CH1101, Autumn 2024
Midsem Exam
25.09.2024, 3-4:30 pm
Total marks: 50
Special instruction: You must attempt all questions.

1. If you are given with only the radial part of the wavefunction for the 3d orbital of a H atom, which of the following information you can extract out of it? [2]
   (i) The shape of this orbital.
   (ii) The size of this orbital.
   (iii) The energy level of this orbital.
   (iv) Both options i and iii.
   (v) Both options ii and iii.
   (vi) None of the above.

2. For an 1s electron of He, what could possibly be the effective nuclear charge (Z_{eff})? [2]
   (i) $0 < Z_{eff} < 1$
   (ii) $1 < Z_{eff} < 2$
   (iii) $Z_{eff} = 0$
   (iv) $Z_{eff} = 1$
   (v) None of the above.

3. Which of the following statements is CORRECT regarding the photoelectric effect? [2]
   (i) The kinetic energy of an electron ejected (KE_{Max}) from a metal surface when irradiated with a radiation is independent of the frequency of the radiation.
   (ii) Photons of IR radiation have more energy than photons of UV radiation.
   (iii) A less intense violet light could eject a few electrons but their $KE_{Max} >> KE_{Max}$ of the electrons ejected by intense light of longer wavelength.
   (iv) The energy of a photon is directly proportional to the wavelength of the radiation.
   (v) None of the above.

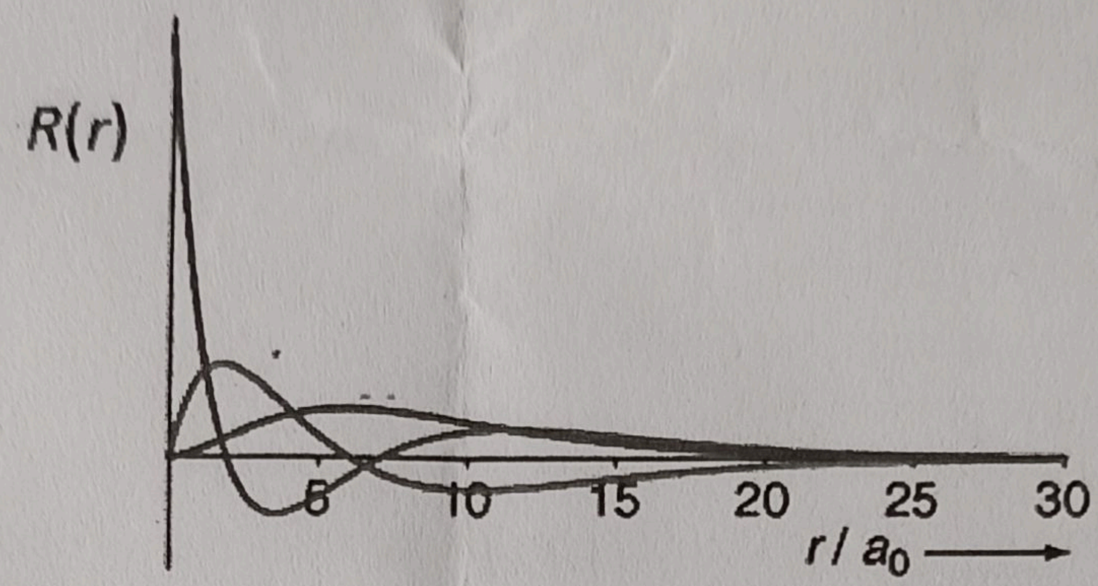
4. Consider the following radial function and identify the possible position of the major maxima in the corresponding RDF plot. [2]

$$R_{3,1}(r) = N_{3,1}\left[6\left(\frac{r}{a_0}\right) - \left(\frac{r}{a_0}\right)^2\right]\exp\left(-\frac{r}{3a_0}\right).$$

   (i) At $r < 3a_o$
   (ii) At $r = 3a_0$
   (iii) At $r > 6a_0$
   (iv) In between $3a_0$ and $6a_0$
   (v) At $r < 6a_0$

5. Which of the following is the correct order of ranking for the 2p orbital energy of Ne, B, N, Na, and Al? [2]
   (i) Ne < B < Na < N < Al
   (ii) Al > B > Ne > B > N
   (iii) B > N > Ne > Na > Al
   (iv) Al < Ne < N < B < Na
   (v) Na > B > Al > Ne > N

6. Draw the equal probability iso-surface plots of 3s and $3p_z$ with proper labelling of axes, sign of the wavefunctions, and radial/angular nodes. [**5+5**]
7. In the illustration below, the radial parts of three wavefunctions for n = 3 of a H atom are shown. Identify their quantum number *l* and assign their orbital designation as appropriate. Sketch their Radial Probability Distribution Functions (RDFs) in a single graph and label the nodes and maxima for each. [**2 + 5 + 2×4**]



(a) From the RDF plot, rank them in the order of their penetrating ability towards the nucleus.
(b) How these plots will change with the change in θ and ϕ?
(c) For the corresponding wavefunctions (ψ), how many angular node(s) would you expect in each case?
(d) Calculate the corresponding energies of these three wavefunctions and compare them.

8. The 1st ionization energy of carbon is 11.26 eV. Calculate the Z_{eff} for one of its outermost electrons. Hint: R_H = 13.6 eV. [**5**]

9. Using the concepts of electron screening and penetration, briefly justify why the ground state electronic configuration of Li is $1s^2 2s^1$ and not $1s^2 2p^1$. [**5**]

10. Despite having a higher positive nuclear charge, oxygen has a lower 1st ionization energy than nitrogen. Justify this based on the exchange interaction. [**5**]
