

## Module 1 : Atomic Structure

### Lecture 2 : Particle In A Box

#### Objectives

- Schrodinger Equation for a particle in a one dimensional "box".
- Solutions for appropriate boundary conditions.
- Wave functions and obtain transition energies between various states.
- Values of average quantities such as position, momentum and energy.
- The  $\pi$  - electron spectrum for models of linear polyenes.

#### 2.1 A One Dimensional (1-d) Box

A small particle such as an electron or a proton confined to a box constitutes the particle in a box problem, which we are about to study. This is one of the few problems for which there are exact solutions, i.e., the solutions can be expressed in terms of known mathematical functions. The fact that the particle cannot come out of the box is mathematically expressed as the potential,  $V = \infty$  outside the box and also at the boundary of the box.

A simpler problem is a particle in a one dimensional box. Here, the particle can move only on a line of finite length, say  $L_x$ . An example close to this situation is an electron moving "in" a very thin wire or in a long chain molecule. The analogy is imperfect; yet, a lot of useful information can be derived from this idealized problem. To solve this problem, we write the Schrodinger equation, apply appropriate boundary conditions (that the particle is confined to the box), find and interpret the solutions.

#### 2.2 The Schrodinger Equation

The Schrodinger equation is  $H \Psi = E \Psi$ , where  $H = T + V$ .  $T$  and  $V$  are the operators for the kinetic and potential energies respectively. In one dimension, the kinetic energy for the  $x$  direction  $T_x = p_x^2 / 2m$  and the operator for it is  $T = -(\hbar^2 / 2m) \partial^2 / \partial x^2$ . Verify this by replacing  $p_x$  by  $(\hbar / i) \partial / \partial x$  in the formula for  $T_x$ . The operator for the potential energy is

$$V(x) = V(x)$$

$$V(x) = 0 \text{ for } 0 < x < L_x \quad (2.1)$$

and

$$V(x) = \infty \text{ for } x \leq 0 \text{ and } x \geq L_x \quad (2.2)$$

The Schrodinger equation becomes,

$$-(\hbar^2 / 2m) \partial^2 / \partial x^2 = E \Psi \quad (2.3)$$

#### 2.3 Boundary conditions

The above equation can be easily solved for the given boundary conditions. We look for those functions whose second derivatives are a negative constant multiplied by the function itself. The possible functions are  $\exp(iax)$ ,  $\cos(ax)$  and  $\sin(ax)$  and linear combinations of them. The boundary conditions require that the function goes to zero at the boundary of the box, i.e.,

$$\Psi(0) = \Psi(L_x) = 0 \quad (2.4)$$

Not only is the wavefunction zero at the boundary, but it is zero everywhere outside the box. If it were not so, the particle would be found outside the box and this contradicts with the fact that we are studying the problem of a particle confined inside a box. Only the sine function satisfies the condition for  $x = 0$ . It will also satisfy the boundary condition at  $x = L_x$  if  $(a L_x)$  is a multiple of  $n\pi$  or  $a = n\pi / L_x$  where  $n$  can take on only integer values.

## 2.4 The Solution

Substituting the function in the Schrodinger equation,

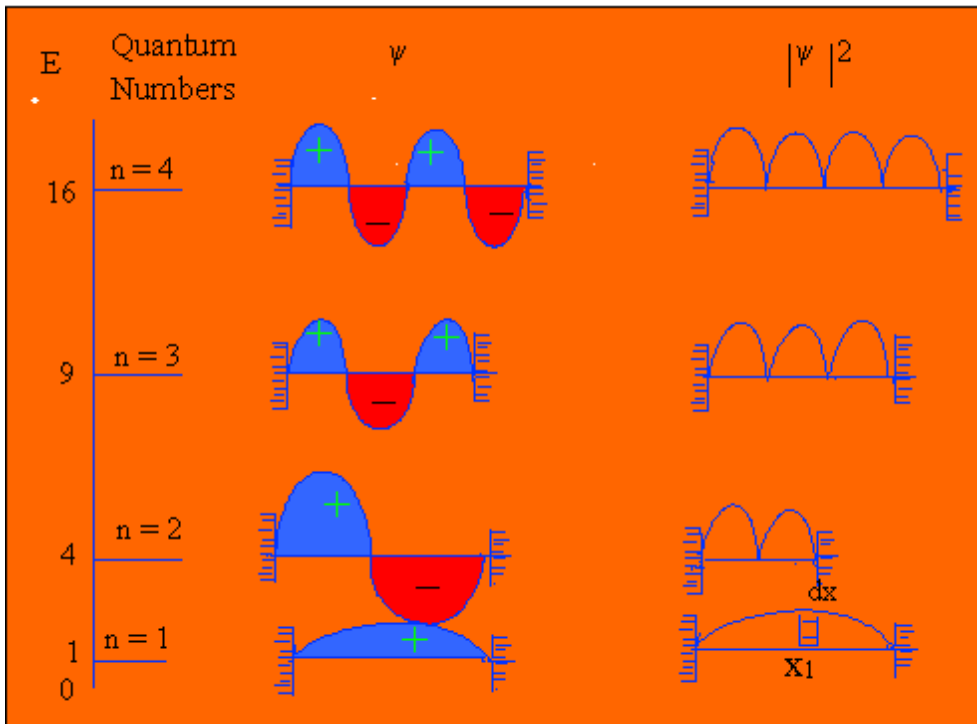
$$\begin{aligned} -(\hbar^2 / 2m) \partial^2 / \partial x^2 \sin(n\pi x / L_x) &= -(\hbar^2 / 2m) (n\pi / L_x) \partial / \partial x \cos(n\pi x / L_x) \\ &= (\hbar^2 / 2m) (n^2 \pi^2 / L_x^2) \sin(n\pi x / L_x) \\ &= E \sin(n\pi x / L_x) \end{aligned} \quad (2.5)$$

