Assignment 2 (CML100)

1. (a) Calculate the energy levels for n = 1, 2, and 3 for an electron in an infinite potential well of width 0.25 nm. (b) If an electron makes a transition from n = 2 to n =1 what will be the wavelength of the emitted radiation.

2. (a) Calculate the separation between the lowest energy levels for an oxygen molecule in a 1-D box of length 5cm. (b) At what quantum number n does the energy of the molecule equal $kT/2$ when T = 300K. [*1.24 x* 10^{-39} *J; 2.2 x* 10^{9}]

3. What is the probability of finding a particle in a 1-D box of length L: (a) in the right half of the box (b) in the central third of the box and (c) between $x = 0$ and $x = L/n$ when it is in the n-th state? Does this probability depend on the quantum number labeling the state of the particle? Useful Integral:
$$\int \sin^2(by)dy = \frac{y}{2} - \frac{1}{4b}\sin(2by)$$

4. Consider a 1D infinite square well potential of length L. A particle is in n = 3 state of this potential well. Find the probability that this particle will be observed between $x = 0$ and $x = L/6$. Can you guess the answer without solving the integral? Explain how.

5. Find the expectation values of x, x^2, p, p^2 for the ground state and the first excited state of a particle in a one-dimensional box.

6. (i) To a crude first approximation, a π electron in linear polyene may be considered to be a particle in a one-dimensional box. The polyene in β- carotene contains 22 conjugated C atoms and the average internuclear distance is 140 pm. Each state upto n = 11 is occupied by two electrons. Calculate (a) the separation energy between the ground state and the first excited state in which one electron occupies the state with n = 12 and (b) The frequency of the radiation required to produce a transition between these two states. [*1.6 x* 10^{-19} *J; 2.41 x* $10^{14} s^{-1}$]

   (ii) When β- carotene is oxidized, it breaks into half and forms two molecules of retinal (vitamin A) which is a precursor to the pigment in the retina responsible for vision. The conjugated system for retinal consists of 11 C atoms and one O atom. In the ground state of retinal, each level upto n = 6 is occupied by 2 electrons. Treating everything else to be similar repeat calculations for parts (a) and (b) of the previous problem keeping in mind that in this case the first excited state has one electron in the n = 7 state. [*3.3 x* 10^{-19} *J; 4.95 x* $10^{14} s^{-1}$]

   Comments on your results from 6(i) and 6(ii).

7. What are the most likely locations of a particle in a box of length L in the state n = 3.

8. Consider a particle of mass m in a 1D box of length a. Its average energy is given by $\langle E \rangle = \frac{\langle p^2 \rangle}{2m}$. Using the uncertainty principle sow that the energy must be at least as large as $\hbar^2/8ma^2$ because σ_x, the uncertainty in x, cannot be larger than a.

9. Set up the problem of a particle in a box with its walls located at $-L$ and $+L$. Show that the energies are equal to those of a box with walls located at 0 and $2L$. Show however that the wavefunctions are not the same. Comment on the results thus obtained by you.

10. Consider a free particle constrained to move over the rectangular region $0 \le x \le a$, $0 \le y \le b$. Show that if the system is in one of its eigenstates, then $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = 0$.

11. A particle of mass m is confined to move on the two-dimensional strip $-a < x < a$, $-\infty < y < \infty$ by two impenetrable walls at $x = \pm a$. (a) What is the minimum energy of the particle that measurement can find? (b) Suppose that two additional walls are inserted at $y = \pm a$. Can measurement of the particle's energy find the value of $3\pi^2 h^2/8ma^2$?

12. For a particle in a 2D box, determine $\left[\hat{X}, \hat{P}_y\right]$, $\left[\hat{Y}, \hat{P}_y\right]$, $\left[\hat{X}, \hat{P}_x\right]$ and $\left[\hat{Y}, \hat{P}_x\right]$.

13. Discuss the source and nature of degeneracy for a particle in a 2-D and 3-D box.

14. Consider a particle in a cubic box. What is the degeneracy of the level that has an energy 14/3 times that of the lowest level?

15. Consider a particle in a 1D box defined by $V(x) = 0$, $a > x > 0$ and $V(x) = \infty$, $x \geq a$, $x \leq 0$. Explain whether the following functions are acceptable wavefunctions for this particle:
    (a) $A\cos(n\pi x/a)$ (b) $B(x+x^2)$ (c) $C\,x^3(x-a)$ (d) $D/\sin(n\pi x/a)$

16. The function $\psi(x) = Ax[1 - \frac{x}{a}]$ is an acceptable wavefunction for the particle in the one dimensional infinite depth box of length a. Calculate the normalization constant A and the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$.

17. Are the eigenfunctions of $\hat{H}$ for the particle in a 1D box also eigenfunctions of the position operator $\hat{x}$? Calculate $\langle x \rangle$ for the quantum numbers $n = 3$ and $n = 5$. For this problem use the following standard integral:
    $$\int x\sin^2(bx)dx = \frac{x^2}{4} - \frac{\cos(2bx)}{8b^2} - \frac{x\sin(2bx)}{4b}.$$

18. Derive an expression for the probability that a particle characterized by the quantum number n is in the first quarter ($0 \leq x \leq L/4$) of an infinite depth box. Show that this probability approaches the classical limit as $n \to \infty$.

19. Find the average position of a particle in a 3D box of sides a, b, c.

20. Show that a particle in a box of length L satisfies the uncertainty principle.

21. If the wave function describing a system is not an eigenfunction of the operator $\hat{A}$, measurements on identically prepared systems will give different results. The variance of this set of results is defined in error analysis as $\sigma_A^2 = \left\langle \left(A - \langle A \rangle\right)^2 \right\rangle$ where A is the value of the observable in a single measurement and $\langle A \rangle$ is the average of all measurements. Using the definition of average value from the quantum mechanical postulates, show that $\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2$.

<u>Other integrals</u>:

$$\int \sin(bx)\cos(bx)\,dx = \frac{\cos^2(bx)}{2b}$$

$$\int x^2 \sin^2 x dx = \frac{x^3}{6} + \frac{1}{4}x^2\sin 2x + \frac{1}{4}x\cos 2x - \frac{1}{8}\sin 2x$$