CHEM F213: Physical Chemistry-II

Date: October 12, 2023 **Time: 90 minutes**
Mid-semester Test (Closed Book) **Max. Total Marks 60**

General Instructions: *1.Write your name, ID no., Course No., Course Title, Date and Day legibly, correctly and completely on the main answer-sheet as well as on the supplement(s) (if any) used. 2. All the questions are compulsory. You may solve the questions in any order. However, solve all the sub-questions of a question before going to new question.3. Only scientific and non-programmable calculators may be used for numerical calculations. Use of mobile phones is strictly prohibited.*

Useful data: $a_0=\frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$; *Standard integral:* $\int_0^\infty x^n e^{-\beta x}dx=\frac{n!}{\beta^{n+1}}$

1. (a) The variable, ϕ , defines the angular position of a particle of mass, μ , confined to move in a circular orbit of the fixed radius, r .

(I) Evaluate $[\hat{L}_z,\hat{\phi}]$. **[3]**

(II) Find the product of minimum uncertainties in simultaneous measurements of the angular position and angular momentum of the particle in a given energy level. **[5]**

(b) A one-dimensional quantum harmonic oscillator of mass μ and the force constant, k , is found to be in a normalized state defined by $\Psi(x,t)=\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-(i\pi\nu t+\alpha x^2/2)}$, where, ν is the fundamental vibrational frequency and $\alpha=\frac{\sqrt{k\mu}}{\hbar}$.

(I) Is this a stationary state? Justify your answer mathematically in no more than four lines. Can you identify this state without action of any operator on it? **[4]**

(II) Find the total energy of the oscillator in the given state and also find the minimum displacement (in positive x-direction) so that the oscillator is found in the classically forbidden region. **[4]**

(III) Find the net probability current in the given state of the oscillator. **[4]**

(c) Recall that for s -type orbitals, the orbital angular momentum is zero and the kinetic energy operator for a hydrogen atom takes the reduced form: $\hat{T}_e=-\frac{\hbar^2}{2m_e}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)$. The normalized $1s$ orbital of this atom is expressed as $\psi_{1s}=\frac{e^{-r/a_0}}{(a_0^3\pi)^{1/2}}$.

(I) Determine $\langle\hat{T}_e\rangle$ in the given state. **[6]**

(II) Using the potential energy operator form: $\hat{U}(r)=-\frac{\hbar^2}{m_e a_0 r}$, determine $\langle\hat{U}\rangle$ in the given state. **[4]**

2. (a) Answer the questions based on the operators, $\hat{A}=\hbar\left[z\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)-(x+iy)\frac{\partial}{\partial z}\right]$; $\hat{B}=\hbar\left[-z\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)+(x-iy)\frac{\partial}{\partial z}\right]$; and the given function, $f(x,y,z)=z$.

(I) If $f_A=\hat{A}f(x,y,z)$; $f_B=\hat{B}f(x,y,z)$; $f_{BA}=\hat{B}\hat{A}f(x,y,z)$; $f_{AB}=\hat{A}\hat{B}f(x,y,z)$; then find f_A ; f_B ; f_{BA} and f_{AB} . **[8]**

(II) Using the same convention, find f_{AA} and f_{BB} . **[4]**

(III) Based on your observations in I and II, above, can you recognize the operators $\hat{A}$ and $\hat{B}$? Also identify the significance of the functions, f_A and f_B . **[4]**

(b) Suppose the trial function, $\tilde{\psi}=c_1e^{-\alpha r}+c_2e^{-\alpha r^2}$ were used to carry out variational calculation for the ground state of hydrogen atom and E_{min} was the lowest root of the energies obtained, then, without explicitly doing any calculation, guess the values of c_1 , c_2 and α corresponding to the energy, E_{min} . **[6]**

(c) A two dimensional translation operator $\hat{T}_{a,b}$ is defined as $\hat{T}_{a,b}f(x,y)=f(x+a,y+b)$.

(I) Is it a linear operator? Justify your answer mathematically. **[3]**

(II) Define inverse of the operator. **[3]**

(III) If $g(x,y)=\sin(x+y)$; then what choice(s) of c and d would give $\hat{T}_{c,d}g(x,y)=-g(x,y)$? **[2]**

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