Therefore,

$$E = E_n = n^2 \hbar^2 / 8mL_x^2 \quad (2.6)$$

where we have used the fact that  $\hbar = h / 2\pi$  and associated  $E$  with a subscript  $n$  to indicate the  $n^{\text{th}}$  energy level with quantum number  $n$ .

The function  $\sin(n\pi x / L_x)$  is called an eigenfunction and the energy  $E_n = n^2 \hbar^2 / 8mL_x^2$  is called an eigenvalue. The eigenvalues and the eigenfunctions for this problem for value of  $n = 1, 2, 3$  and  $4$  are shown in the accompanying figure. The values of the square of the eigenfunctions (which are also the wavefunctions in this case) are also shown in the figure.



**Figure 2.1 Plots of the wavefunctions of a particle in a two dimensional box.**

The y axis gives energy in units of  $\hbar^2 / 8mL_x^2$ . The energies, quantum numbers,  $\Psi$  and  $\Psi^2$  are shown in the four segments of the figure.

As was mentioned earlier, the wavefunction contains all the possible microscopic information of

the system that can possibly be obtained. It is not possible to obtain simultaneously the position and the momentum of the particle (this is the uncertainty principle). We may however ask questions such as:

- 1) What is the average position of the particle in the box?
- 2) What is the probability of finding the particle between  $x_1$  and  $x_1 + dx$  for any value of  $x_1$ ?
- 3) What is the average momentum of the particle in the box?
- 4) What is the mean square deviation of the particle's position from its average value?
- 5) What is/are the most probable position/s of the particle in the box?

We will find the answers to these questions as we go along. Quantum mechanics allows us to answer all these questions. Let us consider first an important and convenient requirement for the wavefunction which is referred to as normalization.

## 2.5 Normalization

The probability of finding the particle somewhere in the box has to be unity (else, the particle can escape from the box!). This is called the normalization condition, i.e., when the probability density is integrated over the relevant space, which in this case is the length of the box, we should get 1. But integrating  $\sin^2(n\pi x / L_x)$  between 0 and  $L_x$  gives

$$\int \sin^2(n\pi x / L_x) dx = L_x / 2 \quad (2.7)$$

Therefore integrating the square of the function  $\sqrt{(2 / L_x)} \sin(n\pi x / L_x)$  gives unity. In general if  $\int f(x)^2 dx = N$ , then  $\int (1/\sqrt{N})^2 f(x)^2 dx$  gives unity. The quantity  $(1/\sqrt{N})$  in the function

$$(1/\sqrt{N}) f(x) \quad (2.8)$$

is called the normalization constant. If the function is complex, then, in place of  $f(x)^2$ , the modulus square of the function  $|f(x)|^2$ , or  $f(x) \cdot f^*(x)$  is used. Here,  $f^*(x)$  is the complex conjugate of  $f(x)$ .

