Exam II
C441, Fall 2000

Instructions:

You may use any resource ***except*** each other, which is strictly forbidden. For maximum partial credit show **all** of your work, and clearly indicate the answer to numerical problems. Clearly label the axes and title of any graph you include, and choose appropriate ranges. Submit the problems **in numerical order**.

If you have questions, please contact me. I am willing to point you in the right direction, but if you ask me about an answer, I will suddenly become very quiet. (Or charge you more money than you are willing to part with. I generally charge 10x what you can afford...).

The exam is due on **Friday, Oct. 20 at the end of class. NO EXCEPTIONS!**

Good Luck!

1. Do example 11.10 on pg 251 of *Physical Chemistry Using Mathcad*. You will have to define the constants yourself. The zero-tolerance is adjusted in Mathcad 8 by changing the zero threshold (in the Format results pull down menu). Extend the example to compute J_{ave} and the rotational period for each diatomic in Table 5.1 (pg. 169 of McQuarrie and Simon). Tabulate the moments of inertia, J_{ave} and the rotational period. Is there a trend?

2. Do example 11.12 on pg 252 of *Physical Chemistry Using Mathcad.* Compare the populations at T = 300 K and 30 K for CO, I_2 and H_2. What can you say about rotational state populations compared to vibrational state populations (from our in-class harmonic oscillator work).

3. Define commutor, and explain the significance of commutors in quantum mechanics.

4. In your own words, define orthonormal, and describe what an orthonormal set of functions is.

5. In your own words, describe what a well-behaved function is.

6. Prove that the following functions are orthonormal over the interval $-\infty \le x \le \infty$:

$$\psi_0(x) = \pi^{-1/4} e^{-x^2/2}; \quad \psi_1(x) = \left(\frac{4}{\pi}\right)^{1/4} x e^{-x^2/2}; \quad \psi_2(x) = (4\pi)^{-1/4}\left(2x^2 - 1\right) e^{-x^2/2}$$

7. The frequency of the J = 0 to J = 1 transition of $^{12}C^{16}O$ is 1.153 x 10^5 MHz. Determine the bond length of CO in pm.

8. Determine the expectation value of the displacement, $\langle x \rangle$, of a harmonic oscillator in the state

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

(the wave function is normalized). Comment on the physical significance of the result.

9. Calculate the probability that a hydrogen 1s electron will be found within a distance of $2a_0$ from the nucleus.

10. Find the average value of r in the 1s and 2s orbitals of a hydrogen like atom.