Problem Set 3
CHM102A

1. Assuming particle in a 1-D box model, calculate the energy separation between the lowest two levels for a particle confined in a box of length 3 nm (consider the particle to be the H_2 molecule). In this model, at what quantum number, *n*, does the energy of the molecule equal k_BT when T=300K. Compare the results to the case of nitrogen molecule whose mass is 14-times higher.

2. Consider a system of two non-interacting particles of mass m_1 and m_2 confined along the x-axis such that:

$$V(x_1, x_2) = \begin{cases} 0 & if\ 0 < x_1 < L, and\ 0 < x_2 < L \\ \infty & otherwise \end{cases}$$

where x_1 and x_2 are coordinates of particles 1 and 2.

- Solve the Schrodinger equation for this problem.
- How many quantum numbers are required to specify a state of this system?
- Can degenerate states appear for this problem as special case? Explain.
- Sketch the ground state wave function.
- For the ground state, sketch the probability density for finding both particle 1 and particle 2 simultaneously at the same point for 0 < x < L?

3. For the ground state of a quantum mechanical 1-D simple harmonic oscillator, compute the expectation value of Kinetic Energy $\langle T \rangle$.

4. Assuming a particle in a 1-D box model, calculate the separation between the lowest two energy levels for a $^{14}N_2$ molecule in a box of length 3 nm. In this model, at what quantum number, *n*, does the energy of the molecule equal k_BT when T = 300K.

5. Consider the wavefunction $\psi = A\cos\left(\frac{n\pi x}{a}\right)$, where *n* is a nonzero positive integer and '*a*' is the length of the box as a possible solution for a particle in a 1D box with infinite potential. Under what condition, if any, will ψ be an allowed wavefunction for this 'particle in a 1D box'.

6. For a 3D rigid rotor with quantum number $l = 1$, what are the possible angles (θ) the angular momentum vector with the z-axis?