Fig. 2.1 gives the quantum numbers, energy levels, wavefunctions and probability densities for a particle in a one dimensional box of length  $L_x$ . In one dimension  $|\Psi(x)|^2 dx$  gives the probability of finding the particle in a length  $dx$  at location  $x$ . A shaded area between  $x_1$  and  $x_1 + dx$  is shown in Fig 2.1 for the  $n = 1$  state. The probability is

$$|\Psi(x)|^2 dx = (2 / L_x) \int_{x_1}^{x_1 + dx} \sin^2(n\pi x / L_x) dx \quad (2.9)$$

This is the reason that  $|\Psi(x)|^2$  is called as the probability density. In one dimension, it is the probability per unit length and thus, the dimension of  $\Psi(x)$  in one dimension is  $(1/\sqrt{\text{Length}})$ .

### Example 2.1

What is the probability of finding an electron in a box of length  $2 \text{ \AA}$  in the middle of the box in an interval of length  $0.1 \text{ \AA}$ ? This probability may be represented as  $P(0.95 \text{ \AA} \leq x \leq 1.05 \text{ \AA})$

### Solution:

A simple and approximate way of calculating this probability is to use the square of the wavefunction at the midpoint of the box and multiply it by the interval  $0.1 \text{ \AA}$

$$|\Psi(x = 1 \text{ \AA})|^2 \cdot dx = (2 / 2)^{1/2} \sin(1\pi \cdot 1/2) \cdot 0.1 = 0.1$$

A precise way of calculating this probability is to integrate the square of the wavefunction from

0.95 Å to 1.05 Å. This is necessary because the wavefunction is not constant over this interval (as was assumed in the above approximate calculation).

$$\int_a^b \left( \frac{2}{L} \right) \sin^2 \left( n \pi x / L \right) dx = \frac{1}{2} \int_a^b [1 - \cos(2 \pi n x / L)] dx$$

$$= (b - a) / L - (1 / 2 \pi n) \sin(2 \pi n x / L) \Big|_a^b$$

In our problem  $L = 2 \text{ Å}$ ,  $b = 1.05 \text{ Å}$ ,  $a = 0.95 \text{ Å}$  and  $n = 1$

$$\therefore P(0.95 \text{ Å} \leq x \leq 1.05 \text{ Å}) = (1.05 - 0.95) / 2 - (1 / 2 \pi) [-0.1544 - 0.1564]$$

$$= 0.05 + 0.0498$$

$$= 0.0998$$

In the present case, the approximate calculation is good since the wavefunction is not varying very much in this interval. When the wavefunction changes rapidly, the approximate method will not give good results.

## 2.6 Average Quantities

In the quantum mechanical world, exact values of dynamical variables such as position, linear momentum, angular momentum or energy can not be measured. What can be measured however is the average value of a dynamical variable. The measurement of a variable is made in several repeated observations and from these, the average value is obtained. This value is called the expectation value. As the name suggests, this is the expected value when a measurement is made. It does not mean that every measurement gives this value! The expectation values are very easy to compute if the wavefunction is known.

If  $\Psi(x)$  is the wavefunction (which really represents a quantum mechanical state of a given system) then, the expectation value of the operator  $O$  in this state is given by

$$\langle O \rangle = \int \Psi(x)^* O \Psi(x) dx \quad (2.10)$$

The notation  $\langle \rangle$  is used to denote the expectation value. As an example, consider the position operator  $x$ . Its expectation value is given by

$$\langle x \rangle = \int \Psi^*(x) x \Psi(x) dx \quad (2.11)$$

When the function  $\sqrt{(2/L_x)} \sin(n \pi x / L_x)$  is used for  $\Psi(x)$ , verify that  $\langle x \rangle$  is equal to  $L_x / 2$ . This seems to make sense. The potential energy is zero inside the box and there is no reason to expect that the particle is to be found on the average, favourably in any special position inside the box. The expectation value of position is an average value over many measurements. It is not the most probable value of the position in any state. The most probable of position is determined by the largest value of the wavefunction in the box. We can use Eq. (2.10) for other operators as well. For energy, we have,

$$E = \langle H \rangle = \int \Psi^*(x) H \Psi(x) dx \quad (2.12)$$

Verify that the average value or the expectation value of energy in each state  $n$  is indeed  $n^2 h^2 / 8mL_x^2$ .

The mean square deviation in the position (with respect to the average position in any state is given by  $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$ . This is always a positive quantity. This is like the square error in the measurement of  $x$ , and  $\Delta x$  may be treated as the uncertainty in the measurement of  $x$ . Similarly,  $\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2}$  is the uncertainty in the measurement of  $p_x$ . It is indeed very satisfying that the product  $(\Delta x) (\Delta p_x)$  is indeed of the order of  $\hbar / 2$ . This means that the Schrodinger equation is consistent with the uncertainty principle. If this were not the case, we would have to change at least one of them!

