Nov. 9, 2009 Keye to the Midterm Exam.

1. a. Wave-Particle Duality:

All matters possess both the wave and particle natures.

b. Uncertainty principle:

At the same instant, both the position and momentum of matter can be known to only a certain minimal number but not zero.

c. physical meaning of wave functions:

At an instant t, if a measurement is made to locate the particle associated with the wave function $\Psi(x,t)$, then the probability $P(x,t)dx$ that the particle will be found at a coordinate between x and $x+dx$ is equal to $\Psi^*(x,t)\Psi(x,t)dx$.

d. Electron spin:

An electron spin is an intrinsic angular momentum associated with the electron, having an intrinsic magnetic dipole moment. So, it can be detected by the application of a magnetic field.

e. Covalent bond:

It is one type of binding between atoms. The bond is formed betwen atoms by sharing of their electrons.

2. (a) For He^+, $Z = 2$

$$E_n = -13.6 \left(\frac{Z^2}{n^2}\right) eV = -\frac{54.4 (eV)}{n^2}$$

$$E_1 = -54.4 \text{ eV}$$

$$E_2 = -13.6 \text{ eV}$$

$$E_3 = -6.06 \text{ eV}.$$

(b) Transitions:

$E_3 \to E_1$ $\quad \nu_{31} = \frac{E_3 - E_1}{h} = \frac{48.34}{4.14\times10^{-15}} \approx \underline{1.17\times10^{16} \text{ Hz}}$

$E_3 \to E_2$ $\quad \nu_{21}$ $\quad \lambda_{31} = \frac{c}{\nu_{31}} = \frac{3\times10^{8}}{1.17\times10^{16}} \sim 2.6\times10^{-8} \text{ m} \sim \underline{26 \text{ nm}}$

$E_3 \to E_2$ $\quad \nu_{32} = \frac{E_3 - E_2}{h} = \frac{7.54}{4.14\times10^{-15}} \sim \underline{1.8\times10^{15} \text{ Hz}}$

$\lambda_{32} = \frac{c}{\nu_{32}} = \frac{3\times10^{8}}{1.8\times10^{15}} \sim 1.6\times10^{-7} \text{ m} \sim \underline{160 \text{ nm}}$

$E_2 \to E_1$ $\quad \nu_{21} = \frac{E_2 - E_1}{h} = \frac{40.8}{4.14\times10^{-15}} \sim \underline{9.9\times10^{15} \text{ Hz}}$

$\lambda_{21} = \frac{c}{\nu_{21}} = \frac{3\times10^{8}}{9.9\times10^{15}} \sim 3.1\times10^{-8} \text{ m} \approx \underline{31 \text{ nm}}$

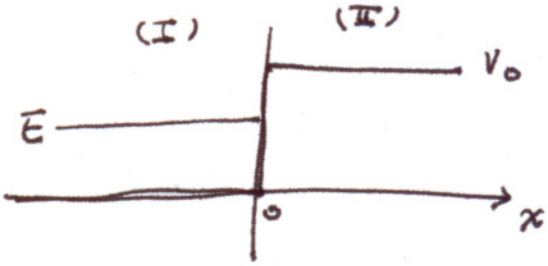
(c) The maximum radial probability is found at $r = \underline{4a_0}$

The expectation value of the radial coordinate is at $\underline{r = 5a_0}$.

There is no fixed orbital for an electron in an atom as envisioned by a classical model. The distribution of probability represent the likelyhood an electron will be detected at a certain position. The expectation value represents the average radial distance of an electron to the nucleus.

3. (a) $\underline{E < V_0}$

In regim (I)



$$\psi(x) = A e^{ik_1x} + B e^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad , \quad x \leq 0$$

In regim (II)

$$\psi(x) = C e^{-k_2x} \quad , \ x > 0 \qquad k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

By applying continuity boundary conditions:

$$\begin{cases} A + B = C \\ A - B = \frac{ik_2}{k_1} C \end{cases}$$

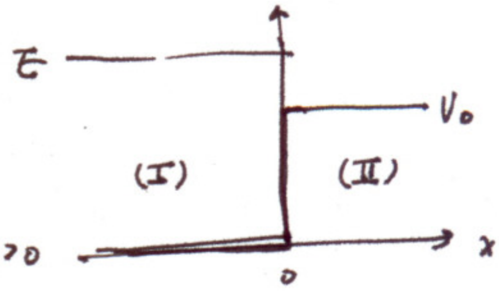
$$\Rightarrow A = \frac{C}{2}\left(1 + \frac{ik_2}{k_1}\right)$$

$$B = \frac{C}{2}\left(1 - \frac{ik_2}{k_1}\right)$$

$$\Rightarrow \psi(x = \begin{cases} \frac{C}{2}\left(1+\frac{ik_2}{k_1}\right)e^{ik_1x} + \frac{C}{2}\left(1-\frac{ik_2}{k_1}\right)e^{-ik_1x} & , \ x \leq 0 \\ C e^{-k_2x} & , \ x > 0 \end{cases}$$

