Computational Physics
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Lecture – 36
Differential Equation for Quantum Mechanical Problems: Numerov Algorithm
Part 01

So, in this module what we will do is the aim of this module is to tell you about some simple methods which will allow us to solve another class of second order differential equations which are known as Schrodinger equations. So, this we will do for one dimension.

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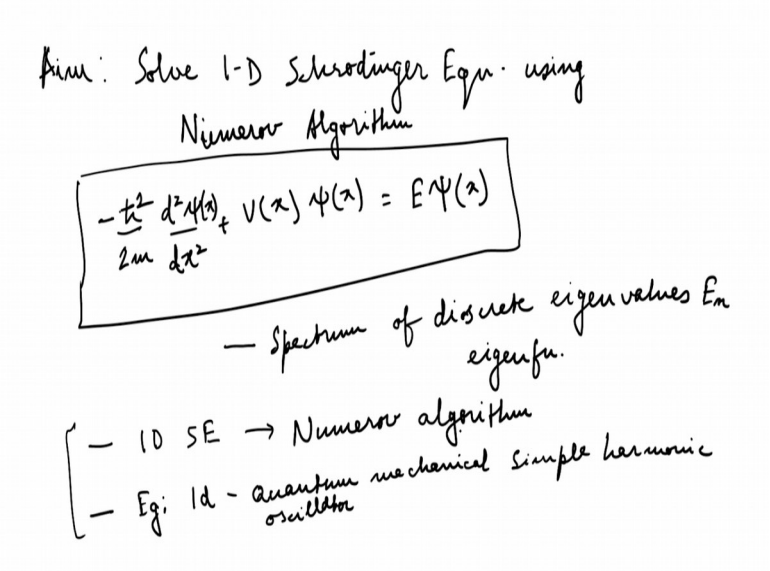

So, the aim is solve one dimensional Schrodinger equation using the Numerov algorithm. So, we are all aware of the what a Schrodinger equation is, but just for the sake of completeness I am writing it down once again minus h cut square by twice m d 2 psi dx 2 plus V as a function of x psi is also a function of x here equals to E psi x.

So, this is my 1-D Schrodinger equation. So, if you look at it ,this is again nothing, but a second order differential equation and you have learnt already in the previous modules how to handle it. But, there are some other its additional complexities to the system while that is the reason why it needs some special treatment. So, we will talk about that.

So, the focus here is sort of to get; so, what do you get? If you if you are able to solve the Schrodinger equation analytically, you get a spectrum of discrete eigen values for which there exists a unique eigen function.

So, our aim is to obtain these eigenvalues and eigen functions numerically because in most of the practical cases, we will not be able to solve this Schrodinger equation analytically. So, in this part of this course what we will learn is we will learn for the special case of one 1-D Schrodinger equation and the algorithm which we will discuss is known as the Numerov algorithm. And then what we will do is we will take an example and the example will be basically my 1-D quantum mechanical simple harmonic oscillator.

So, this is the plan of what we are going to cover in this part of the course. So, but before we go into this, these two parts , that is before we talk about the Numerov algorithm and before we take a practical example and apply the Numerov algorithm. So, what I would like to discuss is now the additional problems which one typically faces when one solves this type of a differential equation particularly in the area of quantum mechanics.

So, one issue is already there is that you do not know how to do the integration analytically to get the solution that is how; I mean what is the function as a function of x. So, for that the Numerov algorithm is already there which we will see, but in addition to that there are two more problems which are associated in solving this type of Schrodinger's equation particularly in the context of quantum mechanics.

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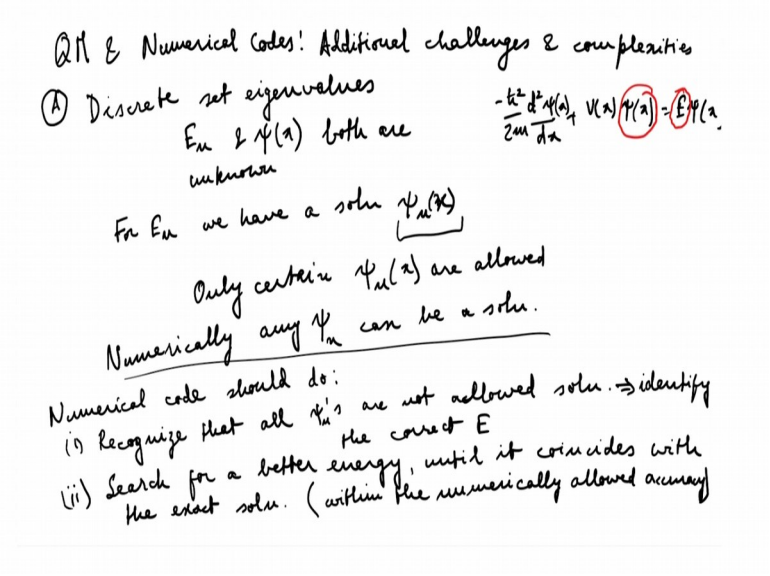

So, basically so, it will be more like a sort of a overview. So, what is what we are going to talk about is quantum mechanics and the issues with numerical codes. That is what are the additional challenges and complexities; primarily there are two types of additional challenges and complexities which one come across here. The first at complexity which is pertain to the fact that when we solve a quantum mechanical Schrodinger equation what we end up at the end of the day is discrete set of eigenvalues which I am calling as En.

