

NAME _____

Grades: points/possible points

I /50

II /30

III /50

IV /50

V /20

Total: /200

This is a closed book, closed notes exam. You may use calculators.**Make sure you show all your work! You will get partial credit.**Useful data and equations:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)$$

1 dimensional Schrödinger equation: $(\eta = \hbar/2\pi)$ $|\psi(x)|^2$ is the Probability per unit length. Kinetic Energy = $1/2 mv^2 = p^2/2m$ (for a plane wave = $\eta^2 k^2/2m$) de Broglie: $\lambda = h/p$; wave number $k = 2\pi/\lambda$ Photon energy $E = hf = \hbar\omega/2\pi$ Quantum mechanical angular momentum $|L| = [\lambda(\lambda+1)]^{1/2}\eta$ and $L_z = m_l \eta$ Transition and photon selection rule: $\lambda \rightarrow \lambda \pm 1$ Atomic electron spectroscopic notation: principal quantum number $n = 0, 1, 2, \dots$; orbital angular momentum quantumnumber symbol $\lambda = 0, 1, 2, \dots, n-1$, with notation $\lambda = 0 \rightarrow s, 1 \rightarrow p, 2 \rightarrow d, 3 \rightarrow f, \dots$; magnetic quantum no. $m_\lambda = -l, -l+1, \dots, l-1, l$ Spin $m_s = -1/2, +1/2$ Electric dipole moment $p_{E1} = Q r$ ($Q = \text{charge}$)Rydberg Constant = $13.6 \text{ eV} = k_{EM}^2 e^4 m/2\eta^2 = -E_0$ ($= -E_1$, ground state energy of Hydrogen)Atomic electron around nucleus of charge Z , $E_n = -Z^2|E_0|/n^2$ Magnetic moment - orbital: $\mu_L = [\lambda(\lambda+1)]^{1/2} \mu_B$ spin: $\mu_S = g_s[s(s+1)]^{1/2} \mu_B$ Magnetic moment along z-axis $\mu_{Lz} = -m_\lambda \mu_B$ and $\mu_{Sz} = -g_s m_s \mu_B$ with $g_s = 2$ and $\mu_B = 5.79 \times 10^{-5} \text{ eV/Tesla}$ Interaction Energy $U = -\boldsymbol{\mu} \bullet \mathbf{B} = -\mu_z B$ $c = 3.00 \times 10^8 \text{ meter/sec}$ electron charge: $e = 1.60 \times 10^{-19} \text{ Coul}$ $h = 6.63 \times 10^{-34} \text{ J sec} = 4.14 \times 10^{-15} \text{ eV sec}$ $\eta = 6.58 \times 10^{-16} \text{ eV sec}$

$$k_{EM} = \frac{1}{4\pi\epsilon_0} = 8.99 \times 10^9 \text{ Nm}^2/\text{Coul}^2 \quad hc = 1.24 \times 10^6 \text{ eV m} \quad \eta c = 1.97 \times 10^{-7} \text{ eV m}$$

Rest energy of electron = $m_e c^2 = 5.11 \times 10^5 \text{ eV}$ Rest mass of electron = $m_e = 9.11 \times 10^{-31} \text{ Kg}$

I. Multiple choice -- circle the one best answer.

- 1) The Schrödinger equation is
 - a. a wave equation for Electromagnetic waves.
 - b. a wave equation for photons.
 - c. a differential equation for the time evolution of position.
 - d. the relativistic version of Newton's second law equation.
 - e. a wave equation for non-relativistic electrons.

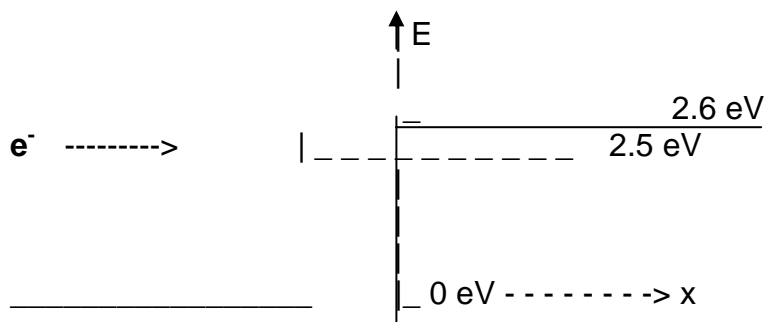
- 2) The element ${}^7\text{N}$ (Nitrogen) has a ground state configuration
 - a. $1s^2 1p^2 2s^3$
 - b. $1s^2 2s^2 3s^2 3p^1$
 - c. $1s^2 2s^2 2p^2 3s^1$
 - d. $1s^2 2s^2 2p^3$
 - e. $1s^2 2s^2 2p^1 3d^2$

