HW #6 (221A), due March 8, 5pm

1. Consider a one-dimensional problem of two heavy particles at x_1 and x_2 of mass M and one light particle at x_3 of mass m attached by springs, with the light particle in the middle: $x_1 < x_3 < x_2$. The Hamiltonian of the system is

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2M} + \frac{p_3^2}{2m} + \frac{1}{2}k(x_3 - x_1 - d)^2 + \frac{1}{2}k(x_2 - x_3 - d)^2. \quad (1)$$

   Here, d is the natural length of the spring and k the spring constant. Answer the following questions.

   (a) Use Bohr–Oppenheimer approximation to study the system. First, fix the positions of heavy particles x_1 and x_2, and find the energy eigenvalues in the $M \to \infty$ limit. Second, consider the energy eigenvalues (as a function of x_1 and x_2) as a potential energy for the heavy particles and work out energy eigenvalues for the heavy particles.

   (b) One can also solve this system exactly. Identify the basic oscillation modes, rewrite the Hamiltonian in terms of them, and obtain the energy eigenvalues exactly.

   (c) Compare two results and see what corrections are missed in Bohr–Oppenheimer approximation.

2. Consider $2s$ and $2p$ wave functions of the hydrogen atom. Answer the following questions. Try to use Mathematica for visualization as much as possible.

   (a) Show that one can take linear combinations of states $|2p, m = \pm 1\rangle$ to obtain orbitals elongated along x or y axis (or equivalently, $\phi = 0$ and $\phi = \pi/2$ directions).

   (b) Show that one can further combine $|2s\rangle$ state to obtain orbitals elongated along $\phi = 0$, $\phi = 2\pi/3$, and $\phi = 4\pi/3$ directions. They are sp^2 mixed orbitals used for carbon atoms in ethylene, etc.

   (c) Similarly, show that one can combine all three $2p$ states and $2p$ state to obtain orbitals elongated along the axes of a tetrahedron. They are sp^3 mixed orbitals used in methane etc.