

## CHM102-Assignment-1

1. Which of the following wave functions represent stationary states? (1)  $\Psi_1(t) = Ce^{i\omega t}$ ,  $\Psi_2(x) = C \sin x$ ,  $\Psi_3(x, t) = Cx^2 \sin \omega t$  (C is a complex constant).
2. Is  $\psi(x) = xe^{-ax^2}$  an eigen function of the operator  $\left( \frac{d^2}{dx^2} - 4a^2 x^2 \right)$ ?
3. Consider the wave function,  $\Psi(x) = A(ax - x^2)$  for  $0 \leq x \leq a$   
 (a) Normalize the wave function (b) Find  $\langle x \rangle, \langle x^2 \rangle$  and  $\Delta x$  (deviation).
4. Consider a system whose state is expressed in terms of a complete orthonormal set of basis functions  $\phi_1, \phi_2, \phi_3, \phi_4, \phi_5$  as follows:  

$$\Psi = \frac{1}{\sqrt{19}}\phi_1 + \frac{2}{\sqrt{19}}\phi_2 + \sqrt{\frac{2}{19}}\phi_3 + \sqrt{\frac{3}{19}}\phi_4 + \sqrt{\frac{5}{19}}\phi_5$$
 . If the  $\phi_i$  's satisfy the following relation,  
 $\hat{H}\phi_n = n\epsilon_0\phi_n$  where  $n=1,2,3,4,5$ , calculate  
 (a) the average energy of the system.  
 (b) if the energy is measured on a large number of identical systems that are initially in the same state  $\Psi$ , comment on the possible energies that could be measured along with their probabilities.
5. An electron in a stationary state of a 1D-box of length  $3 \text{ \AA}$  emits a photon of frequency  $5.05 \times 10^{15} \text{ s}^{-1}$ . Find the initial and final quantum numbers for this transition.
6. Consider a one-dimensional particle with wave function  $\Psi(x, t) = \sin\left(\frac{\pi x}{a}\right)e^{-i\omega t}$  confined within the region  $0 \leq x \leq a$ . Calculate the probability of finding the particle in the interval  $a/4 \leq x \leq 3a/4$ .
7. If an electron in a certain excited energy level in a 1D-box of length  $2 \text{ \AA}$  makes a transition to the ground state emitting a photon of wavelength  $8.79 \text{ nm}$ , find the quantum number of the excited state.
8. Consider a particle confined in a 1D-box of length 'a' and described by a wave function  $\Psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$ . Show that the uncertainty relation  $\sigma_x \cdot \sigma_{p_x} > \frac{\hbar}{2}$ .  $\sigma_x, \sigma_{p_x}$  represent the standard deviation of the position and momentum along the x-direction respectively.

Note:  $\int_0^l x \sin^2 \frac{n\pi x}{l} dx = \frac{l^2}{4}$ ,  $\int_0^l x^2 \sin^2 \frac{n\pi x}{l} dx = \left( \frac{l}{2n\pi} \right)^3 \left[ \frac{4n^3\pi^3}{3} - 2n\pi \right]$ ,  $\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2$

9. Employing the following operators,  $\hat{P} = \sqrt{\frac{1}{m\omega\hbar}} \hat{p}_x$ ,  $\hat{Q} = \sqrt{\frac{m\omega}{\hbar}} \hat{x}$ ,  $\hat{a} = \sqrt{\frac{1}{2}}[\hat{Q} + i\hat{P}]$ ,  $\hat{a}^\dagger = \sqrt{\frac{1}{2}}[\hat{Q} - i\hat{P}]$ , evaluate (a)  $[\hat{P}, \hat{Q}]$  (b)  $[\hat{a}^\dagger, \hat{a}]$ . **Note:**  $\hat{p}_x$ ,  $\hat{x}$  denote the x-component of momentum and displacement.

10. An electron in a 1D-potential well, defined by  $V(x) = 0, -a \leq x \leq a$  and  $V(x) = \infty$  otherwise, makes a transition from the  $n=4$  to the  $n=2$  level. The frequency of the emitted photon is  $3.43 \times 10^{14}$  Hz. Calculate the width of the box.

11. A system is initially prepared in the state  $\Psi = \frac{1}{\sqrt{7}}[\sqrt{2}\phi_1 + i\sqrt{3}\phi_2 + \phi_3 + \phi_4]$ , where  $\phi_n$  are eigen states of the system's Hamiltonian, such that  $\hat{H}\phi_n = n\varepsilon_0\phi_n$ .

(a) If energy is measured, what values will be obtained and with what probabilities? Also, calculate the mean energy and the most probable energy for this state?

(b) If the system is in state  $\phi_3$ , what values of energy and the observable A will be obtained if we measure (i) H first and then A (ii) A first and then H, given that  $\hat{A}\phi_n = na_0\phi_{n+1}$

12. Find the value of the constant 'a' that makes  $e^{-ax^2}$  an eigen function of the operator  $\left(\frac{d^2}{dx^2} - Bx^2\right)$ , where 'B' is a constant. What is the corresponding eigenvalue?

13. Suppose, we have 810 identical systems, each of which is in the state  $\Psi$ , given by,  $\Psi = \frac{\sqrt{3}}{3}\phi_1 + \frac{2}{3}\phi_2 + \sqrt{\frac{2}{9}}\phi_3$  (where  $\phi_1, \phi_2$  and  $\phi_3$  are orthonormal basis functions). If measurements are to be done on all of the systems, predict the occupancy of the states  $\phi_1, \phi_2$  and  $\phi_3$ .

14. Compare the probability density profiles for a system described by the following states:

(a)  $\Psi(x) = \phi_1(x)$  (b)  $\Psi(x) = \phi_2(x)$  (c)  $\Psi(x) = \frac{1}{\sqrt{2}}(\phi_1(x) + \phi_2(x))$

(Note:  $\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$  are the basis states for the 1D-box of length 'a'.)

15. Consider the following operators:  $\hat{A}\phi(x) = x^3\phi(x)$ ,  $\hat{B}\phi(x) = x\frac{d\phi(x)}{dx}$ . Find the commutator relation  $[\hat{A}, \hat{B}]$ .