**Chem 361**
**Quantum Chemistry**
**Midterm Exam**
**October 13, 2004**

**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 -

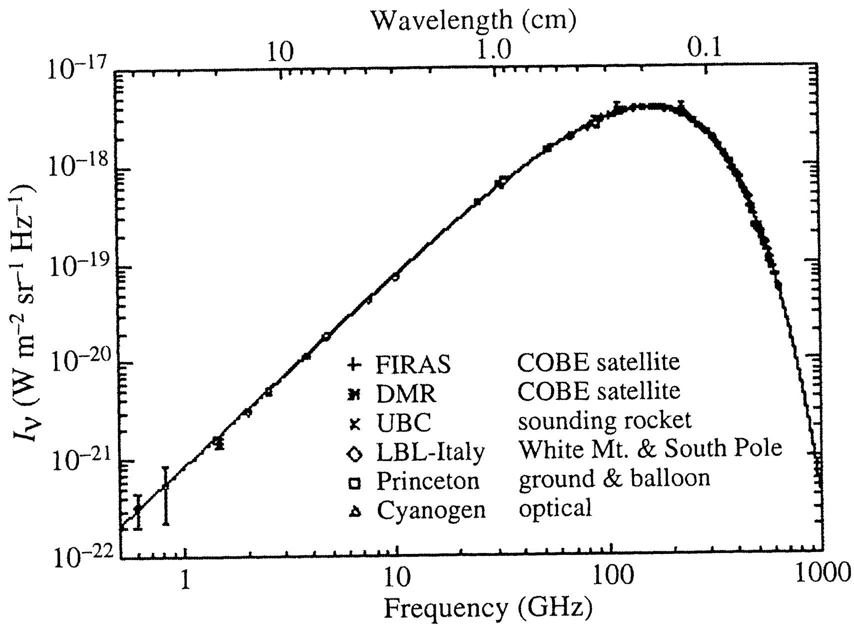
**Honor Statement**

**I have neither give nor received aid in this examination.**

**Full signature ________________________________**

**Problem 1 (20 points)**

Astrophysicists have been studying what is known as background radiation of the Universe, the rennet of the Big Bang. Recent observations have yielded the following energy distribution.




The figure shows that the background radiation follows the blackbody distribution. From the figure estimate the temperature of the background radiation of the Universe.

WIEN DISPLACEMENT LAW $\lambda_{max} T = 2.899 \times 10^{-3}\, m\, K$

OR $\dfrac{hc}{\lambda_{max} k_B T} \simeq 5 \Rightarrow \lambda_{max} T \simeq \dfrac{1}{5} \dfrac{hc}{k_B}$

$$T = \frac{2.899 \times 10^{-3}\, m\, K}{\lambda_{max}} \simeq \frac{2.899 \times 10^{-3}\, m\, K}{1.8 \times 10^{-3}\, m}$$

$T \simeq 1.6\, K$

**Problem 2 (30 points)**

A certain one-dimensional quantum system in $0 \le x \le \infty$ is describe by the Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2\,m}\frac{d^2}{d\,x^2} \quad - \quad \frac{q^2}{x} \ ,.$$

where q is a constant.

One of the wave functions is known to be

$$\Psi(x) = \mathrm{A\,x\,e}^{-\alpha\,x} \ ,$$

where

$\alpha = \dfrac{m\,q^2}{\hbar^2}$ and A is a constant.

$$\hat{H}\Psi = E\Psi$$

a) Find the corresponding energy eigenvalue in terms of $\hbar$, m and q.
b) Find the value of A which normalizes the wave function according to

$$\int_0^\infty |\Psi(x)|^2\,dx = 1 \ ,$$

You may require the definite integrals

$$\int_0^\infty x^n\,e^{-a\,x}dx = \frac{n!}{a^{n+1}} \ ,$$

where the factorial of n is given by: n! = 1*2*3*…(n-2)*(n-1)*n.

$$-\frac{\hbar^2}{2m}\frac{d}{dx}\frac{d}{dx}\left(Axe^{-\alpha x}\right) - \frac{q^2}{x}Axe^{-\alpha x} = EAxe^{-\alpha x}$$

$$-\frac{\hbar^2}{2m}\frac{d}{dx}\left[-\alpha Axe^{-\alpha x} + Ae^{-\alpha x}\right] - q^2Ae^{-\alpha x} = EAxe^{-\alpha x}$$

$$-\frac{\hbar^2}{2m}\left[\alpha^2Axe^{-\alpha x} - 2\alpha Ae^{-\alpha x}\right] - q^2Ae^{-\alpha x} = EAxe^{-\alpha x}$$

$$-\frac{\hbar^2\alpha^2}{2m}Axe^{-\alpha x} + \frac{\hbar^2\alpha}{m}Ae^{-\alpha x} - q^2Ae^{-\alpha x} = EAxe^{-\alpha x}$$

$$-\frac{\cancel{\hbar^2}}{2\cancel{m}}\frac{m^{\cancel{2}}q^4}{\hbar^{\cancel{4}2}}Axe^{-\alpha x} + \underbrace{\frac{\cancel{\hbar^2}}{\cancel{m}}\frac{\cancel{m}q^2}{\cancel{\hbar^2}}Ae^{-\alpha x} - q^2Ae^{-\alpha x}}_{0} = EAxe^{-\alpha x}$$

