Name:

Quiz 2

Chemistry 3BB3; Winter 2006

When we performed the Born-Oppenheimer approximation for the Hydrogen molecule, we separated the Schrödinger equation for the molecule into an electronic Schrödinger equation and a nuclear Schrödinger equation.

1. **Write the electronic Schrödinger equation for the Hydrogen atom in SI units, showing the dependence on $\hbar$, e, m_e, etc..**

2. **Write the radial Schrödinger equation for the Hydrogen atom in *atomic* units, showing the dependence on the angular momentum quantum number, l.**

3. **The general solutions to the radial equation (which you wrote in problem #2) can be written in terms of a factor of r to some power, times an exponential, times a _______ polynomial.**
   (a) Legendre
   (b) Chebyschev
   (c) Hermite
   (d) Laguerre
   (e) associate Legendre
   (f) associated Chebychev
   (g) associated Hermite
   (h) associate Laguerre
   (i) Schrödinger
   (j) Pauling
   (k) Gauss
   (l) Euler

Supernovae are responsible for most of the heavy elements (specifically, elements past Iron) in the universe. However, due to the extremely strong radiation near supernovae, almost all of the atoms around them are ionized: i.e., the atomic nuclei have few, if any, electrons around them.

4. **The atomic number of Thorium is 90. If a Thorium atom is exposed to radiation with a wavelength of .1 nm (i.e., 1 Å), will this be sufficient to remove its 1s electrons? [Hint: the energy of a photon with wavelength .1 nm is 456 Hartree.]**
   (a) Yes
   (b) No

Name:

In class we talked a lot about things like $4d_0$ orbitals, and $2p_{-1}$ orbitals, etc.. Remember that (a) the first number is the principle quantum number; (b) the second number represents the total orbital angular momentum, and (c) the subscript is related to the orbital angular momentum around the z-axis.

Suppose you are given the following information about the <u>wavefunction</u> of the <u>Hydrogen</u> atom:

- very close to the nucleus, the wave function has the form r^4.
- very far from the nucleus, the wave function decays like $e^{-r/5}$.
- the orbital angular momentum around the z axis is $-1\hbar$.

5-7. What type of orbital is this?

Now suppose you are given the following information about the <u>probability of observing an electron</u> in the <u>*Lithium dication*</u> (with atomic number equal to three).

- very close to the nucleus, the probability of observing an electron is proportional to r^4.
- very far from the nucleus, the probability of observing an electron decays as $e^{-r/5}$.

8-9. The electron in this Lithium atom is in what type of orbital. (Note that you don't know enough to place the subscript on the "letter" part of the orbital; don't worry about it. A lot of the time we talk about 2p, or 4f, or 6s orbitals without worrying about specifying the m_l value.)

10. What is the energy of this state of the Lithium atom?

Name:

Quiz 2 KEY

Chemistry 3BB3; Winter 2006

When we performed the Born-Oppenheimer approximation for the Hydrogen molecule, we separated the Schrödinger equation for the molecule into an electronic Schrödinger equation and a nuclear Schrödinger equation.

1. **Write the electronic Schrödinger equation for the Hydrogen <u>atom</u> in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..**

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2-\frac{Ze^2}{4\pi\varepsilon_0 r}\right)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

2. **Write the radial Schrödinger equation for the Hydrogen atom in *<u>atomic</u>* units, showing the dependence on the angular momentum quantum number, *l*.**

$$\left(-\frac{1}{2r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}\right)R(r)=ER(r)$$

3. **The general solutions to the radial equation (which you wrote in problem #2) can be written in terms of a factor of *r* to some power, times an exponential, times a _______ polynomial.**

(a) Legendre	(e) associate Legendre	(i) Schrödinger
(b) Chebyschev	(f) associated Chebychev	(j) Pauling
(c) Hermite	(g) associated Hermite	(k) Gauss
(d) Laguerre	**(h) associate Laguerre**	(l) Euler

Supernovae are responsible for most of the heavy elements (specifically, elements past Iron) in the universe. However, due to the extremely strong radiation near supernovae, almost all of the atoms around them are ionized: i.e., the atomic nuclei have few, if any, electrons around them.

4. **The atomic number of Thorium is 90. If a Thorium atom is exposed to radiation with a wavelength of .1 nm (i.e., 1 Å), will this be sufficient to remove its 1s electrons? [Hint: the energy of a photon with wavelength .1 nm is 456 Hartree.]**
   (a) Yes
   (b) No

Name:

In class we talked a lot about things like $4d_0$ orbitals, and $2p_{-1}$ orbitals, etc.. Remember that (a) the first number is the principle quantum number; (b) the second number represents the total orbital angular momentum, and (c) the subscript is related to the orbital angular momentum around the *z*-axis.

Suppose you are given the following information about the __wavefunction__ of the __Hydrogen__ atom:

- very close to the nucleus, the wave function has the form r^4.
- very far from the nucleus, the wave function decays like $e^{-r/5}$.
- the orbital angular momentum around the *z* axis is $-1\hbar$.

5-7. What type of orbital is this?

From the first piece of information, we know that we have a "g" orbital ($l = 4$).
From the second piece of information, we know that the principle quantum number is 5 ($n = 5$).
From the third piece of information, we know that $m_l = -1$.

So we have a $5g_{-1}$ orbital.

Now suppose you are given the following information about the __probability of observing an electron__ in the __*Lithium dication*__ (with atomic number equal to three).

- very close to the nucleus, the probability of observing an electron is proportional to r^4.
- very far from the nucleus, the probability of observing an electron decays as $e^{-r/5}$.

8-9. The electron in this Lithium atom is in what type of orbital. (Note that you don't know enough to place the subscript on the "letter" part of the orbital; don't worry about it. A lot of the time we talk about 2p, or 4f, or 6s orbitals without worrying about specifying the m_l value.)

The probability of observing an electron is given by the square of the wave function.
From the first piece of information, we know that we have a *d* orbital (since $r^4 = \left(r^2\right)^2$).
From the second piece of information, we know that $n = 30$ since $\left(e^{-(3/30)r}\right)^2 = e^{-(1/10)(2)r} = e^{-r/5}$.
So we have a $48d$ orbital.

10. What is the energy of this state of the Lithium atom?

$$E = -\tfrac{Z^2}{2n^2} = -\tfrac{3^2}{2(30)^2} = \tfrac{-1}{2(10)^2} = \tfrac{1}{200} = .005 \text{ Hartree}$$