### Example 2.2

Obtain the values of  $\Delta p_x$  and  $\Delta x$  for the  $n = 1$  state of a particle in a one dimensional box of length

$$L_x = 1 \text{ Å}.$$

**Solution:**

$$\langle x \rangle = \left( \frac{2}{L_x} \right) \int_0^{L_x} \sin^2 \left( n \pi x / L_x \right) x \, dx = \left( \frac{2}{L_x} \right) \int_0^{L_x} x \sin^2 \pi x \, dx$$

$$= 1/2.$$

We have used  $\int x \sin^2 x \, dx = x^2/4 - x/4 \sin 2x - \cos 2x/8$  which can be easily showing by integrating by parts

$$\langle x^2 \rangle = \left( \frac{2}{L_x} \right) \int_0^{L_x} x^2 \sin^2 \left( n \pi x / L_x \right) dx = 1/3$$

$$\text{where we have used } \int x^2 \sin^2 x \, dx = x^3/6 - x^2 \sin 2x/4 - x \cos 2x/4 + \sin 2x/8$$

$$\therefore \Delta x = [\langle x^2 \rangle - \langle x \rangle^2]^{1/2} = 1/\sqrt{12} \text{ in Å units.}$$

$$\langle p_x \rangle = \int_0^{L_x} \left( \frac{2}{L_x} \right)^{1/2} \sin \left( n \pi x / L_x \right) \left( \hbar / i \partial / \partial x \right) \left( \frac{2}{L_x} \right)^{1/2} \sin \left( n \pi x / L_x \right) dx$$

$$= \left( \hbar / i \right) \left( n \pi / L_x \right) \left( \frac{2}{L_x} \right) \int_0^{L_x} \sin \left( n \pi x / L_x \right) \cos \left( n \pi x / L_x \right) dx$$

= 0 as the cos and sin function are "orthogonal" over one period.

$$\langle p_x^2 \rangle = \int \psi_x \left( \hbar / i \partial / \partial x \right)^2 \psi_x \, dx$$

$$- \hbar^2 \partial / \partial x^2 \sin(n \pi x / L_x) = \left( \hbar^2 / L_x^2 \right) n^2 \pi^2 \sin n \pi x / L_x$$

$$\therefore \langle p_x^2 \rangle = \hbar^2 / 4, \Delta p_x = \hbar / 2; \Delta x \cdot \Delta p_x = \hbar / 2 \sqrt{12}$$

$$= 0.144 \hbar \geq \hbar / 2 = 0.08 \hbar$$

## 2.7 Particle in two and three dimensions

The Schrodinger equation in two and three dimensions is given below

$$- \left[ \left( \hbar^2 / 2m \right) \partial^2 / \partial x^2 + \left( \hbar^2 / 2m \right) \partial^2 / \partial y^2 \right] \Psi(x, y) = E \Psi(x, y) \quad (2.13)$$

$$- \left[ \left( \hbar^2 / 2m \right) \partial^2 / \partial x^2 + \left( \hbar^2 / 2m \right) \partial^2 / \partial y^2 + \left( \hbar^2 / 2m \right) \partial^2 / \partial z^2 \right] \Psi(x, y, z) = E \Psi(x, y, z) \quad (2.14)$$

In eq. (2.13), the operator for the y component of kinetic energy has been added (with reference to eq (2.3)), and in eq. (2.14), the operators for the y and z components of kinetic energy have been added. The variables in parentheses following  $\Psi$  refer to all the independent variables (or coordinates) characterizing the particle. A common method of solving the problem is known as the method of separation of variables. In two dimensions, we have

$$\Psi(x, y) = \psi_x(x) \psi_y(y) \quad (2.15)$$

The subscripts on the right hand side following  $\Psi$  once again distinguish between the independent variables x and y, and  $\psi_x$  and  $\psi_y$  need not be the same and  $\psi_x(x)$  and  $\psi_y(y)$  are different functions. Substituting Eq. (2.15) into eq. (2.13) and dividing each term by  $\psi_x(x) \psi_y(y)$  from the left hand side, we get (Since we are dealing with operators, multiplying or dividing from the left side is different from doing the same operation from the right side and great caution has to be always exercised),

$$- \left( \frac{1}{\psi_x(x)} \right) \left( \hbar^2 / 2m \right) \partial^2 / \partial x^2 \psi_x(x) - \left( \frac{1}{\psi_y(y)} \right) \left( \hbar^2 / 2m \right) \partial^2 / \partial y^2 \psi_y(y) = E \quad (2.16)$$

Let us illustrate that dividing from the left side of a term can be different from dividing from the right side as can be easily seen when you divide  $\partial / \partial x$  by x. If you divide from the left side, you

get  $(1/x) \partial / \partial x$ . When you divide from the right side, you get  $\partial / \partial x (1/x)$  which equals  $-1/x$ . In the first case, we have an operator and in the second case, we have a "simple" function.