(b) $\underline{E > V_0}$

In regim I is the same as that in (a)



In regim II,

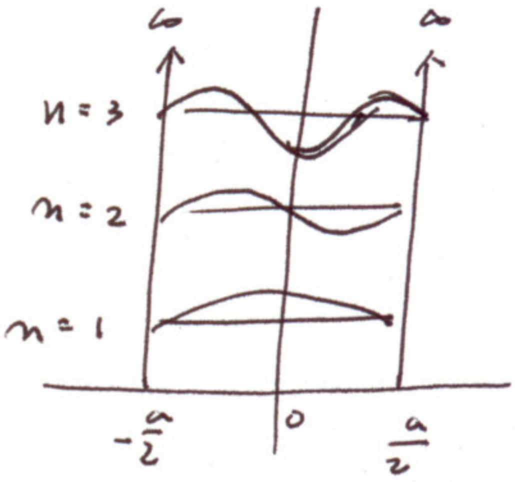
$$\psi(x) = C e^{ik_2x} \ , \quad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar} \ , \quad x > 0$$

applying the continuity boundary conditions:

$$\begin{cases} A + B = C \\ k_1(A-B) = k_2 C \end{cases} \Rightarrow \begin{cases} A = \frac{C}{2}\left(1 + \frac{k_2}{k_1}\right) \\ B = \frac{C}{2}\left(1 - \frac{k_2}{k_1}\right) \end{cases}$$

$$\Rightarrow \psi(x) = \begin{cases} \frac{C}{2}\left(1+\frac{k_2}{k_1}\right)e^{ik_1x} + \frac{C}{2}\left(1-\frac{k_2}{k_1}\right)e^{ik_1x} & , \ x \leq 0 \\ C e^{ik_2x} & \ x > 0 \end{cases}$$

4.



a) $\psi_n(x) = A\cos k_n x$

$\psi_n(\frac{a}{2}) = \psi_n(-\frac{a}{2}) = 0$

$\Rightarrow \quad k_n\frac{a}{2} = n\frac{\pi}{2}$, n=1,2..

$k_n a = n\pi$

$\psi_1(x)$ and $\psi_3(x)$ are even function

$\Rightarrow \psi_1(x) = A\cos\frac{\pi}{a}x \qquad E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$

$\psi_3(x) = A\cos\frac{3\pi}{a}x \qquad E_3 = \frac{\hbar^2 k_3^2}{2m} = \frac{\hbar^2}{2m}(\frac{3\pi}{a})^2$

ψ_2 is an odd function

$\Rightarrow \psi_2 = B\sin k_2 X$

$k_2\frac{a}{2} = \pi \Rightarrow k_2 = \frac{2\pi}{a}$

$\Rightarrow \psi_2 = B\sin\frac{2\pi}{a}x$, $E_2 = \frac{\hbar^2 k_2^2}{2m} = \frac{\hbar^2}{2m}(\frac{2\pi}{a})^2$

b) From the above results. we derive

$$E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$$

$$\Delta E_n = E_{n+1} - E_n = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2((n+1)^2 - n^2)$$

$$= \frac{\hbar^2}{2m}(\frac{\pi}{a})^2(2n+1)$$

$$\Rightarrow \frac{\Delta E_n}{E_n} = \frac{2n+1}{n^2}$$

c) In classical limit, $n \to \infty \Rightarrow \Delta E \to 0$.

5. (a) $^{19}K : 1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 = [Ar] 4s^1$.

$^{17}Cl : 1s^2 2s^2 2p^6 3s^2 3p^5$.

(b) Potassium K has an electronic structure with a closed shell and one extra electron, so the tendency is to release this electron easily.

Cl is just the opposite, it requires one more electron to close a shell, so the tendency here is to grab an electron.

Ionic bond is formed between K and Cl because the abovementioned natures associated with their eletronic structure; and once they become ions, an extra electrostatic force occurs, and further reducing their formation energy.

(c) The energy required to dissociate a KCl molecule is just opposite to the energy gain in the formation of this molecule.

Formation energy of KCl $= 4.34 - 3.82 - \frac{14.4}{2.79} = -4.64$ (eV).

So, the dissociation energy of an KCl molecule is

$\underline{4.64\ \text{eV}}$.