

HW #7 (221B), due Mar 9, 4pm

1. Consider a one-dimensional problem of two heavy particles of mass M at x_1 and x_2 and one light particle of mass m at x_3 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 $M \rightarrow \infty$ 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.
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, benzene, etc.
 - (c) Similarly, show that one can combine all three $2p$ states and $2s$ state to obtain orbitals elongated along the axes of a tetrahedron. They are sp^3 mixed orbitals used in methane etc.