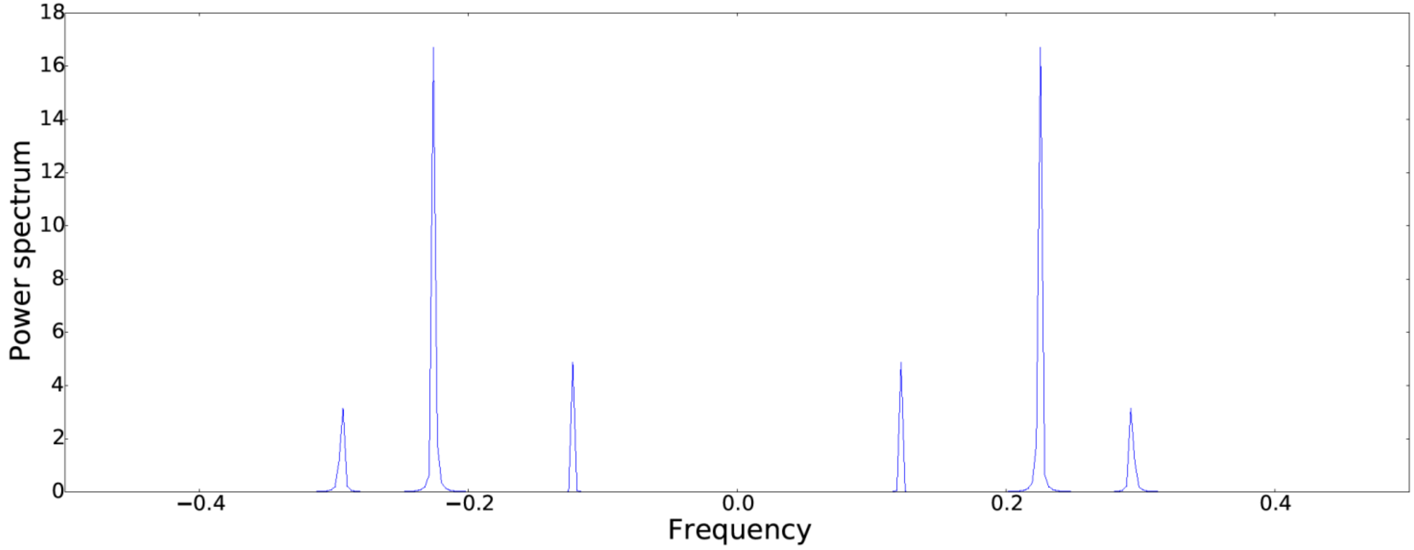
Coupled harmonic oscillators





Coupled harmonic oscillators





Coupled harmonic oscillators

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