Due: Thursday, February 2, 2017 by 11pm

Put homework in mailbox labelled 223B on 1st floor of Broida (by elevators).

If you do not have access to Ashcroft and Mermin please let me know, and I can scan and upload the relevant problems.

#### 1.) HUNDS RULES

Ashcroft and Mermin, Chapter 31, Problem 3

## 2.) CRYSTAL FIELD EFFECTS

For an atom (or ion) in a solid the effects of the electric fields from the neighboring atoms breaks the rotational symmetry. For a partially filled atomic 3d orbital these inter-atom "crystal field" effects can be significantly larger than the intra-atomic spin-orbit interactions. Suppose that within a set of (2L+1)(2S+1) lowest lying atomic states the crystal field can be represented in the form,

$$H_{cryst} = aL_x^2 + bL_y^2 + cL_z^2,$$
 (1)

with a, b and c all different (and positive). For the special case of L = 1 show that if the crystal field is the dominant perturbation (compared with the spin orbit interaction) it breaks the (2L+1)(2S+1) degeneracy, giving a (2S+1)fold degenerate manifold of ground states in which every matrix element of every component of  $\vec{L}$  vanishes. This is an example of a complete quenching of the orbital angular momentum.

## 3.) SINGLET GROUND STATE OF (SPIN-INDEPENDENT) TWO ELECTRON HAMILTONIAN

# Ashcroft and Mermin, Chapter 32, Problem 2

This method of showing that the 2-electron ground state is a singlet, can be used to show that the ground state wavefunction of N Bosons,  $\Psi(r_1, r_2, \dots, r_N)$ , interacting via a density-density interaction (as in 4-He) is nodeless, that is  $\Psi \geq 0$ . See, for example, Section 11.3 in Feynman's Statistical Mechanics book.

#### 4.) HUBBARD MODEL OF THE HYDROGEN MOLECULE

Ashcroft and Mermin, Chapter 32, Problem 5 (parts a-e and two extra parts, f and g, below)

(f) Find the unique triplet (spatially anti-symmetric) state of the two-electron problem, and show that it has energy  $E_t = 2\epsilon$ .

(g) Show that the appropriate spin Hamiltonian for this two-electron problem, valid in the limit U >> t, is

$$H_{spin} = J\vec{S_R} \cdot \vec{S_{R'}},\tag{2}$$

with exchange  $J = E_t - E_s$  where  $E_s$  is the ground state (singlet) energy. (This Hamiltonian acts in a projected Hilbert space where there is no double occupancy.) Plot the antiferromagnetic exchange coupling J versus U at fixed t, and show that  $J = 4t^2/U$  in the large U/t limit.