Lesson: USEFUL QUANTUM MODELS IN CHEMISTRY

PROBLEM SHEET: QUESTIONS

1. (♦◇◇) Calculate the probability of finding a particle in an one-dimensional box in the right half and show that it is independent of the quantum number.

2. (♦◇◇) Calculate the probability of finding a particle in an one-dimensional box in the $(L/3, 2L/3)$ interval for the first 40 quantum states and plot it. Discuss the evolution of the probabilities with the quantum number.

3. (♦♦◇) Calculate the average values of the $\hat{x}$ and $\hat{p}$ operators for the eigenfunctions of the particle in an one-dimensional box. Discuss the results.

4. (♦♦◇) The following function
$$\Psi(x) = Ae^{icx} + Be^{-icx}$$
where A, B and c are constants is proposed to describe a particle in an one-dimensional box.

   a) Find the values of the constants so that $\Psi(x)$ is an eigenfunction of the system.

   b) Evaluate the constants so that $\Psi(x)$ is well-behaved.

5. (♦♦◇) The following function
$$\Psi(x) = a\,(1 - \cos(b\,x))^{1/2}$$
where a and b are constants is proposed to describe a particle in an one-dimensional box. Evaluate the constants so that $\Psi(x)$ is well-behaved.

6. (♦♦◇) The following function
$$\psi(x) = Ax^2 + Bx + C$$
where A, B and C are constants is proposed to describe the ground state of a particle in an one-dimensional box.

   - Evaluate the constants so that $\psi(x)$ is well-behaved.
   - Calcualte the mean value of the nergy and the error with respecto to the accurate energy.
   - Plot the probability densities of $\psi(x)$ and the accurate eigenfunction assuming $L = 1$.

7. (♦◇◇) Calculate the probability of finding the particle in a ring in the first quadrant.

8. (♦♦♦) Let us consider the following physical model: A particle with mass m moving freely in a semicircumference with radius R so that the potential energy is null for $0 \leq \phi \leq \pi$ and infinite otherwise ($\pi < \phi < 2\pi$). Find the eigenfunctions and eigenvalues for the energy.

9. (♦◇◇) Show that the spherical polar and cartesians coordiantes are related through the following expressions:

$$x = r \,\mathrm{sen}\, \theta \, \cos \phi$$
$$y = r \,\mathrm{sen}\, \theta \,\mathrm{sen}\, \phi$$
$$z = r \, \cos \theta$$

10. (♦♦◇) Plot using polar coordinates the $Y_1^0(\theta, \phi)$ spherical harmonic in the xz plane.

11. (♦♦◇) Let us consider the following state function

$$\psi(\theta, \phi) = A \sin^2 \theta \, \sin(m\phi)$$

where A is a normalization constant. Prove whether this function is, in any case, an eigenfunction of the operators $\hat{L}^2(\theta, \phi)$ and $\hat{L}_z(\phi)$.

12. (♦♦◇) The following functions are spherical harmonics

$$F_A(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta$$
$$F_B(\theta, \phi) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$$

Find their corresponding quantum numbers and prove that they are orthogonal.

13. (♦♦♦) A particle in a one-dimensional box is described by the following state function

$$\psi(x) = \sqrt{\frac{30}{l^5}} \, x(x - l)$$

Calculate the probability of meassuring the values of energy E_n ($n = 1, 2, \ldots ...$).

14. (♦♦◇) Let us consider that the six p electrons of benzene move in a ring with radius equatl to the C-C bond distance(0.139 nm). Calculate the energy required to excite one electron in the higher occupied level into the next one. Compare the result with the experimental meassurement which wavenumber is 49019 cm^{-1}.

Dificulty level: (♦◇◇) Easy, (♦♦◇) Normal, (♦♦♦) To think a bit.

Problem sheet: Solutions

Question 1 ⇒ 0.5

Question 2 ⇒ $\frac{1}{3} - \frac{1}{2n\pi}\left(\sin\frac{4n\pi}{3} - \sin\frac{2n\pi}{3}\right)$

Question 3 ⇒ $\langle\hat{x}\rangle = \frac{l}{2}$, $\langle\hat{p}\rangle = 0$

Question 4 ⇒ $A = -B = \frac{1}{2i}\sqrt{\frac{2}{l}}$, $c = \frac{n\pi}{l},\ n = 1, 2, \ldots$

Question 5 ⇒ $B = \frac{n\pi}{l},\ n = 2, 4, 6, \ldots$, $A = \frac{1}{\sqrt{l}}$

Question 6 ⇒ $A = \sqrt{\frac{30}{l^5}}$, $B = -\sqrt{\frac{30}{l^3}}$, $C = 0$, $\langle\hat{H}\rangle = \frac{5h^2}{4\pi^2 ml^2}$

Question 7 ⇒ $\frac{1}{4}$

Question 12 ⇒ $l_A = 1$, $l_B = 2$, $m_A = m_B = 0$

Question 13 ⇒ 0 if n is even and $\frac{960}{(n\pi)^6}$ if n is odd.

Question 14 ⇒ λ = 47672 cm^{-1}. Error = 2.7 %