

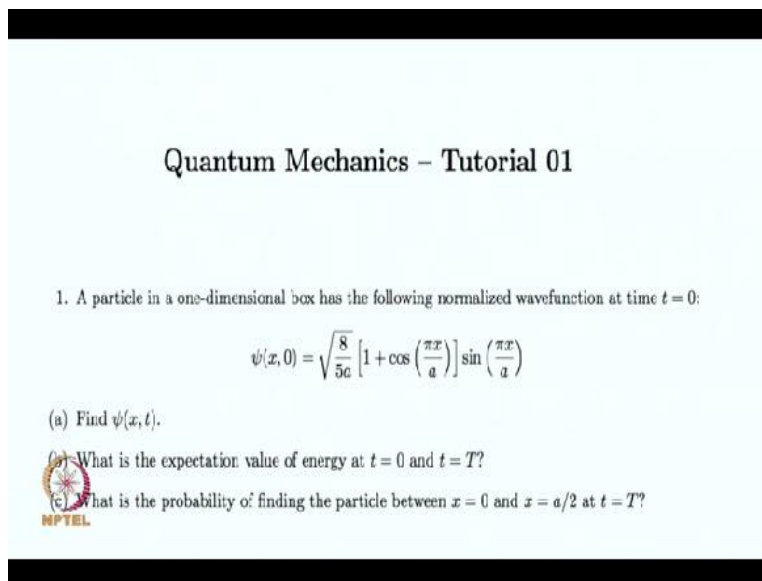
Quantum Mechanics
Prof. P. Ramadevi
Department of Physics
Indian Institute of Technology - Bombay

Lecture – 05
Tutorial 1 - Part I

I am Jai More and I will be doing TA this quantum mechanics course conducted by professor Ramadevi and in the tutorials, after every 4 lectures as you know that there will be 1 tutorial. And these tutorials will consist of 4 to 5 problem based on the lectures which you have seen, which will be posted before the tutorials.

And then from tutorials, we will basically help you to understand more the theoretical part. So I will try to put important steps while discussing the tutorial and then there will be some in between step that you can work out and then understand the problems in a better way. So let us get started to the tutorials.

(Refer Slide Time: 01:15)



Quantum Mechanics – Tutorial 01

1. A particle in a one-dimensional box has the following normalized wavefunction at time $t = 0$:

$$\psi(x, 0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right)$$

(a) Find $\psi(x, t)$.

(b) What is the expectation value of energy at $t = 0$ and $t = T$?

(c) What is the probability of finding the particle between $x = 0$ and $x = a/2$ at $t = T$?

NPTEL

This first tutorial consist of 5 problems based on what we have already seen in last 4 lectures which will basically have more problems on particle in 1-dimensional box, find out the probability, density, expectation value, etc. So as you can see the first problem is divided into 3 parts. So the first, let me read out the question, a particle in 1-dimensional box has the following normalized wavefunction at time $t=0$.

So time-independent wavefunction is given to you. And you are asked to find out the time-dependent wavefunction. And then the second part of this question is what is the expectation value of the energy at time $t=0$ and at another time where t is some T . And the third part of the question is what is the probability of finding the particle between the position $x=0$ to $x=a/2$ at some instant of time, okay. So let us get started with the problem.

(Refer Slide Time: 02:26)

$$\begin{aligned} \psi(x,0) &= \frac{8}{\sqrt{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right) \\ &= \frac{8}{\sqrt{5a}} \sin\left(\frac{\pi x}{a}\right) + \frac{2}{\sqrt{5a}} \sin\left(\frac{2\pi x}{a}\right) \\ &= \frac{4}{\sqrt{5}} \underbrace{\left(\frac{2}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) \right)}_{\phi_1(x)} + \frac{1}{\sqrt{5}} \underbrace{\left(\frac{2}{\sqrt{a}} \sin\left(\frac{2\pi x}{a}\right) \right)}_{\phi_2(x)} \end{aligned}$$

So first problem wavefunction, time-independent wavefunction is given to us which is this constant times, this is given to us and in the next step, we will try to write this in a simplified way. So I will just open up these brackets. So this will give me, $\pi x/a$, here I will simplify this $2 \cdot \cos(\theta) \sin(\theta)$ will give us $\sin 2\theta$. So I will just write it in this form that will be $\sin\left(\frac{2\pi x}{a}\right)$, okay.

