Quiz 1

Chemistry 3BB3; Winter 2004

Name/PID:

1. **Write the Schrödinger Equation for the Hydrogen atom in SI units, showing the dependence on $\hbar$, e, ε_0, and m_e. You may use the Born-Oppenheimer approximation.**

Using separation of variables, the wave function for the hydrogen atom can be written as

$$\Psi_{n,l,m}(\boldsymbol{r}) = R_{n,l}(r)\, Y_l^m(\theta,\phi).$$

2. **Write the Schrodinger equation for radial wave function, $R_{n,l}(r)$, in the hydrogen atom. You may use atomic units.**

3. $Y_l^m(\theta,\phi)$ **is called a(n)**
   (a) associated Legendre polynomial
   (b) associated Laguerre polynomial
   (c) associated Lagrange polynomial
   (d) Linus-Pauling polynomial
   (e) Legendre polynomial
   (f) Laguerre polynomial
   (g) Lagrange polynomial
   (h) spherical harmonic

4. **Let $\hat{L}(\theta,\phi)$ denote the angular momentum operator. What is the eigenvalue of this operator (fill in the blank).**

$$\hat{L}^2(\theta,\phi)\, Y_l^{(m)}(\theta,\phi) = \hbar^2 \left[\qquad\qquad\qquad\qquad \right] Y_l^{(m)}(\theta,\phi)$$

The radial wave function of the hydrogen atom is given by

$$R_{n,l}(r) \propto (Zr)^l\, L_{n-l-1}^{2l+1}(2Zr)\, e^{-\left(\frac{Z}{n}\right)r}.$$

5. $L_n^k(x)$ **is called a(n)**
   (a) associated Legendre polynomial
   (b) associated Laguerre polynomial
   (c) associated Lagrange polynomial
   (d) Linus-Pauling polynomial
   (e) Legendre polynomial
   (f) Laguerre polynomial
   (g) Lagrange polynomial
   (h) spherical harmonic

6,7. Suppose $l = 3$. What is the energy and ground state wave function of the lowest-energy state. You may use atomic units and, additionally, you do not have to normalize the wave function.

8. For which of the following systems is the Born-Oppenheimer approximation most justified? In other words, neglecting all other effects, for which system do you expect corrections to the Born-Oppenheimer approximation will be least important.

(a) C_{60}
(b) H_2
(c) C_6H_6
(d) Si_{60}

9. A computational chemist gives you an estimate for the activation energy of a chemical reaction and tells you that the calculation is in error by .2 Hartree. Is this result likely to be accurate enough to reliably predict the rate of the chemical reaction?

(a) yes
(b) no

10. Below, sketch the 5s and 6s orbitals for the Hydrogen atom.

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Name/PID: **KEY**

1. **Write the Schrödinger Equation for the Hydrogen atom in SI units, showing the dependence on $\hbar$, e, ε_0, and m_e. You may use the Born-Oppenheimer approximation.**

$$\left(\frac{-\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right)\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r})$$

Using separation of variables, the wave function for the hydrogen atom can be written as

$$\Psi_{n,l,m}(\boldsymbol{r}) = R_{n,l}(r)\,Y_l^m(\theta,\phi).$$

2. **Write the Schrodinger equation for radial wave function, $R_{n,l}(r)$, in the hydrogen atom. You may use atomic units.**

$$-\frac{1}{2}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} - \frac{Z}{r}\right)R_{n,l}(r) = E_{n,l}R_{n,l}(r)$$

3. $Y_l^m(\theta,\phi)$ **is called a(n)**

(a) associated Legendre polynomial
(b) associated Laguerre polynomial
(c) associated Lagrange polynomial
(d) Linus-Pauling polynomial
(e) Legendre polynomial
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(g) Lagrange polynomial
(h) spherical harmonic

4. **Let $\hat{L}(\theta,\phi)$ denote the angular momentum operator. What is the eigenvalue of this operator (fill in the blank).**

$$\hat{L}^2(\theta,\phi)\,Y_l^{(m)}(\theta,\phi) = \hbar^2\left[\quad l(l+1)\quad\right]Y_l^{(m)}(\theta,\phi)$$

The radial wave function of the hydrogen atom is given by

$$R_{n,l}(r) \propto (Zr)^l\,L_{n-l-1}^{2l+1}(2Zr)\,e^{-\left(\frac{Z}{n}\right)r}.$$

5. $L_n^k(x)$ **is called a(n)**

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6,7. Suppose $l = 3$. What is the energy and ground state wave function of the lowest-energy state. You may use atomic units and, additionally, you do not have to normalize the wave function.

$E = \frac{-Z^2}{2n^2}$. But $n \geq l + 1$. So the lowest energy state is $n = l + 1 = 3 + 1 = 4$. Thus

$$E = -\frac{Z^2}{2(4)^2} = \frac{-Z^2}{32}$$

Similarly, the wave function is

$$\psi(\boldsymbol{r}) \propto r^l e^{-\frac{Z}{n}r}$$

when l has its maximum value for a given principle quantum number. Thus

$$\psi(\boldsymbol{r}) = r^3 e^{-\frac{Z}{4}r}$$

8. For which of the following systems is the Born-Oppenheimer approximation most justified? In other words, neglecting all other effects, for which system do you expect corrections to the Born-Oppenheimer approximation will be least important.

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(c) C_6H_6

(d) Si_{60}

(Remember that the Born-Oppenheimer approximation is perfect when the nuclear masses are infinity; it is most accurate when the nuclear masses is small and least accurate when they are large (that is, for Hydrogen.) The order of quality here is roughly

$$(d) \gg (a) \gg (b) \approx (c)$$

9. A computational chemist gives you an estimate for the activation energy of a chemical reaction and tells you that the calculation is in error by .2 Hartree. Is this result likely to be accurate enough to reliably predict the rate of the chemical reaction?

(a) yes

(b) no

10. Below, sketch the 5s and 6s orbitals for the Hydrogen atom.