Now, both  $\Psi_x(x)$  and  $\Psi_y(y)$  are independent functions. If the sum of two independent functions is constant, then each function has to be constant. E.g, if  $(y^3 + y^2) + x^2 + x = \text{constant}$ , then both  $y^3 + y^2$  and  $x^2 + x$  have to equal to separate constants. Therefore,

$$- (1/\Psi_x(x)) (\hbar^2 / 2m) \partial^2 / \partial x^2 \Psi_x(x) = \text{constant} = E_x \quad (2.17)$$

$$- (1/\Psi_y(y)) (\hbar^2 / 2m) \partial^2 / \partial y^2 \Psi_y(y) = \text{another constant} = E_y \quad (2.18)$$

$$\text{with } E = E_x + E_y \quad (2.19)$$

Now, both equations (2.17) and (2.18) are identical to eq. (2.3) with appropriate substitutions for the corresponding terms. The two dimensional problem has thus been reduced to two one-dimensional problems. The energies and the wavefunctions in the y and z directions are

$$E_y = n_y^2 \hbar^2 / 8mL_y^2 \quad (2.20)$$

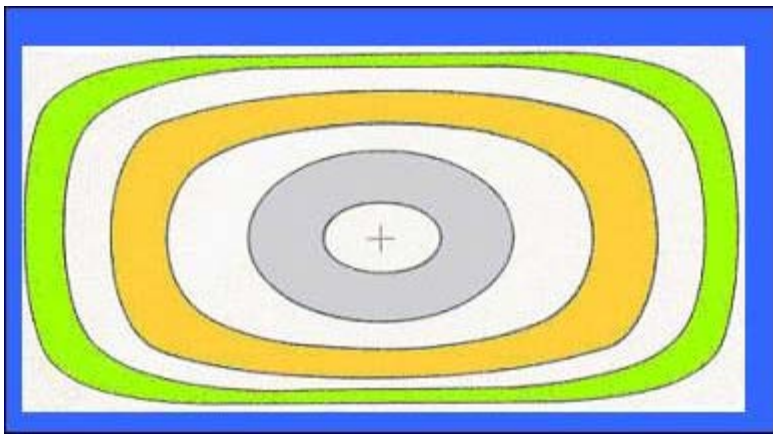
$$E_z = n_z^2 \hbar^2 / 8mL_z^2 \quad (2.21)$$

The total normalized wavefunction in two dimensions is

$$\Psi(x, y) = \sqrt{4 / L_x L_y} \sin(n_x \pi x / L_x) \sin(n_y \pi y / L_y) \quad (2.22)$$

The quantum numbers  $n_x$  and  $n_y$  are in general different and correspond the the translational motion in different directions.

