Indian Institute of Technology Goa

CH 107 End Semester Examination

September 13, 2017 1430–1730

Final marks will be awarded out of best 50, considering this paper and quiz together

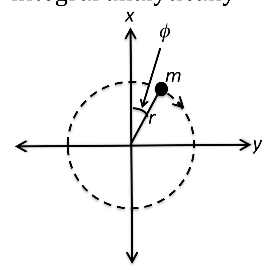
Question 1

(a) Kinetic Energy operator for a particle of mass m moving along x-direction is $\widehat{T_x} = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2}$. Knowing this, arrive at the expression for the linear momentum operator for this particle, $\widehat{p_x}$. **2**

(b) Sketch a plot of $\psi(x) = \frac{\sin x}{x}$ on y-axis and x on x axis. Discuss if $\psi(x)$ is an acceptable wavefunction or not. **2**

(c) Sketch any two wavefunctions of a particle in a one-dimensional box. Mention the quantum numbers for the two wavefunctions. Prove that they are orthogonal, using this sketch and without working out any integral analytically. **2**

(d) The adjacent figure depicts particle of mass m, moving in xy-plane, around a center in a circular path of fixed radius r. For this system, Hamiltonian operator is $-\frac{h^2}{8\pi^2 m r^2}\frac{d^2}{d\phi^2}$.



- i) Propose a suitable wavefunction for this system. **0.5**
- ii) Write the appropriate boundary condition. **0.5**
- iii) Determine the allowed values of the quantum number. **1**
- iv) Normalize the wavefunction. **1**
- v) Determine the allowed values of energy **1**

Question 2

(a) Derive an expression for the volume of a very small volume element in spherical polar co-ordinates. **2**

(b) $\psi_{1s} = \frac{1}{\sqrt{\pi}a^{3/2}}.e^{-r/3a}$, where a = Bohr radius. What is the most probable radius of this orbital? **2**

(c) $\psi_{3,2,2} = \frac{r^2}{162\sqrt{\pi}a^{7/2}}.e^{-r/3a}.sin^2\theta.e^{2i\phi}$ and $\psi_{3,2,-2} = \frac{r^2}{162\sqrt{\pi}a^{7/2}}.e^{-r/3a}.sin^2\theta.e^{-2i\phi}$ for atomic orbitals with n = 3, l = 2, m = +2 and –2 respectively. a = Bohr radius.

- i) Generate an orbital with no imaginary part, by taking an appropriate linear combination of these orbitals. **2**
- ii) Express it in terms of Cartesian co–ordinates, x, y and z. **1**
- iii) Identify the angular node(s) of the orbital generated in the previous part. **0.5**
- iv) What is the name of this orbital? **0.5**
- iv) Draw a contour plot of this orbital. **2**

Question 3

(a) Fill in the table in the supplied sheet and construct the polar part for an orbital for which $\Theta = sin^2\theta.\cos\theta$. Show the signs of each lobe of the wavefunction. **4**

(b) Write the Hamiltonian operator for the electronic part of Be atom. **2**

(c) Identify the term(s) in the Hamiltonian operator that make Schrödinger equation not exactly solvable for Be. Explain how this problem is tackled. (**Note:** Do not try to solve any equation) **1**

(d) *W*rite the wavefunction of the ground state of Li atom as a Slater determinant. Hence, show that no more than two electrons can reside in the *1s* orbital. **3**

Question 4

(a) Write the electronic wavefunction of H_2 molecule, from Valence Bond Theory, with proper explanation. **2**

(b) Draw a schematic plot of the overlap integral, as a function of internuclear distance, for δ-bond formation involving two *3d* orbitals. **2**

(c) Derive an expression for the expectation value of energy for antibonding molecular orbital of H_2^+ **4**

(d) Draw an energy diagram for formation of molecular orbitals of HF by appropriate linear combination of atomic orbitals of H and F atoms. **2**

Question 5

(a) The H–C=O bond angles in formaldehyde are 121^o. It is a planar molecule. Find the coefficients of the valence shell orbitals of the central carbon atom in the hybrid orbitals used for sigma bonding, considering the molecule to be in *zx* plane, with the C=O bond along positive *z* axis. Calculate percent s and p character for each of these hybrid orbitals. **5**

(b) Write down the Hamiltonian for a linear H_3^+ molecular ion (*hypothetical*, with equal H – H bond lengths). Write the complete expression for the lowest energy MO (include spin). Draw a qualitative sketch of bonding and antibonding MOs using 1s AOs . **3**

(c) What is the experimental evidence for the superiority of the delocalized MOT approach over the localized MOT approach for methance? **2**

End of question paper

Roll Number: ______________________________

Please attach this sheet with the answer booklet

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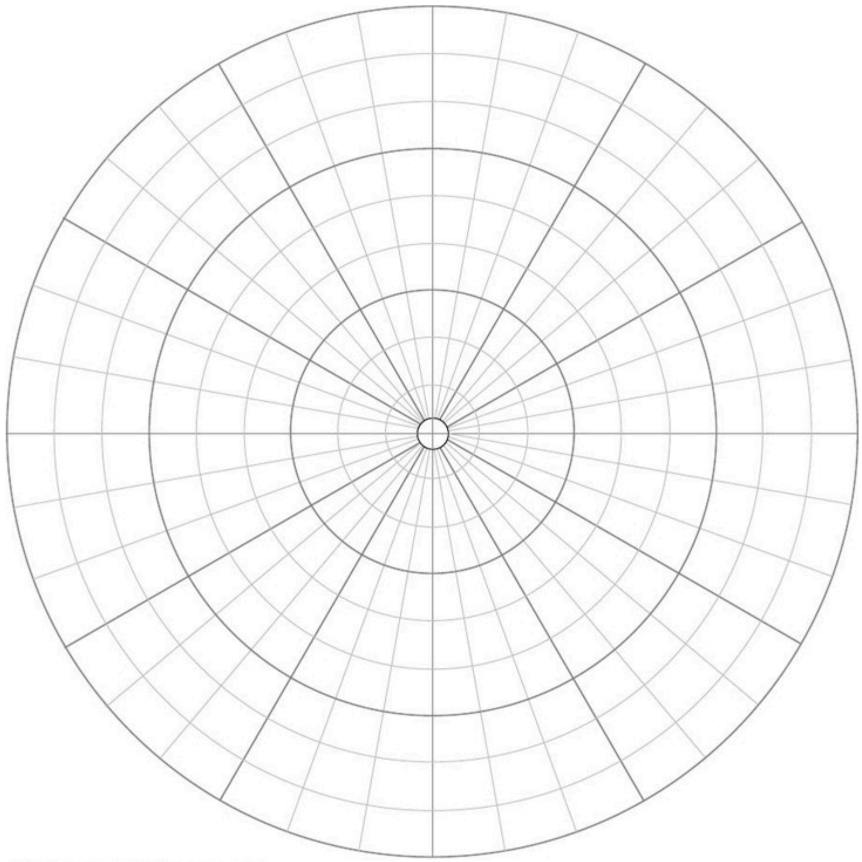
0^{0}		
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