Question	*Score*	*out of*
1		4
2		6
3		5
Total		**15**

Name:________________

Student Number:________________

Chem 3PA3 - Fall 2013

1st Midterm Practice

Time: 50 min
Calculators are allowed!
No notes, books or personal paper are allowed!
Attempt all questions.
In answering the questions, show all steps of your reasoning and calculation!
This exam is worth a total of 15%, i. e. you should be scoring on average 0.3% per minute!

Potentially Useful Numbers and Formulas: *(Note the difference between h and h-bar!)*

h = 6.6261 x 10^{-34} Js; m_e = 9.1094 x 10^{-31} kg; e = 1.6022 x 10^{-19} C; c = 2.9979x10^{8} m/s;
N_A = 6.022x10^{23} mol^{-1}; k_B = 1.38066 x 10^{-23} J/K; a_0 = 5.291772x10^{-9} cm; $l_{C=C,\ Benzene}$ = 0.14 nm;
1 nm = 10^{-9} m; 1 J = 6.242x10^{18} eV = 5.034 x 10^{22} cm^{-1}

Rigid Rotor: $B=\frac{h}{8\pi^2 c\mu r^2}$ Harmonic Oscillator: $\psi_0(x)=\sqrt[4]{\frac{\beta^2}{\pi}}e^{\frac{-(\beta x)^2}{2}}$; $\beta^2=\frac{\sqrt{(km)}}{\hbar}$

$$\psi_1(x)=\frac{\sqrt[4]{\frac{\beta^2}{\pi}}}{\sqrt{2}}(2\beta x)e^{\frac{-(\beta x)^2}{2}};\beta^2=\frac{\sqrt{(km)}}{\hbar} \qquad \psi_2(x)=\frac{\sqrt[4]{\frac{\beta^2}{\pi}}}{\sqrt{8}}(4(\beta x)^2-2)e^{\frac{-(\beta x)^2}{2}};\beta^2=\frac{\sqrt{(km)}}{\hbar}$$

Potentially Useful Integrals:

$$\int_0^\infty e^{-cx^2}dx=\frac{1}{2}\sqrt{\frac{\pi}{c}} \; ; \; \int_0^\infty x^2 e^{-cx^2}dx=\frac{1}{4}\sqrt{\frac{\pi}{c^3}} \; ; \; \int_0^\infty x e^{-cx^2}dx=\frac{1}{2c} \; ; \; \int_0^\infty x^{2n+1}e^{-cx^2}dx=\frac{n!}{2c^{n+1}}$$

$$\int_0^\infty x^{2n}e^{-cx^2}dx=\frac{(2n-1)(2n-3)...(3)(1)}{2^{n+1}}\sqrt{\frac{\pi}{c^{2n+1}}} \; ; \; \int_{-\infty}^0 x^n e^{-cx^2}dx=(-1)^n\int_0^\infty x^n e^{-cx^2}dx$$

$$\int \sin^2(cx)dx=\frac{x}{2}-\frac{\sin(2cx)}{4c} \; ; \; \int x\sin^2(cx)dx=\frac{x^2}{4}-\frac{x\sin(2cx)}{4c}-\frac{\cos(2cx)}{8c^2}$$

$$\int x^2\sin^2(cx)dx=\frac{x^3}{6}-\left(\frac{x^2}{4c}-\frac{1}{8c^3}\right)\sin(2cx)-\frac{x\cos(2cx)}{4c^2}$$

1) *(4)* **Operators.**

(a) *(2)* Evaluate $[\hat{p}_x, (\hat{x})^2]$ and $[\hat{p}_y, (\hat{x})^2]$

(b) *(2)* Define the term "Linear Operator" and give one counter-example. Prove that your example is not a linear operator.

2) *(6)* **Particle in a 3D box.**
For a particle in an oblong 3-dimensional box with infinitely tall walls and dimensions such that $a = l_x = l_y = 0.5\, l_z$, consider the energy range $E < 10h^2/8ma^2$.
(a) *(2)* Write out expressions for the overall wavefunction and total energy of this particle as a function of all its quantum numbers!
(b) *(2)* How many states lie in the given energy range? (What are the states?)
(c) *(2)* How many energy levels lie in the given energy range? (What are they and what is the degree of degeneracy for each?)

3) *(5)* **Particle in a 1D box.**
Consider a one-dimensional box of length l with infinitely tall walls. ($V \to \infty$ for $x \leqslant 0$ and $x \geqslant l$)
(a) *(1)* What is the normalized eigenfunction of the associated Hamiltonian operator with the smallest eigenvalue? What is the smallest eigenvalue?
(b) *(2)* Now assume a particle with a wavefunction of the form $\psi(x) = A\,x(l-x)$ for the region $0 < x < l$. Find the value of the normalization constant A and the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$.
(c) *(2)* Is the function in question 3b an eigenfunction of the Hamiltonian? Prove your answer. If it is an eigenfunction of the Hamiltonian, find the associated eigenvalue. If it is not an eigenfunction, find the expectation value of the Hamiltonian for this function. How does the eigenvalue or expectation value of this function compare to the eigenvalue of the function from question 3a? Which one is bigger and by how much?