We can simplify this expression again by writing it into the known form. What is the known form? That is we know what is the solution of 1-dimensional, of a particle in 1-dimensional box. So we will write the normalized wavefunction as, this we all know. We have seen already in the lectures, $\sin\left(\frac{\pi x}{a}\right)$, okay. This is one term. The second term I will rewrite as $\sin\left(\frac{2\pi x}{a}\right)$.

(Refer Slide Time: 04:24)

$$\phi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad n=1, 2, \dots \quad (2)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \rightarrow E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

$$\psi(x, 0) = \sqrt{\frac{4}{5}} \phi_1(x) + \sqrt{\frac{1}{5}} \phi_2(x)$$

$$\psi(x, t) = \sqrt{\frac{4}{5}} \phi_1(x) e^{-iE_1 t} + \sqrt{\frac{1}{5}} \phi_2(x) e^{-iE_2 t}$$

So for this just recollect what was the solution for particle in 1-dimensional box. ψ of x was given by or rather, let us call it as $\phi(x)$. $\phi(x)$ was given by $\frac{2\pi}{L} \sin\left(\frac{n\pi x}{L}\right)$, this was the general solution where n can take any value, okay. And the corresponding energy E_n was given by $\frac{n^2 \pi^2 \hbar^2}{2mL^2}$ where L was the length of the box or the width of the box.

In this case, we have it as a. So now what do we have? So using this, you can see in the first expression we had this was my $\phi_1(x)$, this is nothing but $\phi_2(x)$, okay. So your $n=2$, your $n=1$. So now what I can do is, coming back to this, I can write this wavefunction as, we have the constant as $\sqrt{\frac{4}{5}} \phi_1(x)$, we have $\sqrt{\frac{1}{5}} \phi_2(x)$. Now we have to evaluate the time-dependent wavefunction, that is $\psi(x, t)$.

So now you can see from this relation. So E_1 will just correspond to $\frac{\pi^2 \hbar^2}{2mL^2}$ and similarly for E_2 you can evaluate. So this can be written as $4/5$. This is my $\phi_1(x)$ and I have to put the time component which is $e^{iE_1 t}$ + the latter part will have $\phi_2(x) e^{iE_2 t}$.

This is nothing but the time-dependent wavefunction, okay. This is the simple way. So this is the first part where we have to calculate the time-dependent wavefunction, okay. So now let us go to the second part of the problem. In the second part of the problem, you are asked to find out the

expectation value of energy.

(Refer Slide Time: 07:03)

Handwritten derivation on a whiteboard:

$$\begin{aligned} (b) \langle \hat{E} \rangle &= \int_{-a}^a \psi^*(x,t) E \psi(x,t) dx \\ &= \frac{4}{5} E_1 + \frac{1}{5} E_2 \\ &= \frac{4}{5} E_0 + \frac{4}{5} E_0 \\ \langle \hat{E} \rangle &= \frac{8}{5} E_0 \end{aligned}$$

Additional notes on the right side of the whiteboard:

$$\begin{aligned} \hat{p} &= -i\hbar \frac{\partial}{\partial x} \\ \hat{E} &= i\hbar \frac{\partial}{\partial t} \\ E_n &= \frac{\pi^2 \hbar^2 k^2}{2ma^2} \\ E_0 &= E_1 \\ &= \frac{\pi^2 \hbar^2}{2ma^2} \end{aligned}$$

That is the energy operator, how does you calculate the expectation value? The standard way of writing this is $\psi^*(x, t)E\psi(x, t)$. This operator E we can write it as $i\hbar \frac{\partial}{\partial t}$. This is the representation of the energy operator, okay. As you know that momentum operator is represented as $-i\hbar \frac{\partial}{\partial x}$. Similarly, the energy operator is represented by $i\hbar \frac{\partial}{\partial t}$. So now what we do is we will solve this.