**Figure 2.2 (a)**



$\Psi$  11

**Figure 2.2 (b)**

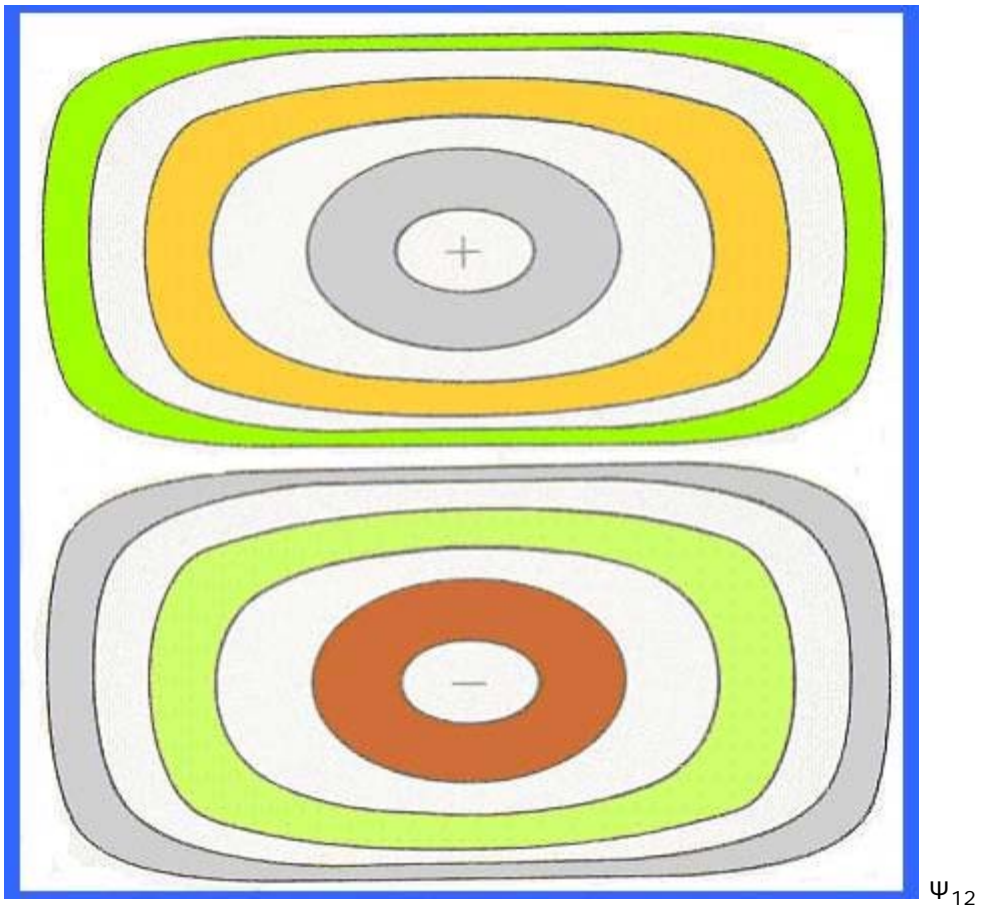


Figure 2.2 (c)

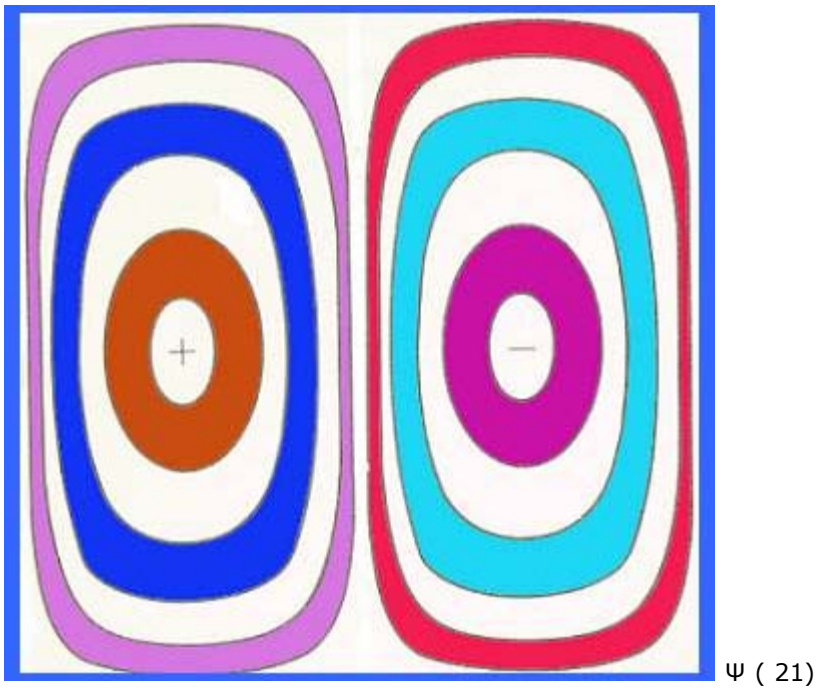
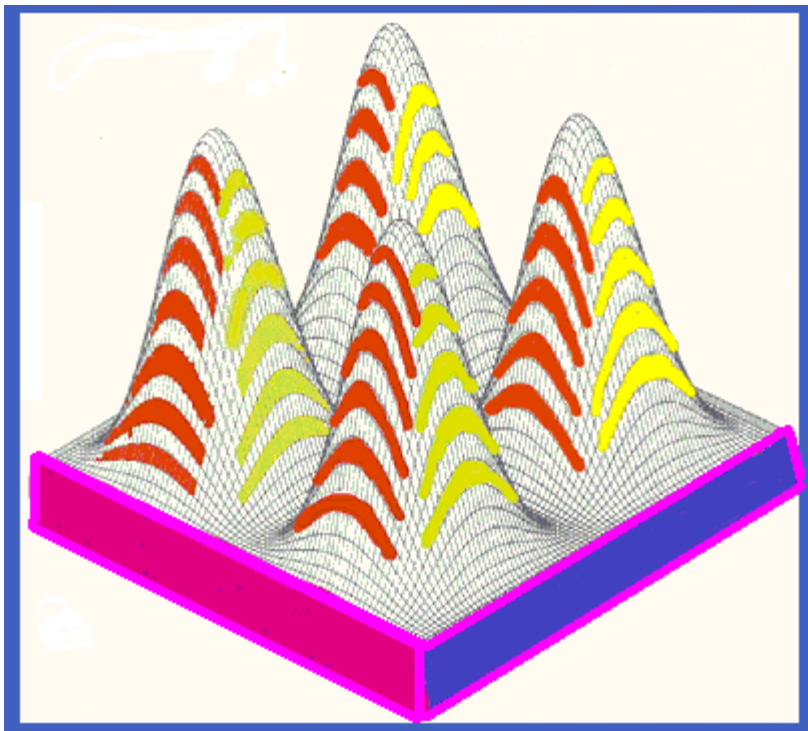


