Chem 3060

Fall 2005

Final Exam

December 16, 2005

Name: ______________________________

Uid#: _______________________________

Signature: ___________________________

1. For each of the following statements, identify whether the statement is true or false by circling the appropriate answer.

a). If two operaters commute, then there exist states for which both of the (5 pts) correspondingproperties are precisely known.

True False

b). When the uncertainty is calculated for the position coordinates x and y for a particle, the resulting values Δ x and Δ y, must obey the equation
(5 pts.)

$$\Delta x * \Delta y = \frac{\hbar}{2}$$

True False

c). Every linear combination of solutions of the time-dependent Schrödinger equation
(5 pts.)

$$\hat{H}\Psi(x,t) = ih\frac{\partial \Psi(x,t)}{\partial t}$$

is a solution of this equation.

True False

2. In class we discussed simple systems in order to characterize real physical problems. For each portion of this problem suggest a model system discussed in class that would be appropriate for the system.

(a) The states of the electron in a rectangular slab of metal.
(5 pts.)

(b) The internal rotation of methyl rotors in dimethylacetylene, $H_3C-C=C-CH_3$
(5 pts.)

(c) The π-orbitals of octatetraene, $H_2C=CH-CH=CH-CH=CH-CH=CH_2$.
(5 pts.)

(d) The bending vibration of the linear molecule CO_2
(5 pts.)

(e) The π-orbitals of the benzene molecule.
(5 pts.)

3. A particle of mass *m* is free to move in the x-y plane, subject to the potential:

$$V(x,y) = 0 \qquad \text{for } x^2 + y^2 \leq r_0$$

$$V(x,y) = \infty \qquad \text{for } x^2 + y^2 > r_0$$

According to this potential, the particle is free to move within a circle of radius r_0, but is rigorously excluded from the space outside this circle.

One may also consider this system in terms of the polar coordinates *r* and Φ, giving

$$V(r,\phi) = 0 \qquad \text{for } r \leq r_0$$

$$V(r,\phi) = \infty \qquad \text{for } r > r_0$$

For this system the time-dependent Schrödinger equation is:

$$-\frac{\hbar}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Psi}{\partial r}\right)\right] - \frac{\hbar^2}{2mr^2}\frac{\partial^2 \Psi}{\partial \phi^2} + V(r,\phi)\Psi = E\Psi$$

(a) What are the boundary conditions for this system?
(10 pts.)

(b) For this system, the solution to $\hat{H}\Psi = E\Psi$ may be factored into a radial factor times an angular factor, as
(5 pts.)

$$(r,\phi) = R(r)\Phi(\phi)$$

What are the angular wavefunctions, $\Phi(\phi)$, for this system? [Hint: You should be able to guess these solutions by noting a similarity between this system and one of the model systems we have studied in this course. If you have to solve the differential equation, you aren't thinking about this system correctly.]

4. The ground state wavefunction for a one electron atom or atomic ion with nuclear charge Z is given by
(6 pts.)

$$\Psi_{1s}(r,\Theta,\Phi) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a}}$$

Write down the detailed expression that you would use to calculate the expectation value of the distance of the electron from the nucleus for this system. Do not evaluate any integrals that may appear in your expression.

5. List all symmetry elements of the following molecules:
(15 pts, 5 pts for each molecule)

	Cl		F		F	H		CH_3
	B			Xe			C C	
Cl		Cl	F		F	H_3C		H

Then classify then into by the point group symmetry (use flow chart provided).

6. Consider the π-orbitals of an allyl anion, CH_sCHCH_2- by using only ψ_1, ψ_2, and ψ_3 (2p_z orbital on each carbon atom) in the Huckel theory.
(24 pts, 4 pts for each answer)

a. show the form of the Huckel secular determinant
b. the (ψ_1, ψ_2, and ψ_3) set belong to the C_s symmetry point group. What is the

   reducible representation for this set?
c. Reduce this reducible representation
d. What would be the expected form of the Secular determinant if we use symmetry?
e. Derive the three symmetry orbitals
f. Find the orbital energy of the antisymmetric orbital belong to the A'' irreducible representation.

C_s	E	σ
A'	1	1
A''	1	-1