Physics 221B
Spring 2008
Homework 16
Due Friday, February 1 at 5pm

Reading Assignment: Sakurai, pp. 357–368; Notes 24, 25; lecture notes for 1/24/08.

1. A problem on the hydrogen molecule.

(a) In classical statistical mechanics, each degree of freedom contributes an amount $\frac{1}{2}Nk$ to the specific heat C_v, where N is the number of particles and k is the Boltzmann constant. In this context, a "degree of freedom" means a quadratic term in the Hamiltonian, for example, $p^2/2$ or $x^2/2$. For example, the three translational degrees of freedom of a molecule contribute $\frac{3}{2}Nk$, and the two rotational degrees of freedom of a diatomic contribute Nk more (the third rotational degree of freedom about the axis of the molecule is frozen out because of the small moment of inertia).

Use quantum statistical mechanics to compute the rotational contribution to the specific heat C_v of H_2 gas in both the low and high temperature limits. In each case, just give the dominant term at low or high temperatures. Give a quantitative condition as to what "low" and "high" temperatures mean in this case, and work out a characteristic temperature in Kelvins that separates the two temperature regimes. Hint: in the high temperature limit, evaluate the sum by regarding it as a Riemann sum approximation to an integral. Then do the integral.

(b) Do the same for D_2 gas (deuterium).

2. In working the previous problem, you may have noticed that when you combine equal spins, say, $j_1 = j_2 = j$, according to $\mathbf{S} = \mathbf{J}_1 + \mathbf{J}_2$, then the states $s = 2j$, that is, the states $|sm_s\rangle$ for $s = 2j$, are symmetric under exchange E_{12}, the states $s = 2j - 1$ are antisymmetric, etc. In the following problem you must not use any properties of the Clebsch-Gordan coefficients, only general properties of operators such as S^2, S_z, E_{12}, etc.

(a) Prove that the states $s = 2j$ are symmetric under exchange (all of them, that is, all $2s + 1$ of them).

(b) Prove that as the total value of s is decreased from its maximum of $2j$ to its minimum of 0, the states $|sm_s\rangle$ alternate between symmetric and antisymmetric under exchange. Hint:

Review the general proof for the addition of angular momenta, that says when you combine angular momenta according to $\mathbf{S} = \mathbf{J}_1 + \mathbf{J}_2$, you get $j = |j_1 - j_2|, \ldots, j_1 + j_2$. In the present case we are interested in $j_1 = j_2 = j$. Think of the square of $(2j+1)^2$ lattice points in the m_1-m_2 plane, representing the uncoupled basis $|m_1\rangle|m_2\rangle$.

3. The bound states of helium are shown in Fig. 25.3.

(a) How would this diagram be different if the electron were a spin 0 particle? If it were a spin $\frac{3}{2}$ particle? You do not need to be quantitative, but if some levels go up or down, say which ones and which way. If some levels appear or disappear, say which ones. What are the degeneracies of the levels in actual helium? What would they be if the electron were a spin-0 particle?

(b) The electric dipole operator for a multielectron atom is defined by Eq. (20.15), where the charges are the electrons (with $q = -e$). Electric dipole transitions between two states are governed by the matrix element of the electric dipole operator between the states in question. Explain why there are no electric dipole transitions between ortho and para eigenstates of the Hamiltonian (25.1).

Remark: The eigenstates of the Hamiltonian (25.1) are not exactly the eigenstates of real helium because of the neglect of small terms, notably, the fine structure terms. When these are included, it turns out that electric dipole transitions are allowed between ortho and para states, but the amplitude is small and the lines are very weak. For this reason, it was thought at one time on spectroscopic grounds that parahelium and orthohelium were two different species of helium. The weak spectral lines connecting the ortho and para states are called "intercombination lines."

4. Consider a simple "one-dimensional" hydrogen atom that obeys the equation,

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} - Z\delta(x)\psi = E\psi. \tag{1}$$

[Units such that $m = \hbar = 1$, and the Coulomb potential is replaced by $-Z\delta(x)$].

(a) Find the ground state energy and wave function $\psi_0(x)$, and verify that

$$\langle T\rangle = -E = -\frac{1}{2}\langle V\rangle. \tag{2}$$

(b) Now consider the one-dimensional "helium" atom which obeys

$$H\psi(x_1, x_2) = -\frac{1}{2}\frac{\partial^2\psi}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2\psi}{\partial x_2^2} - Z\delta(x_1)\psi - Z\delta(x_2)\psi + \delta(x_1 - x_2)\psi = E\psi, \tag{3}$$

where x_1, x_2 are the coordinates of the two "electrons" on the x-axis. First treat $\delta(x_1 - x_2)$ as a perturbation and find the ground state energy to first order. Compare to 3-dimensional helium.

Save your results for this problem, it will be continued next week.