392K March 3, 2020
Midterm 1
And now HW 3, due March 10, 2020

Problem 1: In the harmonic approximation the Hamiltonian of a classical N-atom molecule in 3D can be written as:

$$H = \frac{1}{2}\vec{u}\boldsymbol{M}\vec{u} + \frac{1}{2}\vec{u}\boldsymbol{P}\vec{u},$$

where vector ***u*** describes 3N components of the atomic displacements, ***M*** is the diagonal mass matrix and ***P*** is the force constant matrix. Demonstrate that by expanding ***u*** in a basis set of the eigenvectors of ***P***, the Hamiltonian is transformed to that of 3N independent oscillators:

$$H = 1/2 \sum_f^{3N} \left(\dot{d}_f^2 + \omega_f^2 d_f^2\right),$$

Where d_f's are the expansion coefficients. (*Remember, this is a generalized eigenvalue problem*).

Problem 2: Consider a ground state of Li. In the independent electron approximation, construct a wave function describing two electrons in the 1s state *u(r)* and one electron in the 2s state *v(r).*

Problem 3: Describe a ***diamond*** lattice with as small as possible tetragonal lattice with a basis. Find the lattice and basis vectors for this new cell.

Problem 4: Find symmetry group of a water molecule H_2O. Construct the multiplication table.