Note that in my Schrodinger equation if I just write it down here and so, that we have it for our reference d 2 psi dx 2 plus V x psi. So, psi's are function of x is to E psi x. So, one of our unknowns is this quantity which is my psi x. In addition to that we have another unknown which is E n. So, we do not know what the energy eigenvalues are. So, we only know that these are a set of discrete energy eigenvalues.

So, hence both en and psi x both are unknown here. What we know is that the fact that for each E n, we have a solution psi n and another important fact is, but the complexity lies in the fact that there is only certain values eigen functions which are there are that is there the only certain psi n which are which are allowed based on the type of the problem and the boundary conditions we are we are facing we are applying.

So, only certain psi n sorry this will be x are allowed; however, if you solve this numerically so, numerically any psi n are maybe a solution to my problem. Numerically

any psi n can be a solution, but that solution may not be physically correct. They are not give because we should remember that psi the wave function of a particle the one physical interpretation of the wave function of the particle is that it gives me a probability of finding a particle at a given position x.

So, once we know the wave function we can find the probability of the particle at a given position x. So, what this particular statement means that numerically any psi n can be a solution is that we might end up with an unphysical solution where the wave function may diverge. For example, if we are in the position space; if we are in at a point where the classically the wave function is forbidden or classically the particle is forbidden to stay there.

So, in from a classical picture it is impossible, the probability of finding the particle there at that particular point is 0, but quantum mechanically what you would expect is because of the tunneling phenomena, there is a finite probability of finding the particle. So, the wave function at that point, the correct physical behavior of the wave function is that it should decay exponentially to 0 at that point in space, but there might be possible that there is another numerical solution which is another numerical wave function. The code can find where instead of it decaying, it just simply diverged at that point.

So, this is one of the complexities which I m talking about for this type of codes for quantum mechanical methods. So, when we write a code what we need to keep in mind are the following things. So, basically your numerical code should be able to do the following things. So, first of all it should recognize the fact that we discussed above.

It should recognize that all psi n's are not solutions are not allowed solutions which in other word means that it should ident; it should be able to identify the correct values of E. Only if it identifies the correct value of E, then only can it identify the correct corresponding solution. And in order to do so, what it should be able to do is it should be able to search for a better (value of) energy until it coincides with the exact solution.

So, remember here I am using exact ……..when I say exact I mean exact within the numerical accuracy because numerically in most cases we will never get, we will never get the exact solution; we can be close to the exact solution because there will be always some numerical errors present with the same.

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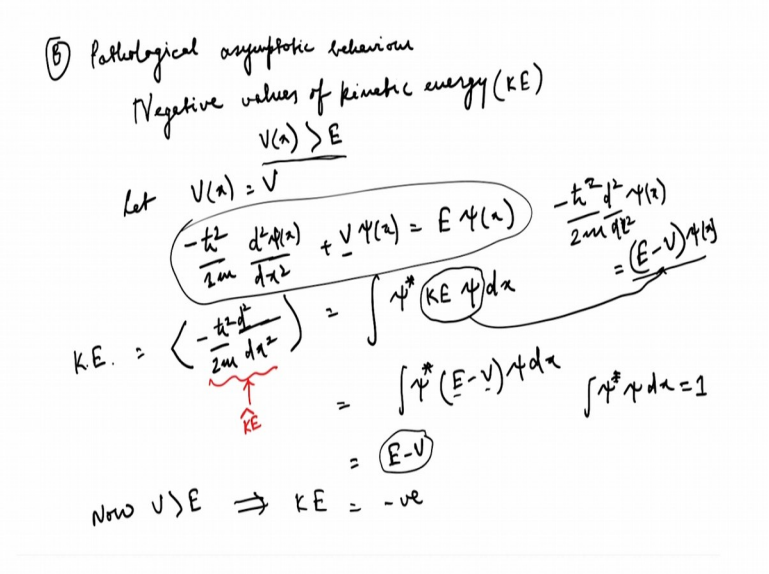

So, this is one problem and second problem. It is a sort of a, one can say, it is a pathological problem in quantum mechanics is that as it has a pathological asymptotic behaviour. So, what does do we mean to by that? So, by the statement that in the problems in quantum mechanics have a pathological asymptotic behaviour. So, what I am really trying to point out is to the fact that in quantum mechanics unlike classical mechanics, it is possible to have negative values of kinetic energy.

So, so, what I mean is it is possible to have negative values of kinetic energy. So, when this is possible? So, this is possible when my potential say potential at a given point x is greater than the energy of the particle. So, how this is possible? So, we will let me just explain to you in by taking a simple example. So, let us assume that my potential V x is a constant and let us suppose it to be V. So, if I write my Schrodinger equation. So, what I have is minus h cut square by twice m d 2 psi which is a function of x dx 2 plus now my V is a constant here psi x this gives me E psi x.

