YOUR NAME:

PHY 491 - 2013
Midterm Exam

1. In the intergalactic medium, oxygen ($Z = 8$) can be highly ionized. This has been seen in far-ultraviolet spectroscopy. Consider an oxygen ion where only one electron is left. What is the energy of a photon that it would emit in a transition from the first excited to the ground state, given that the electron binding energy in a hydrogen atom is Ry$\approx$ 13.6 eV; an approximate value is sufficient (10 pt)

2. Consider an atom with the ground-state electron configuration $1s^2\,2s^2\,2p^2$. What is the ground-state term and what is the value of the total momentum J in the ground state, according to Hund's rule? (10 pt) Do you expect the atom to show diamagnetic or paramagnetic response to a magnetic field - provide arguments (3 pt)

3. Consider a diatomic molecule with nuclear masses $\sim M$ and the typical electron binding energy E_e. Consider the quartic term in the expansion of the potential energy in the relative displacement ΔR of the nuclei from the equilibrium position $\Delta U = K_1(\Delta R)^4$. Estimate K_1 in terms of E_e and the electron mass m_e. (10 pt) Using the first-order perturbation theory, estimate the shift of the lowest vibrational energy level $\propto K_1$ (5 pt).

You need 30 pt

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1. An oxygen ion with one electron is described by the same equation as the hydrogen atom, except that the nuclear charge is different, $e \to Ze$. The Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2_{\vec{r}} - \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi(\vec{r}) = E\psi(\vec{r}).$$

Therefore the energy levels are $E_n = -\frac{\hbar^2 Z^2}{2m_e a_B^2}\frac{1}{n^2}$, $n=1,2,\ldots$

The energy difference between the first excited state and the ground state is

$$h\nu = E_2 - E_1 = \frac{3}{4}\frac{\hbar^2 Z^2}{2m_e a_B^2} = \frac{3}{4} Z^2 Ry \simeq 0.65\ keV$$

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2. The only contribution comes from the unfilled shell p^2. We have states $(m_\ell\, s_z)$ like

$$(1\ \tfrac{1}{2})\quad (0\ \tfrac{1}{2})\quad (-1\ \tfrac{1}{2})$$

$$(1\ -\tfrac{1}{2})\quad (0\ -\tfrac{1}{2})\quad (-1\ -\tfrac{1}{2})$$

and look for states with nonnegative total m_ℓ, s_z

We have, for two electrons

$$(2\ 0)\quad (1\ 0)\quad (0\ 0)\quad (1\ 0)\quad (0\ 0)\quad (0\ 0)\quad (1\ 1)\quad (0\ 1)$$

$\Rightarrow$ we have terms ${}^1D$, ${}^3P$, ${}^1S$ $\Rightarrow$ total $5+9+1=15$ states

The largest-spin term is ${}^3P$. Since the shell is less than half-filled, $J=|L-S|=0$. Therefore the ground state is ${}^3P_0$.

With $J=0$, there is a diamagnetic contribution to the ground-state energy $\Delta E = \frac{1}{8m} e^2 \langle 0|(\vec{r}\times\vec{B})^2|0\rangle > 0$.

There is also a second-order correction $\mu_B^2 \sum_n \frac{|\langle 0|\vec{B}(\vec{L}+g\vec{S})|n\rangle|^2}{E_0-E_n}$, which is negative ($n$ enumerates excited states).

If this correction dominates, the atom displays Van Vleck paramagnetism, otherwise it is diamagnetic

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3. If the typical internuclear distance is a, then the electron energy is $E_e \sim \frac{\hbar^2}{m_e a^2}$, or $a^2 \sim \frac{\hbar^2}{m_e E_e}$.

If we stretch the molecule so that the nuclei are shifted by a, the change of the energy should be $\sim$ the energy E_e. Then $K_1 a^4 \sim E_e$, $K_1 \sim \frac{E_e}{a^4} \sim \frac{m_e^2 E_e^3}{\hbar^4}$

The displacement of vibrating nuclei due to quantum fluctuations is $\sim (\hbar / M\omega)^{1/2}$, where M is the nuclear mass and ω is the vibration frequency. As we estimated in class, $\hbar\omega \sim E_e \sqrt{\frac{m_e}{M}}$.

The energy shift is $\sim K_1 \left(\left(\frac{\hbar}{M\omega} \right)^{1/2} \right)^4 \sim \frac{m_e^2 E_e^3}{\hbar^4} \cdot \frac{\hbar^4}{E_e^2 m_e M}$

$$\sim \frac{m_e}{M} E_e$$

$\Rightarrow$ the same as the typical rotational energy