So here you will substitute $\frac{\partial}{\partial t}$ and then when you differentiate $\psi(x, t)$ with respect to t, the energy component, that is E_1 and E_2 will come out in the derivative. So finally what you obtain, you will have to write explicitly ψ^* and ψ and operate E on $i\hbar \frac{\partial}{\partial t}$, okay. And then what exactly you obtain in the end is $\frac{4}{5}E_1 + \frac{1}{5}E_2$, okay. Now here there are two 3 steps involved and it is very easy to work out.

You have to just substitute $\psi^*\psi$ and this operator and work out the steps. And just check whether you obtain this equation, okay. One more remark we have seen that $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ in this case. So what will be E_0 ? we will write for $n=1$, our E_0 is equal to E_1 which is nothing but, okay. This is $\frac{\pi^2\hbar^2}{2ma^2}$ and we can write this E_1 and E_2 in terms of E_0 .

Simply I can write this as $\frac{4}{5}E_1$. I can write it as E_0 , +, so here E_2, E_1 is just E_0 . E_2 will be $n^2 \cdot E_0$ which is nothing but $\frac{4}{5}E_0$. So in the end what I obtain is this, okay. So the second part of this problem is, this is the solution, okay. So this was part b of the problem. And now let us go to the part C, okay. It is again very simple to obtain part C.

(Refer Slide Time: 10:12)

(c) $P = \int \psi^* \psi dx$ (4)

$$P = \int_0^{a/2} \psi^*(x,t) \psi(x,t) dx$$

$$= \int_0^{a/2} \frac{4}{5} |\phi_1|^2 dx + \int_0^{a/2} \frac{1}{5} |\phi_2|^2 dx + \int_0^{a/2} \frac{2}{5} \phi_1^* \phi_2 dx$$

$$+ \int_0^{a/2} \frac{2}{5} \phi_1 \phi_2^* dx. \quad t=T$$

$$P = \frac{1}{2} + \frac{16}{15\pi} \cos\left(\frac{3\pi^2 \hbar^2}{2ma^2}\right) T$$

Which is you have to find out the probability of finding the particle. So probability, how do we obtain probability in general? Probability of finding the particle is $\psi^* \psi dx$, this is the shorthand notation. You will write it as x,t and here also x,t . So let me write it again. $\psi^*(x,t) \psi(x,t) dx$, okay. And for the normalized wavefunction, the probability of finding the particle in the box from 0 to say a length a would be 1.

But here we have to calculate the probability from 0 to $a/2$, okay. So now what do I do? Is again I substitute for ψ^* and ψ in the expression and then I will write, I will skip 1 step. What you obtain basically is $\int_0^{a/2} dx \frac{4}{5} |\phi_1|^2$, I have a $\int_0^{a/2} dx \frac{1}{5} |\phi_2|^2$, okay. And I will have 2 more terms that is $\int_0^{a/2} dx \frac{2}{5} (\phi_1^* \phi_2 + \phi_2^* \phi_1)$, okay.

And these are all real wavefunction. And when you perform this integration, you will obtain, ϕ is a normalized wavefunction. So you will simply obtain $4/5$ and you have integral from 0 to $a/2$.

So you will obtain a factor of 1/2. So adding these 2 terms, you obtain a factor of 1/2, okay. And in the second part, you have to work out these integrations, okay. When you write Φ_2 and Φ_1 , the x part that is the space part will remain the same but the time component will have exponent + or $-E_1 - E_2$ or $E_2 - E_1$.

Depending on that, you will simplify these expression and then after performing the integration from 0 to a/2, you obtain this result. So in between step I expect that you can work out, it is not that difficult. So I have a $\frac{16}{15\pi} \cos\left(\frac{3\pi^2 \hbar^2}{2m a^2}\right)$, okay.

And I have a t, $\cos(\theta)*t$, I mean this $(E_2 - E_1)*t$ but we want to find the probability at t at time t=, we have to find the probability at time t=T. So I will put a T over here. So the probability expression comes out to be this. For a particle in 1-dimensional box, you always need to remember that the normalized wavefunction is given by the expression which I have shown you before that is this, this one and this one.

