PHY801: Survey of Atomic and Condensed Matter Physics Michigan State University

Homework 4

4.1. Consider an atom with the ${}^{3}S_{1}$ ground state. What is the value of the Landé g-factor? Find the magnetization M as a function of magnetic field B (oriented along the z axis), the temperature T, and the concentration n = N/V. Show that in the limit of very high temperatures, where $\mu_{B}B \ll k_{B}T$, the susceptibility is given by $\chi = 8n\mu_{B}^{2}/(3k_{B}T)$.

4.2. An exotic proposal to get nuclear fusion between two deuterons is to use the idea of muon catalysis. One constructs a "Hydrogen molecule ion", only with deuterons instead of protons and a muon in place of an electron. Use your knowledge of the H_2^+ ion to predict the equilibrium separation between the deuterons in the muonic molecule. Explain why the chance of getting fusion is better for muons than for electrons.

4.3. The Schrödinger equation for one electron in an attractive one-dimensional delta-function potential of the form $V(x) = -e^2 \delta(x)$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - e^2\delta(x)\psi(x) = E\psi(x) \;.$$

In atomic units ($\hbar = m = e^2 = 1$), the normalized ground state wave function is $\psi_1(x) = e^{-|x|}$, and the corresponding energy is $E_1 = -1/2$.

- (i) Check that the above wave function and energy are correct.
- (ii) Consider a one-dimensional H₂ molecule with a δ -like both ion-electron (as above) and repulsive electron-electron interaction. The ions are fixed at a distance R. Neglect ion-ion repulsion.
 - (a) Write down the Schrödinger equation for this one-dimensional H_2 molecule.
 - (b) Construct a *gerade* molecular orbital (MO) for this molecule with the correct normalization coefficient.
 - (c) Calculate the ground state energy for the molecule using this MO.
 - (d) Construct a Heitler-London (HL) wave function for the molecule and calculate the energy.
 - (e) Compare the energies obtained using the two approaches and discuss the physics.

Use:

$$\int_{-\infty}^{+\infty} e^{-|x-R/2|} e^{-|x+R/2|} dx = (1+R)e^{-R}$$
$$\int_{-\infty}^{+\infty} e^{-3|x-R/2|} e^{-|x+R/2|} dx = (3e^{-R} - e^{-3R})/4$$
$$(a+b)^4 = a^4 + 4a^3b + 6a^2b^2 + 4ab^3 + b^4$$