Figure 2.2 (d)



$$|\psi(2,2)|^2$$

**Figure 2.2 Plots of the wavefunctions of a particle in a two dimensional box.**

The horizontal direction is  $x$  and the vertical direction is  $y$ . Fig 2.2 (a) shows the contours of  $\psi_{11}(x,y)$ , Fig 2.2 (b) shows the contours of  $\psi_{12}$  and fig 2.2 (c) shows the contours of  $\psi_{2,1}$ . Fig 2.2(d) shows a 3 dimensional plot of  $|\psi(2,2)|^2$

The above problem in two dimensions can be easily generalized to three dimensions and the wave function for a particle in a three dimensional box is given by,

$$\psi(x, y, z) = \sqrt{8/L_x L_y L_z} \sin(n_x \pi x / L_x) \sin(n_y \pi y / L_y) \sin(n_z \pi z / L_z) \quad (2.23)$$

### Example 2.3

For a particle in a three dimensional box, what is the (expectation) value of the energy of the particle if  $L_x = 10 \text{ \AA}$ ,  $L_y = 5 \text{ \AA}$  and  $L_z = 1 \text{ \AA}$ . when  $n_x = 2$ ,  $n_y = 2$  and  $n_z = 1$ ? Comment on the degeneracy of the energy levels of a three dimensional box resulting from the three sides of the box becoming equal. Use  $m = 9.1 \times 10^{-31} \text{ kg}$

### Solution

$$\begin{aligned} E(n_x, n_y, n_z) &= E(2, 2, 1) = 2^2 h^2 / 8mL_x^2 + 2^2 h^2 / 8mL_y^2 + 1^2 h^2 / 8mL_z^2 \\ h^2 / 8m &= (6.626 \times 10^{-34})^2 / (8 \times 9.1 \times 10^{-31} \text{ (J}^2\text{s}^2/\text{kg)}) \\ &= 0.603 \times 10^{-37} \text{ J}^2\text{s}^2/\text{kg} \end{aligned}$$

$$\begin{aligned} L_x &= 10 \text{ \AA} = 10 \times 10^{-10} \text{ m} = 10^{-9} \text{ m}, L_y = 5 \times 10^{-10} \text{ m}, L_z = 10^{-10} \text{ m} \\ E(2,2,1) &= 6.03 \times 10^{-36} (4 / 10^{-18} + (4 / 25) \times 10^{-20} + 1 / 10^{-20}) \text{ J} \\ &= 6.03 \times 10^{-36} \times 10^{20} (400 + 32 + 1) \text{ J} \\ &= 2.61 \times 10^{-13} \text{ J} \end{aligned}$$

If  $L = L_x = L_y = L_z$ , then a number of states can have the same energy. Eg, states with quantum



numbers (i) 1, 2, 3, (ii) 2, 1, 3, (iii) 1, 3, 2, (iv) 2, 3, 1, (v) 3, 1, 2 and (vi) 3, 2, 1 have the same energy of  $(1^2 + 2^2 + 3^2) \hbar^2 / 8 mL^2 = 14 \hbar^2 / 8 mL^2$ . These states are said to be degenerate, similar to the 3 p orbitals of the hydrogen atom being degenerate.

#### Example 2.4:

Treating butadiene to be a linear molecule, estimate the approximate value of its length, treat it as a particle in a box problem with four pi electrons confined to this length and calculate the minimum energy required to excite its outermost electron into a higher level. Comment on the approximations inherent in such a simplified model for understanding the behaviour of pi electrons in a linear chain molecule.