So the normalized wavefunction or the solution for a particle in 1-dimensional box is given by this. And the corresponding energy eigen value E_n is given by this expression. Second problem is also a problem based on 1-dimensional potential box but here we have a potential which is non-0. **(Refer Slide Time: 14:41)**

2. Consider a particle in a one-dimensional potential $V(x)$ which is infinite for $x \leq 0$, zero in the region $0 \leq x \leq a$ and V_0 for $x > a$. Show that the bound state energies are given by the solution of the transcendental equation

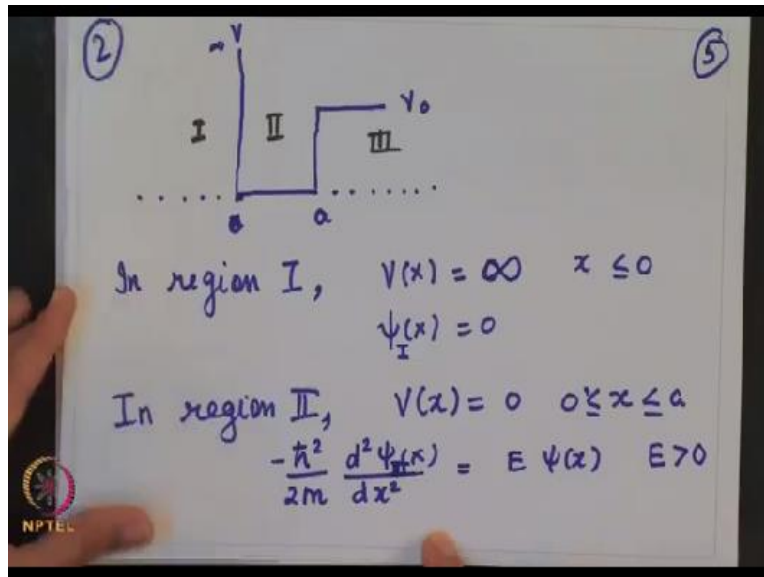
$$\tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = -\sqrt{\frac{E}{V_0 - E}}$$

Sketch the wavefunction.



So you consider a particle in 1-dimensional potential $V(x)$ which is infinity for $x < 0$ and $x > a$. So between 0 and a, the potential is 0. For $x > a$, the potential is V_0 . So let us draw this question 2.

(Refer Slide Time: 15:04)



Let us draw this. So how will the diagram would look like. If you consider between 0 and a, the potential is 0 and so x is 0, x is a, this is the x axis and here V is infinity. So at $x < 0$, V is infinity. So this is your V axis and for $x > a$, $V = V_0$. So this is V, so V will be equal to V_0 , some V_0 , okay. So you are asked to find out some relation between these energies and potential that is show that the bound state energies are given by a transcendental equation.

And you can also, like if once you achieve this transcendental equation, you can actually visualize what will be the form of the wavefunction. We will divide this in 3 regions, okay. So let me call this as region I, this is region II and this is region III, okay. So we will be using our knowledge of what we have learnt in the lectures. So this is the region I. So in region I, what do we have?

In region I, okay, what do we have? V of x is 0, okay for $x < 0$ or $= 0$. So what can you say about the wavefunction? Wavefunction will also be 0, okay. And then in, so let me label this as psi of region I. Then in region II, what can you say about the region II? So in region II, I am sorry, here we have V of x is infinity because I have already drawn it here V goes to infinity in region I. So in region I, V of x is infinity for $x < 0$.

And the wavefunction is 0 at $x=0$ as we know, okay. So for a well-behaved wavefunction, we need to satisfy some conditions. So one of the thing is that the wavefunction will be 0 for $x=0$. So at the

boundary, the wavefunction has vanished. So now let us come to region II. So in region II, we actually had $V(x)$ is 0 and x is between 0 and a , okay. So for this region, we have, we will write down the time-independent Schrodinger equation.

So let us write down the time-independent Schrodinger equation, $\frac{d^2}{dx^2}\psi(x) = E\psi(x)$, okay. So here, you can see that $V(x)$ is 0, so I have directly written down this expression. Again, let me call this as region II, okay. And E , so E has to be greater than 0, okay. So E is greater than V and similarly, you can find out the solution for this wavefunction simply by simple algebra.