$$\boxed{E = -\frac{mq^4}{2\hbar^2}}$$

$$-\frac{mq^4}{2\hbar^2}Axe^{-\alpha} = EAxe^{-\alpha x}$$

$$\int_0^\infty |\Psi(x)|^2 dx = \int_0^\infty A^2 x^2 e^{-2\alpha x} dx = 1$$

$$A^2 \int_0^\infty x^2 e^{-2\alpha x} dx = 1$$

$$A^2 \frac{2!}{(2\alpha)^3} = \frac{A^2 2}{8\alpha^3} = 1$$

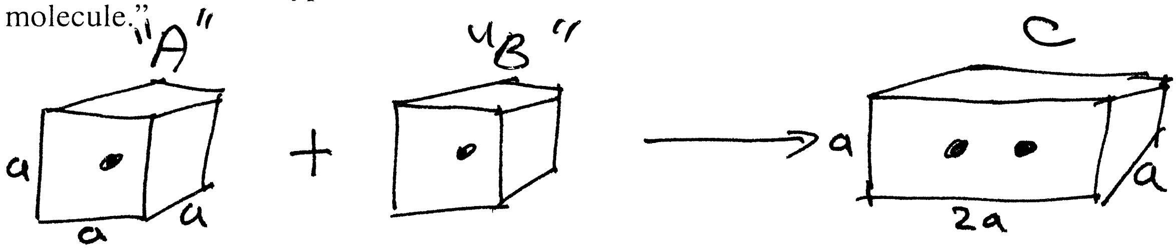
$$A^2 = 4\alpha^3$$

$$A = 2\alpha^{3/2}$$

$$\boxed{\Psi(x) = 2\alpha^{3/2} x e^{-\alpha x}} \qquad \alpha = \frac{mq^2}{\hbar^2}$$

**Problem 3 (20 points)**

Consider the hypothetical chemical reaction of two "cube atoms" to form a "dicube molecule."




Each cube-atom contains one electron. The interaction between electrons can be neglected. Determine the energy change in the above reaction.

FOR "CUBE ATOMS"

$$E_{n_x n_y n_z} = \frac{h^2}{8ma^2}\left[n_x^2 + m_y^2 + n_z^2\right]$$

THE GROUND STATES OF "A" AND "B" YIELD THE FOLLOWING ENERGY

$$E_i \equiv E_A + E_B = 2\left(\frac{h^2}{8ma^2}\right)$$

where $E_A$ OR $E_B$ CAN BE $E_{100}$, $E_{010}$, $E_{001}$

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FOR THE "DICUBE MOLECULE"

$$E_{m_x m_y m_z} = \frac{h^2}{8m}\left[\frac{m_x^2}{(2a)^2} + \frac{m_y^2}{a^2} + \frac{m_z^2}{a^2}\right]$$

DIFFERENT QUANTUM NUMBERS

LOWEST ENERGY $\rightarrow$ $E_{100} < E_{010} = E_{001}$

THUS $E_f = 2E_{100} = \frac{1}{2}\left(\frac{h^2}{8ma^2}\right)$

$$\Delta E = E_f - E_i = \frac{1}{2}\left(\frac{h^2}{8ma^2}\right) - 2\left(\frac{h^2}{8ma^2}\right) = -\frac{3}{2}\left(\frac{h^2}{8ma^2}\right) < 0$$

**Problem 4 (30 points)**

WITH INFINITE PRECISION

Can you measure simultaneously a particle's z-component of linear momentum, $P_z$ , and z-component of the angular momentum, $L_z$? Give proof.

TWO MEASUREMENTS OF TWO DIFFERENT OBSERVABLES CAN BE PERFORMED AT THE SAME TIME WITH INFINITE PRECISION IF AND ONLY IF THE COMMUTATOR OF THE QUANTUM OPERATORS ASSOCIATED WITH THE OBSERVABLES IS EQUAL TO ZERO

$$[\hat{P}_z, \hat{L}_z] = ?$$

$$\hat{L}_z = \hat{x}\hat{P}_y - \hat{y}\hat{P}_x$$

$$\hat{P}_z = -i\hbar \frac{\partial}{\partial z} \qquad \hat{P}_y = -i\hbar \frac{\partial}{\partial y}$$

$$\hat{P}_x = -i\hbar \frac{\partial}{\partial x}$$

$$
\begin{aligned}
[\hat{P}_z, \hat{L}_z]f &= \hat{P}_z\hat{L}_z f - \hat{L}_z\hat{P}_z f \\
&= \hat{P}_z(\hat{x}\hat{P}_y - \hat{y}\hat{P}_x)f - (\hat{x}\hat{P}_y - \hat{y}\hat{P}_x)\hat{P}_z f \\
&= \hat{P}_z\hat{x}\hat{P}_y f - \hat{P}_z\hat{y}\hat{P}_x f - \hat{x}\hat{P}_y\hat{P}_z f + \hat{y}\hat{P}_x\hat{P}_z f \\
&\quad \hat{x}\hat{P}_y\hat{P}_z f - \hat{y}\hat{P}_x\hat{P}_z f - \hat{x}\hat{P}_y\hat{P}_z f + \hat{y}\hat{P}_x\hat{P}_z f \\
&= 0
\end{aligned}
$$

$\Rightarrow$ YES YOU CAN MEASURE SIMULTANEOUSLY $\hat{P}_z$ AND $L_z$

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$$\hat{P}_z\hat{x}\hat{P}_y f = (-i\hbar)^2 \frac{\partial}{\partial z}\left(x \frac{\partial}{\partial y} f\right) = x\frac{\partial^2 f}{\partial z \partial y} = x\frac{\partial^2 f}{\partial y \partial z} = x\frac{\partial}{\partial y}\frac{\partial f}{\partial z}$$

$$= \hat{x}\hat{P}_y\hat{P}_z f$$