Chem 361
Quantum Chemistry
Midterm Exam
October 18, 2006

Name ________

Full credit will be given to correct answers only when ALL the necessary steps are shown. DO NOT GUESS THE ANSWER.

This is a closed book and closed notes exam, and you are responsible to be sure that your exam has no missing pages (6 pages).

If you consider that there is not enough information to solve a problem, you have to specify the missing information and describe the problem solving procedure.

No one can make you feel inferior without your consent

\- Eleanor Roosevelt -

Honor Statement

I have neither give nor received aid in this examination.

Full signature ______________________________

Problem 1 (15 points)

Sirus, one of the hottest known stars, has approximate blackbody radiation with $\lambda max = 2600$ A. Estimate the surface temperature of Sirus.

$$\lambda_{max} T = 2.88 \times 10^7 \text{ K Å}$$

T
2 sig figs

$$T = \frac{2.88 \times 10^7 \text{ K Å}}{2.6 \times 10^3 \text{ Å}}$$

$$\boxed{T = 1.1 \times 10^4 \text{ K}}$$

Problem 2 (15 points)

A muon is an unstable elementary particle whose mass is 207 me, and whose charge is either +e or –e. A negative muon (μ–) can be captured by a nucleus to form a muonic atom.
a) A proton captures a μ–. Find the radius of the first orbit of this atom.
b) Find the ionization energy of the atom.

$$r_n = \frac{4\pi\epsilon_0 \hbar^2}{|q||e|\, m_\mu} n^2 \Rightarrow r_1 = \frac{4\pi\epsilon_0 \hbar^2}{|q||e|\, m_e} \frac{1}{207}$$

$$= \frac{0.5\ \mathring{A}}{207}$$

$$\boxed{r_1 = 2.4 \times 10^{-13}\ m}$$

$$E_n = -\frac{m_\mu |e|^2 |q|^2}{8 \epsilon_0^2 h^2} \frac{1}{n^2}$$

$$IE = 207\left(\frac{m_e |e|^2 |q|^2}{8\epsilon_0^2 h^2}\right) = 207(13.6\ eV)$$

$$\boxed{IE = 2.82\ keV} = 2.82 \times 1.602 \times 10^{-16}\ J$$

$$\boxed{= 4.51 \times 10^{-16}\ J}$$

Problem 3 (30 points)

A particle limited to the x axis has the wave function $\Psi(x) = a\,x$ between $x = 0$ and $x = 1$; $\Psi = 0$ elsewhere.

a) Find the probability that the particle can be found between $x = 0.45$ and $x = 0.55$.

b) Find the expectation value <x> of the particle's position.

$$\int_0^1 \psi^*(x)\,\psi(x)\,dx = 1 = a^2\int_0^1 x^2\,dx = a^2\frac{x^3}{3}\Big|_0^1 = \frac{a^2}{3}$$

$$a = \sqrt{3} = 1.73$$

a) $$P[0.45 < x < 0.55] = \int_{0.45}^{0.55} |\psi|^2\,dx = a^2\frac{x^3}{3}\Big|_{0.45}^{0.55}$$

$$= 0.075$$

b) $$\boxed{\langle x\rangle} = \langle\psi|x\psi\rangle = \int_0^1 x|\psi|^2\,dx = a^2\int_0^1 x^3\,dx$$

$$= a^2\frac{x^4}{4}\Big|_0^1 = \frac{a^2}{4} = \frac{3}{4} = \boxed{0.75}$$

Problem 4 (30 points)

For a particle in a box, find the probability that the particle can be found between 0,45L, and 0.55 L for the ground state and the first excited state.

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$P_n[0.45L < X < 0.55L] = \frac{2}{L}\int_{0.45L}^{0.55L} \sin\left(\frac{n\pi}{L}x\right)^2 dx$$

$n=1$ $$P_1 = \frac{2}{L}\int_{0.45L}^{0.55L} \sin\left(\frac{\pi}{L}x\right)^2 dx = \frac{2}{L}\left[\frac{x}{2} - \frac{L}{4\pi}\sin\left(\frac{2\pi x}{L}\right)\right]_{0.45L}^{0.55L}$$

$$\boxed{P_1 = 0.20}$$

$n=2$ $$P_2 = \frac{2}{L}\int_{0.45L}^{0.55L} \sin\left(\frac{2\pi}{L}x\right)^2 dx = \frac{2}{L}\left[\frac{x}{2} - \frac{L}{8\pi}\sin\left(\frac{4\pi x}{L}\right)\right]_{0.45L}^{0.55L}$$

$$\boxed{P_2 = 6.5 \times 10^{-3}}$$

Problem 5 (10 points)

Prove that for a Hermitian operator **O** its eigenfunctions are orthogonal.

DEF $\hat{O}$ HERMITIAN IF AND ONLY IF

$$\langle m | \hat{O} n \rangle = \langle \hat{O} m | n \rangle$$

$$\int f_m^* (\hat{O} f_n)\, dx = \int (\hat{O} f_m)^* f_n\, dx$$

SINCE $\hat{O} f_i = \lambda_i f_i$ WITH $\lambda_i \in \mathbb{R}$

WE GET FROM THE DEFINITION

$$\lambda_n \int f_m^* f_n\, dx = \lambda_m \int f_m^* f_n\, dx$$

$$(\lambda_m - \lambda_n) \int f_m^* f_n\, dx = 0$$

IF $\lambda_m \neq \lambda_n \Rightarrow \int f_m^* f_n\, dx = 0$

ORTHOGONAL