

Mid Semester Examination II – Monsoon 2017

11-10-2017

IIT-Hyderabad

Subject: Science I (ISC201)

Full Marks: 35

Time: 90 min

Use of non-programmable scientific calculators is allowed

- 1 (a) Compare space quantization diagrams of the Bohr-Sommerfeld orbits with the azimuthal quantum number $k = 3$ and $k = 4$. (Note: You need to specify the respective orientation angles in the diagrams). 3M
- (b) Draw Sommerfeld elliptic orbits for $n=1, 2$ and 3 for the elements H and He. 3M
- (c) Discuss the characteristics of a well-behaved wavefunction. 2M
- 2 (a) Obtain the Schrödinger equation from the plane wave equation. 3M
- (b) Does the curvature of a wavefunction depend on the sign of the wavefunction and relative values of the total energy and potential energy of a quantum system? Justify your answer using schematic diagrams. 2M
- (c) Construct operators for the momentum and kinetic energy of a quantum system. 2M
- 3 (a) Discuss the formation of a chemical bond between two hydrogen atoms to form a H_2 molecule in terms of the symmetry and antisymmetry wavefunctions. 3M
- (b) Consider a quantum system with two electrons (labelled as 1 and 2). If a and b are the two allowed states for these electrons, write possible wavefunctions of the system. Among the possible wavefunctions, identify the wavefunction that obeys the Pauli's exclusion principle. 2M
- (c) The azimuthal wave function for the hydrogen atom is $\psi(\phi) = Ae^{im\phi}$. Show that the value of normalization constant A is $\frac{1}{\sqrt{2\pi}}$ over all angles 0 to 2π . 2M
- 4 (a) Find the expectation values of the operators p_x and p_x^2 for a quantum particle with a wavefunction $\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ in the range 0 to L . 3M
- (b) Write a short note on Born-Oppenheimer approximation. 2M
- (c) Write the Hamiltonian for a hydrogen molecule. 2M
- 5 (a) Show that for a given orthonormal function, the expectation value of the Hamiltonian is greater than or equal to the exact ground state energy. 3M
- (b) Describe the procedure of obtaining a trial wavefunction using the molecular orbital theory. 4M