(Refer Slide Time: 19:07)

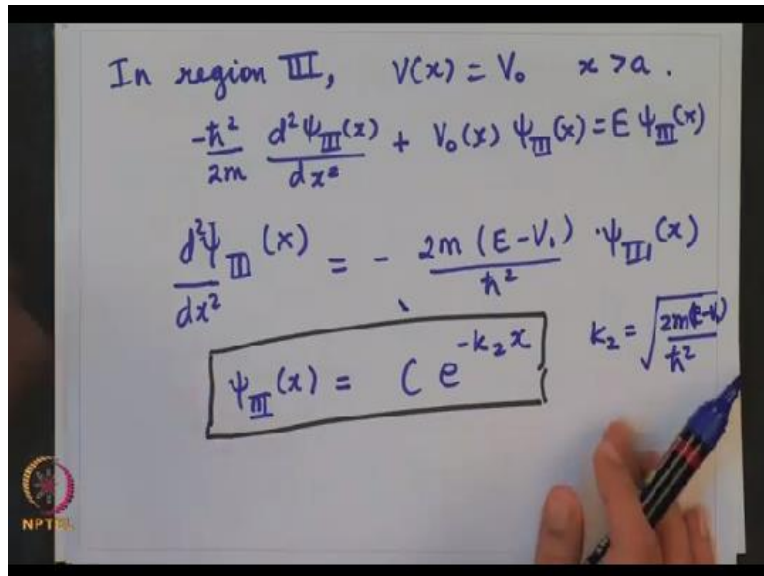
The image shows a whiteboard with handwritten mathematical work. At the top, the wavefunction is given as $\psi_{II}(x) = A \sin k_1 x + B \cos k_1 x$. To the right, the wave number is defined as $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$. Below this, the text says "using boundary condition," followed by the condition $\psi_{II}(x)|_{x=0} = 0$. This leads to the equation $A \sin k_1 x + B \cos k_1 x = 0$. The result $B = 0$ is boxed. Finally, the simplified wavefunction is given as $\psi_{II}(x) = A \sin k_1 x$. A small logo is visible in the bottom left corner of the whiteboard image.

You can find out that this wavefunction which I wrote for region II, can be written as $A \sin(k_1 x) + B \cos(k_2 x)$. This is the general solution for this equation which we have written down before.

$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$, okay. Now we can use boundary condition.

So using boundary conditions, what we can do is, we can write down the correct form of the wavefunction will be. So at boundaries that is at $x=0$, what do we obtain? At $x=0$, $\psi(x)$ is 0. So $A \sin(k_1 x) + B \cos(k_2 x) = 0$. That would imply simply that $B=0$. So this is what we obtain. So let me write what will be my $\psi_{II}(x)|_{x=0}=0$? $\psi_{II}(x)$ will be $A \sin(k_1 x)$. We have region I, wavefunction is 0 in region II. And now let us go to the third region.

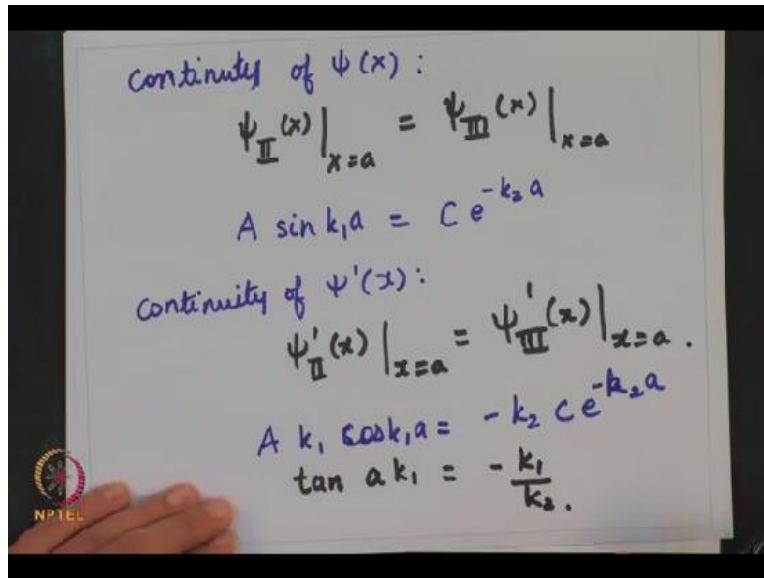
(Refer Slide Time: 20:57)



