7.1: The Problem

7.1 The harmonic Hamiltonian

The Hamiltonian for lattice vibrations, in the harmonic approximation, is

$$\mathcal{H}=\frac{1}{2}\sum_{i=1}^{3N} m_i\dot{x}_i^2+\frac{1}{2}\sum_{i=1}^{3N}\sum_{j=1}^{3N} x_i A_{ij} x_j. \tag{7.1.1}$$

Notice that this Hamiltonian allows the possibility that atoms at different lattice sites might have different masses. Accept the fact that any real symmetric matrix S can be diagonalized through an orthogonal transformation, i.e. that for any such S there exists a matrix B whose inverse is its transpose and such that

$$\mathrm{BSB}^{-1} \tag{7.1.2}$$

is diagonal. Show that the Hamiltonian can be cast into the form

$$\mathcal{H}=\frac{1}{2}\sum_{r=1}^{3N}\left(\dot{q}_r^2+D_r q_r^2\right) \tag{7.1.3}$$

by a linear change of variables. (Clue: As a first step, introduce the change of variable $z_i=\sqrt{m_i}x_i$.)