Physics 449 **HOMEWORK SET 6** Spring 2009

Due Friday March 13

24) The potentials $V(R)$ for the H_2 and D_2 molecules are identical, and it follows that the the effective spring constants, k, are equal. However, the dissociation energies of the two molecules not quite the same – 4.477 eV for H_2 and 4.556 eV for D_2. The reason is that the energy of the lowest quantum state is $\frac{1}{2}\hbar\omega$ above the potential minimum, and ω is different in the two cases because the deuterium nucleus has roughly double the mass of the proton.

(a) Use the given dissociation energies to determine the potential minimum (V_0) for the system and the vibrational energy spacing ($\hbar\omega$) of each molecule.

(b) Predict the dissociation energy of the HD molecule.

25) The equilibrium separation of the nuclei in the H_2 and D_2 molecules is 0.074 nm. Find the energy difference between the lowest rotational state and the next allowed rotational state for:

(a) H_2 with "parallel spins" ($s = 1$).

(b) H_2 with "antiparallel spins" ($s = 0$).

(c) D_2 in any state with a symmetric spin wave function. The deuterium nucleus has spin 1 and is therefore a boson.

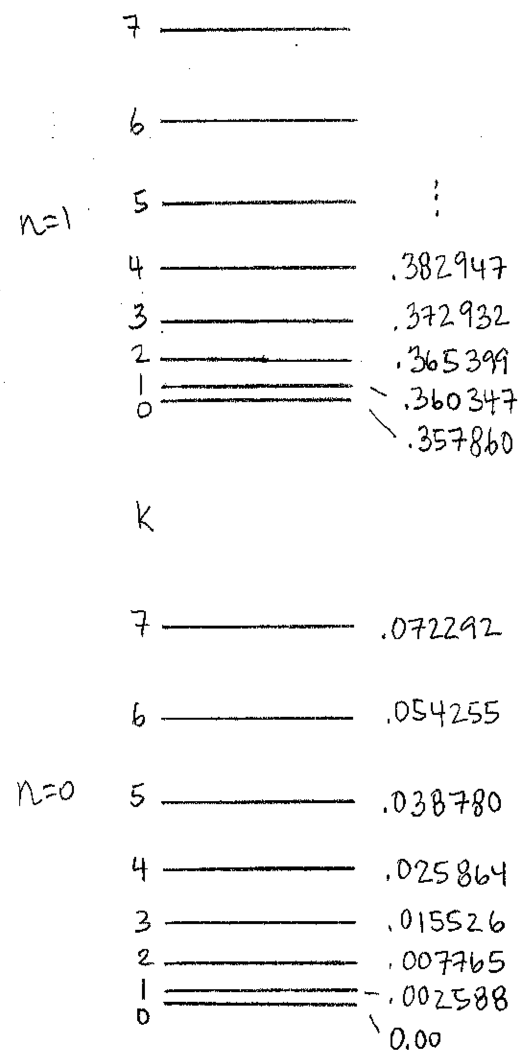
26) In this problem we will use information given in the drawing shown at the right to determine some of the properties of the HCl molecule. Assume that the H and Cl nuclei have masses of 1u and 35u respectively, where $1u = 1.66 \times 10^{-27}$kg. The quantities listed to the right of each level are the energies in units of electron volts.

(a) From the excitation energy of the first $k = 1$ rotational state determine the equilibrium internuclear separation R_0.

(b) From the excitation energy of the $n = 1$ vibrational state determine $\hbar\omega$. Use this and the measured dissociation energy (4.47 eV) to determine the parameters k and V_0 of the effective potential.

(c) We will now try to predict how much the molecule stretches as it rotates. The potential of parts (a) and (b) can be written in the form $V(r) = -V_0 + \frac{1}{2}k(R - R_0)^2$. Add to this the rotational potential $k(k+1)\hbar^2/2\mu R^2$ and then find the new potential minimum for the $k = 7$ rotational state.

(d) To see whether your prediction is correct, extract the value of R_0 for the $k = 7$ rotational state from the observed energy of this state as seen in the diagram.



27) FOR HONORS OR EXTRA CREDIT: Calculation of the hyperfine Zeeman effect in Hydrogen.

As we discussed in class, the Hamiltonian for a hydrogen atom in a magnetic field consists of the usual kinetic and potential energy terms plus the following:

$$H_1 = W_{\text{dd}} + g_e \frac{e}{2m_e} \vec{S}_e \cdot \vec{B} - g_p \frac{e}{2m_p} \vec{S}_p \cdot \vec{B}$$

where W_{dd} is the dipole-dipole interaction

$$W_{\text{dd}} = \frac{\mu_0}{4\pi} g_e g_p \frac{e}{2m_e} \frac{e}{2m_p} \left[\{3(\vec{S}_p \cdot \hat{r})(\vec{S}_e \cdot \hat{r}) - \vec{S}_e \cdot \vec{S}_p\} \frac{1}{r^3} + \frac{2\pi}{3} \vec{S}_e \cdot \vec{S}_p \, \delta^{(3)}(\vec{r}) \right]$$

Use degenerate state perturbation theory to find the zero-order energy eigenfunctions and the first-order energy shifts for the hydrogen ground state as a function of magnetic field. The first part of W_{dd} has a zero expectation value, and so only the δ-function term contributes. You may also ignore the very small $\vec{S}_p \cdot \vec{B}$ term. I believe that the problem is easiest if you use the eigenstates of S^2 and S_z (where $\vec{S} = \vec{S}_e + \vec{S}_p$) as your basis states.