In region III, $V(x)=V_0$ for $x>a$, okay. So what do I have? How will I write this? I will write this as $-\frac{\hbar^2}{2m} \frac{d^2 \psi_{III}(x)}{dx^2} + V_0(x) \psi_{III}(x) = E \psi_{III}(x)$, okay. Now again it is easy to find the solution of this wavefunction. $\psi_{III}(x)$ again what we can do is we can write this as, okay, let me write this as $\frac{d^2 \psi_{III}(x)}{dx^2} = -\frac{2m(E-V_0)}{\hbar^2} \psi_{III}(x)$, okay.

And this term I will write as $\psi_{III}(x)$. So this term I call it as k_2 , okay. So the solution of this is given by $\psi_{III}(x)=C e^{(-k_2 x)}$ where k_2 , so this is nothing but $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$, okay. So this is the third wavefunction, okay. And then now what we do is again here I have skip some steps, you can apply the boundary condition and get this as the final expression.

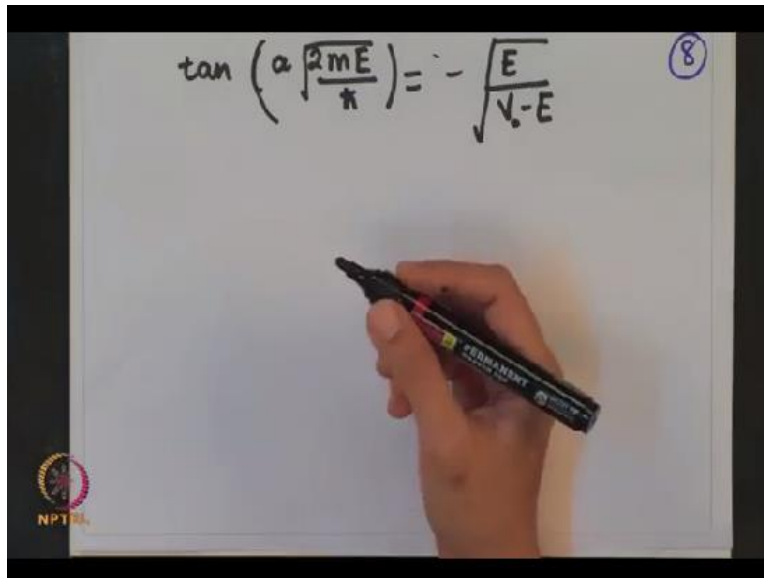
(Refer Slide Time: 23:14)



And in the final step, what we will do is we will use the continuity condition, continuity of $\psi(x)$, okay. What is that? That is at $x=a$, so we had this $\psi(x)$ at $x=a$ should be equal to ψ of, so from region II to region III at $x=a$ should be continuous. So using this, what I obtain is I have $A \sin k_1 a = C e^{-k_2 a}$ and the continuity of $\psi'(x)$, will be, I will do the same thing for $\psi'_{II}(x)|_{x=a} = \psi'_{III}(x)|_{x=a}$.

So this will give me another set of equation. Sin will become $A k_1 \cos k_1 a = -k_2 C e^{-k_2 a}$. So finally what I obtain in the end is when I, just you have to divide the 2 equation and then what you obtain finally is $\tan a k_1 = -\frac{k_1}{k_2}$, okay, which is nothing but what is given to you in the question, okay. So this is the final result.

(Refer Slide Time: 25:32)



We can again rewrite this k_1 to write it in the final step is $\tan\left(a\sqrt{\frac{2mE}{\hbar}}\right) = -\sqrt{\frac{E}{V_0-E}}$ and now you can, using this you can easily sketch the form of the wavefunction, how the wavefunction would be, okay? That I will leave it to you all, okay. So this is what we have done for the tutorial 1 part. This was part 1 and the remaining problem we will discuss in the later part.