Exercise 3.1

Lennard-Jones potential. The Lennard-Jones potential is widely used to describe the interactions between similar atoms or molecules in liquidus or gaseous phases. It has the simple analytical form

$$U(r) = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}],$$

where ϵ is the depth of the potential well, σ is the distance at which the potential between the two atoms is zero, and r is the distance between the two atoms. For argon crystal ($\epsilon = 0.0104\,\text{eV}$ and $\sigma = 3.40\,\text{Å}$),

a) Calculate the equilibrium interatomic distance.

b) Calculate the energy at the minimum (called cohesive energy).

c) Calculate the effective spring constant between two argon atoms.

Exercise 3.2

Phonon spectra of a diatomic lattice chain. Consider a diatomic chain of atoms as shown in figure 1. The masses of the two atoms are different but the spacing and the spring constant between them are the same. Derive the following given expression for the phonon dispersion in this diatomic lattice chain and schematically draw it:

$$\omega^2 = K(\frac{M_1 + M_2}{M_1 M_2}) \pm K\sqrt{(\frac{M_1 + M_2}{M_1 M_2})^2 - \frac{4\sin^2(ka/2)}{M_1 M_2}},$$

where K is the spring constant and k the wavevector with the following values

$$k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, ..., \frac{\pi}{a},$$

and N is the total number of lattice points in the chain.

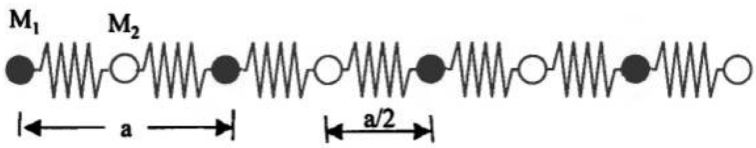

Figure 1: A diatomic lattice chain