#### Solution:

Butadiene has a structure 

Treating this as linear molecule, the length of the molecule may be estimated as  $0.5 + 1.34 + 1.54 + 1.34 + 0.5 = 5.22 \text{ \AA}$ ;  $0.5 \text{ \AA}$  has been added for each of the two end carbons,  $1.34 \text{ \AA}$  for the double bonds and  $1.54 \text{ \AA}$  for the single bond. With this length,

$$\begin{aligned} \hbar^2 / 8 mL^2 &= (6.626 \times 10^{-34})^2 / (8 \times 9.1 \times 10^{-31} \times 5.22^2 \times 10^{-10})^2 \text{ J} \\ &= 2.21 \times 10^{-15} \text{ J} \\ &= q \end{aligned}$$

calling this quantity  $q$ , the first three energy levels will be  $1q$ ,  $4q$  and  $9q$ . The four pi electrons in butadiene may be placed in the levels  $1q$  and  $4q$  (2 each) and the smallest excitation energy is needed to excite an electron from level 2 to level 3 with energy  $5q = 1.107 \times 10^{-14} \text{ J}$

Note that several approximations are implicit in this estimate. The main approximations are that the electrons move in a line, electrons do not interact with one another, as well as with the nuclei, and so on. Yet such approximate results give reasonably good energy levels for many linear polyenes!

## 2.8 Problems

2.1) What is the normalization constant of the function  $\exp(-x)$  if the range of integration is between 0 to infinity? How about  $\exp(-x^2)$ ? (Hint:  $\int \exp(-ax^2) dx = \sqrt{(\pi/a)}$ ).

2.2) Sketch  $\psi_4(x)$  and  $\psi_5(x)$  and their squares as a function of  $x$ . What is the energy needed to take a particle in level 4 to level 5 if  $L_x = 0.5 \text{ nm}$  or 5 Angstroms? In the state  $\psi_3(x)$ , where is the probability of finding the particle largest?

2.3) What are the boundary conditions for  $V$  in eqs. (2.13) and (2.14) (Hint: Let the lengths in the  $y$  and  $z$  directions be  $L_y$  and  $L_z$  respectively. Compare with eqs (2.1) and (2.2).

2.4) What is the expectation value of  $p_x$  for any state of a particle in a one dimensional box? How do you rationalize your answer?

2.5) Find the values of  $\langle x^4 \rangle$  and  $\langle p_x^4 \rangle$  for the state  $n = 1$  of a particle in a one dimensional box.

2.6) Calculate the value of the uncertainty product  $(\Delta x)(\Delta p_x)$  for the  $n = 2$  state of a particle in a one dimensional box.

2.7) Using the separation of variables technique, indicate the steps in the solution of the problem of a particle in a three dimensional box.

2.8) Will it be possible to plot the normalized wavefunction of a particle in a three dimensional box easily?

2.9) Treat hexatriene ( $C_6H_8$ ,  $CH_2 = CH - CH = CH - CH = CH_2$ , length  $7.3 \text{ \AA}$ ) and octatetraene ( $C_8H_{10}$ ,  $CH_2 = CH - CH = CH - CH = CH - CH = CH_2$ , length  $8.5 \text{ \AA}$ ) as linear molecules and calculate the energy levels of pi electrons (6 in hexatriene and 8 in octatetraene) by treating them as particles in one dimensional boxes. Calculate the smallest excitation energies in both molecules. In hexatriene, the wavelength of excitation energy, determined experimentally is 258 nm. Rationalize this observation using your results. (Refer to example 2.4)

## Recap

In this Lecture you have learnt the following

## Summary

In this chapter, we have studied the particle in a box problem. This is probably the simplest problem in quantum theory and the problem is exactly soluble. The Schrodinger equation for a one dimensional box was obtained by replacing the dynamical variable for the kinetic energy by the corresponding operator. The boundary condition in this problem is that the potential energy of the particle is  $\infty$  at the boundary of the box as well as at all points outside the box. It is this boundary condition of confinement of a particle inside the box that causes the quantum numbers to be integers and the energy values to be discrete.

The problem was extended to two and three dimensions and the separation of variables technique was used in solving the problem in two dimensions. The utility of this problem in chemistry was shown by using these formulae in calculating the energy levels of pi electrons of a linear polyene. The one dimensional box problem was also used to obtain the errors or uncertainties in measuring the positions and momenta of particles simultaneously in the box and the result of their product obtained for the  $n = 1$  state was shown to be consistent with the uncertainty principle.

Congratulations, you have finished Lecture 2 : Particle in a Box. To view the next Lecture select it from the left hand side menu of the page