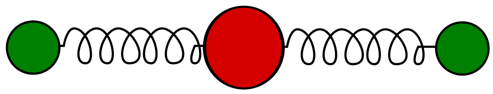
Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 2**

Hand in: Mon 29.10.2018 *(questions marked as ∗ are optional)*
Discussion date: Fri 02.11.2018

2. The oscillations of a linear 3-atomic molecule

A linear 3-atomic molecule is made of 2 masses m connected to another mass M by two springs with constant κ. This can be considered as a simple model of the CO_2 molecule; for simplicity, we only consider the longitudinal motion along the axis of the molecule.



(a) (5pts) Write down the Hamiltonian of the system and derive the differential equation of motion.

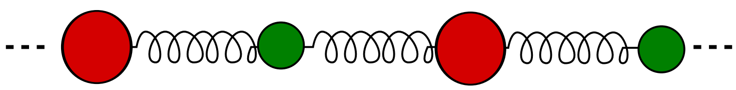
(b) (15pts) Find the eigenmodes of oscillation of the molecule.

(c) ∗ Describe the physical motion of atoms in each mode. Pay attention to the symmetry of the molecule.

(d) ∗ From the infrared absorption spectrum of CO_2, one can extract a peak at wavenumber $k_1 = 2349\text{cm}^{-1}$. Can you predict another wavenumber where CO_2 would interact with electromagnetic wave as well?

3. Linear chains of two atoms per unit cell

Consider a chain of 2 different atoms with masses M and m linked by springs with spring constant κ.



At equilibrium the distance between two consecutive atoms is a, thus the system is periodic with lattice constant $d = 2a$. Again, we only consider the motion of the atoms along the chain.

(a) (20pts) Show that the dispersion relation of the eigenmodes of oscillation is given by

$$\omega^2(q) = \frac{\kappa}{Mm}\left[M + m \pm \sqrt{M^2 + m^2 + 2Mm\cos(qd)}\right]. \tag{1}$$

(b) ∗ Sketch the dispersion relation over the first Brillouin zone. Pay attention to the limits $qd \to 0$ and $qd \to \pi$. What happens when $m = M$? What is the symmetry of the chain, and how is it reflected in the dispersion relation?