Chem 452 – Exam II
October 17, 2007

Cover Sheet
Closed Book, Closed Notes, and NO Calculator

There are 14 total pages. Each part of a question is worth 4 points unless otherwise noted.

Useful Equations:

\[ E_n = -\frac{Z^2 R_H}{n^2} \]

\[ R_H = 109677 \text{ cm}^{-1} = 13.6eV \]

\[ E_m = \frac{m^2 \hbar^2}{2I} \]

\[ E_j = \frac{l(l+1)\hbar^2}{2I} \]

\[ |l - s| \leq j \leq l + s, \text{ in steps of 1} \]
### Point Total

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1. (16 points) Below is the potential energy of the harmonic oscillator with frequency \( \omega \) (\( \omega = (k/m)^{1/2} \)), where \( k \) is force constant, and \( m \) is mass).
a. Write down the Hamiltonian for this system. Give the explicit functional forms for the operators.

b. Sketch on the diagram the energy levels (v = 0 and v = 2). Clearly mark the values of the energy.

c. Identify the zero point energy on the graph and give its value.

d. Does the probability for finding the harmonic oscillator outside of its classical turning points increases, decreases, or remains the same as quantum number, v, increases? Explain your answer.
2. (8 points) For a particle in a ring (2D rotation).

a. What is the value of $l_z$ in energy state with wavefunction $\Psi = \frac{1}{\sqrt{2\pi}} e^{-i3\phi}$?

b. What is the probability of finding the particle at an angle $\phi$? How does the uncertainty principle support your answer?
3. (8 points) For a particle on a sphere with moment of inertia $I$ (3D rotation).

a. What is the energy of the state with $l = 3$.

b. What is the degeneracy of the energy state with $l = 2$. 

4. (8 points) On the vector diagram shown below

a. Calculate and indicate the length of angular momentum vector for \( l = 2 \). For simplicity, you may assume \( h = 1 \).

b. Indicate all possible \( z \)-components of angular momentum.
5. (8 points) Indicate, using sketches and symmetry arguments, whether the following integrals are equal to zero or not.

a. \[ \int_{-\pi}^{\pi} x^3 \sin^2(x) \exp(-x^2) \, dx \]

b. \[ \int_{0}^{\pi} \sin(x) \cos^2(x) \, dx \]
6. (4 points) Suppose the two electrons in an atom occupy the same orbital \( \Psi \), then in the orbital approximation the overall wavefunction is \( \Psi(1)\Psi(2) \). The total wavefunction of the system is of the product of the orbital part and one of the four spin states:

\[
\Psi(1)\Psi(2)\alpha(1)\alpha(1); \Psi(1)\Psi(2)\beta(1)\beta(2); \Psi(1)\Psi(2)\sigma_+ (1, 2); \Psi(1)\Psi(2)\sigma_- (1, 2),
\]

\[
\sigma_+ (1, 2) = \frac{1}{\sqrt{2}} \{\alpha(1)\beta(2) + \beta(1)\alpha(2)\}
\]

\[
\sigma_- (1, 2) = \frac{1}{\sqrt{2}} \{\alpha(1)\beta(2) - \beta(1)\alpha(2)\}
\]

According to the Pauli principle only one of these wavefunctions is acceptable for electrons. Which one? Explain.
7. (4 points) Choose 2 of the 3 to answer. **Clearly mark which part you do not want graded.**

a. One can “add” the orbital and spin angular momenta to obtain the total angular momentum. For a particle free moving on the surface of a sphere with \( l = 2 \) and \( s = 1 \), determine all possible values of \( j \).

b. Assume a particle has total angular momentum quantum number, \( j = 7 \), determine the degeneracy of the total angular momentum state.

c. Assume a particle has total angular momentum quantum number, \( j = 4 \), determine all possible z components of total angular momentum for all states.
8. (4 points) The nucleus $^{23}\text{Na}$ has a spin quantum number of $s = 3/2$. Calculate all possible values of the $z$ component of spin angular momentum.

9. (4 points) What is the Stern-Gerlach experiment? What new property was drawn from this experiment?
10. (12 points) An electron in a He\(^{+}\) ion has a principal quantum number equal to 3.
   
   a. List all the possible values of the other quantum numbers.

   b. Give the degeneracy of this state including spin.

   c. What is the ionization energy from this state?
11. (12 points) Below are three plots of the 2s orbital of a H atom. Identify which plot belongs to the wavefunction, \( \Psi_{2s}(r) \); the probability density, \( \Psi^2_{2s}(r) \); and the radial distribution function, \( r^2\Psi^2_{2s}(r) \). Identify which plot is which function and explain your rationale for the choice. Identify the most probable value of \( r \).
12.  (8 points) Choose 2 of the 3 to answer. **Clearly mark which part you do not want graded.**

Which of the following transitions are allowed or not allowed (forbidden). Give your reason why.

a. H atom, $4p^1$ to $1s^1$

b. Li$^+$ ion, $1s^13p^1$ (triplet state) to $1s^2$ (singlet state)

c. Li$^{2+}$ ion, $4s^1$ to $1s^1$