PHY 491, EXAM #1
October 3, 2011; Time 1 hr
Name:

Magnetization of a multiplet with a given total angular momentum J and Lande g-factor g$_J$

$$M = Ng_J\mu_B J B_J(x); \quad x = g_J\mu_B JB/k_B T$$

Where the Brillouin function $B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{(2J+1)x}{2J}\right) - \frac{1}{2J}\coth\left(\frac{x}{2J}\right)$

Hydrogen atom (Z=1)

Rydberg constant (R) 13.6 eV; Bohr radius (a$_B$) 0.529 A^0

$$R = \frac{me^4}{2\hbar^2}$$
$$a_B = \hbar^2/me^2$$

Problem#1. (5 points)
X-ray Laser pulses can be used to strip atoms of electrons one by one (ionize the atom). What is the energy required to remove the last electron from a K atom? The neutral K atom has 19 electrons. The ionization energy of Hydrogen atom is 13.6 eV. What is the size of the Bohr'r radius for this last electron?

THE LAST ELECTRON SEES Z=19. HYDROGEN ATOM WITH Z=19

IONIZATION ENERGY, E_I, SCALES AS Z^2 AND POSITIVE

E_I=13.6 eVxZ^2=4909.6 Ev

BOHR RADIUS SCHRINKS AND SCALES AS 1/Z. THE NEW BOHR RADIUS IS

a_B=0.52/Z Angstroms=0.0274 Angstroms

Problem#2. (5 points)
Consider an electron trapped in a 3-dimensional harmonic oscillator potential. The Hamiltonian in atomic units ($\hbar = m = e^2 = 1$) is given by

$$H = -\frac{1}{2}\nabla^2 + \frac{1}{2}r^2$$

Let's use a trial wave function for the ground state of the form $\psi(\vec{r}) = \left(1 \middle/ \sqrt{\pi\alpha^3}\right)e^{-r/\alpha}$.

This gives $\dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \dfrac{1}{2\alpha^2} + \dfrac{3}{2}\alpha^2$ (Don't derive this)

What is the best variational ground state energy one can get (in units of Hartree)?

$$E(\alpha) = 1/2\alpha^2 + 3/2\ \alpha^2$$

MINIMIZE E(α) WITH RESPECT TO THE VARIATIONAL PARAMETER α

$$d\ E(\alpha)/d\ \alpha = -2/2\ \alpha^3 + (3/2)\ 2\ \alpha=0$$

THIS GIVES THE BEST VARIATIOAL PARAMETER α^2=1/√3
(MAKE SURE THIS IS A MINIMUM NOT A MAXIMUM)

SUBSTITUTING THIS VALUE OF α^2 IN THE ENERGY EXPRESSION WE FIND

$$E_{min} = E(\alpha^2=1/\sqrt{3}) = \sqrt{3}\ \text{Hartree}$$

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Problem#3. (10 points)

The electronic configuration of nitrogen atom is $1s^2;2s^2;2p^3$. Treat $1s^2;2s^2$ as core electrons and $2p^3$ as valence electrons.

    (i)   What is the total spin angular momentum and total orbital angular momentum of the core? Do these core electrons contribute to the magnetic susceptibility χ of the atoms? If so what is the sign of χ?

                S=0, L=0,J=0: No paramagnetism
                There is a negative (usually) small diamagnetic contribution to the magnetic susceptibility (Langevin diamagnetism)

    (ii)   According to the Hund's rules what is the lowest energy multiplet and what is its degeneracy?

                S=3/2; L=0, J=3/2: ${}^4S_{3/2}$

                Degenaracy of this lowest energy multiplet =2J+1=4

    (iii)   What is the zero-field magnetic susceptibility of 1 mole of notrogen atoms at a temperature T?

                $\chi = N_A [(g_J\mu_B)^2 J(J+1)]/3k_BT$ Curie Law

                Since L=0, g_J=2

                $\chi = N_A [5\mu_B^2]/k_BT$

Problem#4. (5 points)
A He atom is excited to $1s^1 2p^1$ configuration. The one electron spatial wave functions are: $\varphi_{1s}(\mathbf{r})$ and $\varphi_{2pm}(\mathbf{r})$.
What is the total number of 2 electron states corresponding to this configuration?

> Since 1 electron has to be in the 1s with spin either up or down (2 possible ways) and the other in one of the 6 2p states (three space orbitals with spin either up or down- 6 possible ways); the total number of 2 electron states = **12**

Write down the 2-electron spin triplet excited state wave functions associated with this configuration.

> $(1/\sqrt{2})[\varphi_{1s}(\mathbf{r}_1)\varphi_{2pm}(\mathbf{r}_2)- \varphi_{1s}(\mathbf{r}_2)\varphi_{2pm}(\mathbf{r}_1)] \times [\alpha_1\alpha_2; \beta_1\beta_2; (\alpha_1\beta_2+ \alpha_2\beta_1) /\sqrt{2}]$

> m=1, 0, 1

Problem # 5 (5 points)
Write down the wave function for the ground state of H_2 molecule in molecular orbital (MO) approximation? Express your answer in terms of the 1s hydrogen atom wave functions associated with the two protons, $a(\vec{r}); b(\vec{r})$. Draw qualitatively the ground state electronic energy (in atomic units), the repulsive energy between two protons, and the total energy, as function of the inter-nuclear separation R.

> In MO approximation for H2 molecule we first find **single particle** states (molecular orbitals). In the simplest case the molecular orbital is formed out of two atomic hydrogen 1s states associated with two nuclei, denoted as a(r) and b(r) respectively. Since the bonding combination has lower energy we use these bonding orbitals to construct the states for the **two** electrons.

> $$\varphi_B(\mathbf{r})=N[a(\mathbf{r}) +b(\mathbf{r})]$$

If we now put two electrons in this orbital their spins are opposite; **spin singlet**

> $\psi_{MO}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_B(\mathbf{r}_1)\, \varphi_B(\mathbf{r}_2)[(\alpha_1\beta_2- \alpha_2\beta_1) /\sqrt{2}]$

This is just like the ground state of the He atom. Instead of putting the two electrons in the 1s orbital $\varphi_{1s}(\mathbf{r})$, you put them in the bonding orbital $\varphi_B(\mathbf{r})$.

SORRY, I CAN'T DRAW THE FIGURE. WILL DO IT IN THE LECTURE