- 3) Neon, Argon, Krypton, Xenon all belong to the same group in the Periodic Table. Their low chemical activity compared to other groups of elements is related to the fact that
 - a. their highest energy electrons are in complete p-orbitals.
 - b. their highest energy electrons are in complete d-orbitals.
 - c. their ionization energies are relatively small.
 - d. their electrons' mutual interaction energies are large.
 - e. some of their electrons are in incomplete orbitals.

- 4) The wavefunction for two identical spin 1/2 electrons with parallel spin projections $m_s = +1/2$
 - a. must distinguish the two electrons from one another.
 - b. must be symmetric under the interchange of the electrons.
 - c. must vanish when the pair coincide in space.
 - d. must represent the probability for the electrons to be interchanged.
 - e. must be the simple product of two single electron wavefunctions.

- 5) The H_2^+ molecule (singly ionized) has a ground state electron wavefunction that
 - a. collapses from the Coulomb force between the electron and two protons.
 - b. is centered on one proton.
 - c. is symmetrical with respect to the two protons at fixed separations.
 - d. is antisymmetrical with respect to the two protons at fixed separations.
 - e. corresponds to ionic bonding.

II. A free electron of kinetic energy (KE) 2.5 eV is travelling in a straight line to the right. It approaches a region of constant potential of +2.6 eV.



a. What are the wave number k_1 and wavelength λ_1 of the electron in the free region on the left? Use units of meters and m^{-1} .

b. Does the electron propagate into the region of constant potential on the right or does its wavefunction decrease exponentially? If it propagates, what is the wave number k_2 of the electron in this region on the right? If it decays away exponentially, what is the decay constant α in the expression $e^{-\alpha x}$?

I I.c. Does the electron undergo any reflection at $x=0$? Explain in one or two sentences.

III. A neutron (mass $m = 1.67 \times 10^{-27}$ Kg or 9.4×10^8 eV/c²) is confined in a narrow square surface of side $L = 1.0 \times 10^{-11}$ m. Treat this system as two dimensional and time independent.

a. $\psi(x,y) = (2/L)\sin(k_1x)\sin(k_2y)$ is a possible solution to the Schrödinger equation in the square surface layer. What is the relation between the energy E and wave numbers k_1 and k_2 for this actually to be a solution? You can find this or verify your answer by substituting $\psi(x,y)$ into the two dimensional equation with $V(x,y) = 0$ for $0 < x, y < L$ and $V = \infty$ outside.

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,y) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y)$$

11.1.b. What conditions must the k_1 and k_2 satisfy in order that the wavefunction vanish at the sides of the square? You will need to introduce two quantum numbers for this system. Call them n_1 and n_2 .

c. What are the allowed energies of this single electron in terms of the quantum numbers n_1 and n_2 and the length L ? What is the lowest energy state?

d. If three electrons are inserted into the square, what is the lowest allowed total energy for the three particles? Remember that electrons are fermions and assume there are no interactions or forces among the electrons.

e. What would the answer to (d) be if the electrons were bosons?

IV. Consider a Boron (${}_5\text{B}$) atom.

a. What is its electron configuration (in the standard notation) in the ground state? List the n and λ values for each electron.

b. What is the energy of the valence electron (i.e. highest energy electron or highest n and λ values) in eV's, ignoring electron repulsive forces?

c. The measured ionization energy for the valence electron is 8.28 eV. By comparing this to your answer for (b), obtain the effective screened atomic number, Z_{screened} .

d. What is the magnitude of the orbital magnetic moment of the valence electron (in units of Bohr magnetons)?

IV e. Suppose the outer, valence electron is excited to the **4f level**. The electron returns to its lowest allowed state by emitting **two** photons. What will be the energies of the photons? You can assume the same Z_{screened} operates for all excited states.

V. Consider the molecule NaCl.

It has a measured electric dipole moment of 3.00×10^{-29} Coul•m and an equilibrium separation (between the Na and the Cl atoms) of 0.236 nm.

a. If this were a pure ionic molecule, what would be the value of its dipole moment?

b. What percent of the molecular bond is ionic?