Chemistry 542
Fall, 2002
Problem Set 7
Due Wednesday, Oct. 30

Read chapter 6, sections 1-4.

1. Show that the associated Legendre equation is a Sturm-Liouville equation and determine the weighting factor, r(x).

2. Use ladder operators to derive $Y_{2,2}$, $Y_{2,1}$, and $Y_{2,0}$. Don't worry about the normalization.

3. Calculate the rotational population distribution for HCl and H_2 at 300 K. Present your results in the form of a table of P_J vs J. What is the most probable value of J for each molecule? For HCl it is OK to use the equation that we derived in class, but for H_2 the formula is inaccurate. Compare the exact result for with the values predicted by the formula.

4. The alignment of a rotor, *A*, is defined as the expectation value of $\cos^2\theta$.

A. Calculate *A* for a molecule instate J=0.
B. Calculate *A* for J = 2, M = 2 by direct evaluation of the integrals.
C. Use a recursion relation to derive a general expression for the alignment of any J,M state. Show that your equation works for J=1, M= 1 and 0, which were obtained in class.
D. Show that the average over all M gives A = 1/3 for any J. Assume that all M states are equally populated. Hint: $\sum_{M=-J}^{J} M^2 = J(J+1)(2J+1)/3$.

5. Prove that the recurrence time for a rotational wave packet is 1/2Bc.

Also do Levine 6.4 and 6.6.