Quantum Mechanics and Atomic Physics (361)
Final exam, Fall 2011
Name (Please write it legibly): ______________________

**** This exam is composed of four pages, and so if any page is missing, let the proctor know immediately ****

<u>Useful formula</u>

$$\lambda = \frac{h}{p};\ \Delta x \Delta p \geq \frac{\hbar}{2};\ p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x};\ \ H\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t};$$

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i};\ \ \cos(x) = \frac{e^{ix} + e^{-ix}}{2};$$

$$L^2 Y_{l,m} = \hbar^2 l(l+1) Y_{l,m};\ L_z Y_{l,m} = \hbar m Y_{l,m};$$

$$\int sin^2(ax)dx = \frac{x}{2} - \frac{1}{4a}\sin(2ax);$$

WKB approximation: $2\sqrt{2m}\int\sqrt{E - V(x)}dx \approx nh;$

For an infinite potential well covering [0, L], the energy eigen-functions and the corresponding eigen-energies are, respectively, $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$ for $x \in [0, L]$ and $E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$.

Hund's 3rd rule: J = |L-S| if less than half-filled, J=L+S if more than half-filled.

**Table 6.1 Spherical Harmonics**

| | |
|---|---|
| $Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$ | $Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$ |
| $Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$ | $Y_{2,0}(\theta,\phi) = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$ |
| $Y_{2,\pm1}(\theta,\phi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$ | $Y_{2,\pm2}(\theta,\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$ |
| $Y_{3,0}(\theta,\phi) = \sqrt{\frac{7}{16\pi}}(5\cos^3\theta - 3\cos\theta)$ | $Y_{3,\pm1}(\theta,\phi) = \mp\sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta - 1)\, e^{\pm i\phi}$ |
| $Y_{3,\pm2}(\theta,\phi) = \sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$ | $Y_{3,\pm3}(\theta,\phi) = \mp\sqrt{\frac{35}{64\pi}}\sin^3\theta\, e^{\pm 3i\phi}$ |

1. (3pts) In kinetic theory, atoms are modeled as point masses of mass $m$, and the mean speed $v$ of an atom in an environment at absolute temperature $T$ is given by $mv^2 = 3kT$, where $k$ is Boltzmann's constant. Derive an expression for the de Broglie wavelength for an atom of mass $m$ at absolute temperature $T$ in terms of $h$, $k$, $T$ and $m$.

2. (3pts) Suppose that $\psi(x) = A exp(-x^2)$, is known to be a solution of the time independent Schroedinger equation for some energy E. What is the corresponding potential function V(x)?

3. (3pts) Without solving the Shroedinger equation, relying only on the uncertainty principle, estimate the minimum energy of a particle of mass $m$ trapped in an infinite potential well of width L.

4. (3pts) Angular wavefunction of a particle in a central potential is given by $A(\theta, \phi) = C$, where $C$ is a normalization constant. What is the expectation value of $L^2$ and $L_z$ for this state?

5. Consider helium atom with two electrons. For the following questions, assume that one electron is in $\psi_{100}$ state and the other electron can occupy any of the $l$=0 states (that is, $\psi_{n00}$, n=1, 2, 3, …). Also ignore fine-structure or any other higher order effects in the following questions. **Note that single electron has a spin quantum number of ½.**

(a) (2pts) What is the total spin quantum number of the lowest energy configuration? Is the spatial wavefunction of this configuration symmetric or antisymmetric w.r.t. exchange of the two electrons?

(b) (2pts) If you ignore electron-electron interaction, what are the possible total spin quantum numbers of the 2nd lowest energy configuration?

(c) (2pts) If you include the electron-electron interaction, what will be the total spin quantum number of the 2nd lowest energy configuration? Is the spatial wavefunction of this state symmetric or antisymmetric w.r.t. exchange of the two electrons?

(d) (2pts) If the energy of (b) configuration is $E_b$ and that of (c) is $E_c$, which is correct: $E_b > E_c$, $E_b < E_c$ or $E_b = E_c$?

6. In an infinite potential well extending over [0, 2π], the wavefunction of a particle at t=0 is given by

$$\psi(x) = \begin{cases} A\left(1 - e^{ix}\right), & \text{for } x \in [0,2\pi] \\ 0, & \text{else} \end{cases}.$$

(a) (3pts) Find the normalization constant A.

(b) (3pts) Sketch the probability density as a function of $x$.

(c) (3pts) What is the energy expectation value of this state?

(d) (3pts) If you measure the energy of this particle, what is the probability of getting the energy of $E_2$.

7. (3pts) For arbitrarily shaped tunnel barriers, the transmission coefficient is approximately given by $T = \exp\left(-2\int \frac{\sqrt{2m(V(x)-E)}}{\hbar} dx\right)$. For a step potential barrier, given by $V(x) = \begin{cases} V_0, & \text{for } x \in [0,a] \\ 0, & \text{else} \end{cases}$, when an electron with energy between 0 and $V_0$ is injected from left toward this step potential barrier, the transmission coefficient is found to be $T_0$. Now if the width of the step potential is doubled, that is, if '$a$' becomes '$2a$', what will be the new transmission coefficient in terms of $T_0$?

8. Electron in hydrogen atom is prepared in a linearly combined state, $\psi = A(2\psi_{100} - i\psi_{210} + 3\psi_{32-2})$, where $\psi_{nlm}$ stands for the eigen-functions of the hydrogen Schroedinger equation with the quantum numbers ($n$, $l$, $m$).

(a) (3pt) Find the normalization constant A

(b) (3pts) What is the expectation value of $L^2$?

(c) (3pts) What is the expectation value of $L_z$?

(d) (3pts) If you construct a new wavefunction, $\psi_{new} = CL_-(2\psi_{100} - i\psi_{210} + 3\psi_{32-2})$, where C is a normalization constant and $L_-$ is the lowering operator, what are the expectation values of $L^2$ and $L_z$ of this new wavefunction?

9. (3pts) Sulfur has 16 electrons. Using the orbital filling rules as discussed in class, suggest its most likely electron configuration and spectroscopic notation ($^{2S+1}L_J$) of the ground state.

10. (3pts) A particle of mass $m$ is trapped in the linear potential $V(x) = \alpha|x|$
Use WKB approximation to estimate the energy eigenvalues of this particle.

11. (3pts) Consider a perturbed infinite well defined as

$$V(x) = \begin{cases} V_0, & \text{for } x \in [0, \frac{L}{4}] \\ 0, & \text{for } x \in [\frac{L}{4}, L] \\ \infty, & \text{else} \end{cases}$$ , where $V_0$ is small compared with the ground state energy.

Using the first order perturbation theory, estimate the new ground state energy $E_1$. Note that the eigenfunctions and eigenenergies of the unperturbed infinite well, and the necessary integral are given at the beginning of this exam.

12. (4pts) Consider a particle in a tilted infinite-potential well shown below. Without solving the Schroedinger equation, sketch the probability density of the eigenfunctions corresponding to the ground state ($E_0$) and the second excited state ($E_2$): in your sketch, make it clear about the absence/presence of the penetration of the eigenfunction. Note here that the lowest eigenenergy is $E_0$.