So, this is my Schrodinger equation and if I want to compute the kinetic energy, what we need to do is we need to compute the expectation value of my kinetic energy operator which is nothing, but h cut square by twice m d 2 psi x dx 2. So, this is nothing, but so, what I do is I will call this as my kinetic energy operator. So, so what it means is basically we need to evaluate this term and integrate it over the x here because it is a one

dimensional case. Now in order to evaluate this term what we can do is we can take the help of this Schrodinger equation here; this one.

So, from here what we see is that the kinetic energy operator sorry there this psi x going to be here. So, it is this is my operator. So, what we can see here is d 2 dx 2 psi x; this we can write as E minus V psi x. So, what we will do is so, basically in this integral this term, we will replace with this particular term here. So, if we do that so, what we land up with is we have psi star psi E minus V psi dx and this E is also a constant v is also a constant for us. So, we can pull that out. So, we will get this quantity and assuming that my psi's are normalized with the integral. So, integral over psi star psi dx will be equal to 1. So, this is what we will be getting as the expectation value of my kinetic energy.

Now if we go back to the beginning. So, we were talking about this v x greater than E. So, my V is greater than E. So, what this implies is that my kinetic energy which is given by this term E minus V, this will be negative. So, in this case we have a negative value of the kinetic energy. So, now, if we try to find the solution of this so, what we can do is the following we can write it in a simplified form.

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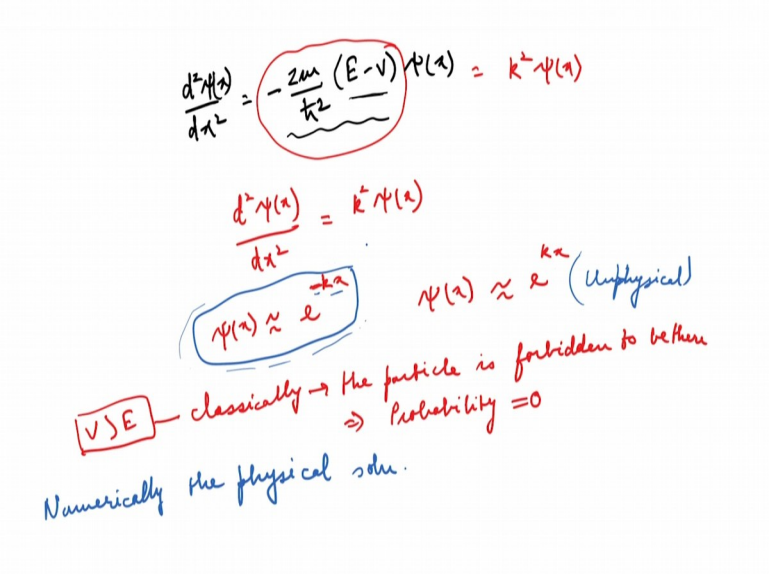

So, what we can do is we can write the Schrodinger equation again in this simplified form where if I go back here. So, what I am doing here is I am taking this term on this side and then this term also on the right hand side and then rewriting the equation again. So, what I will get is minus twice m by h cut square E minus V psi x ok. Now if I look at

this carefully so, this term in the bracket E minus V; this is a negative term and we have a negative sign here. So, this whole term here. So, this whole term the coefficient here we have this is a positive quantity. So, what I can do is I can rewrite as k square phi x.

So, I my Schrodinger equation what I am doing is I am rewriting it in this form k square psi x. Now this type of equation we have already seen earlier and the typical solution. So, there are two possible solutions of psi x. So, one is my psi x is approximately equal to E to the power minus kx or my psi x can go like E to the power k x. Now, the condition that my V is greater than E, so this implies in the classical picture.

So, classically what we have is that it is for with the particle is forbidden to be there which in other word implies that the probability of finding the particle is at that place; at that value of x at those values of x where V is greater than my E this E is equal to 0. But quantum mechanically we know that it is possible to have this tunneling effect.

So, you what you will expect the wave function to behave like is it will have a exponentially it will decay down to 0 instead of abruptly going to going to 0 value. So, the physical picture is the correct physical picture which or the correct physical solution in this case will be this one where my wave function decays exponentially to minus x, but this we can look at the equations and tell that ok. This equation this particular equation is my physical solution while this is unphysical here because here it is diverging exponentially the wave function.

But when you were trying to numerically solve it neither the code nor the computer understands this fact. So, that is gives rise to lots of problems and so the idea is your code should be able to identify numerically the physical solution. The reason for this is that if even if during the when you are at evaluating or evaluating or solving this differential equation although; if there is so, what you are doing is basically you are doing integration.

So, when you are doing integration the problem is if there is a slight amount of numerical noise so, usually what happens is that it gradually builds up and then your solution blows. So, what you might see in these type of problems if you do not take care of. These facts that you are say for example, in this case your wave function should decay exponentially if you do not take care while writing the program to enforce these facts what will happen is that in the classically allowed region you may get the correct

solution while you will yeah while in the classically forbidden region your solutions might diverge.

So, we will see when we will do the example of the Schrodinger equation how I mean how if not, if we do not want to do not take care of this particular aspect of the quantum mechanical problem; how you can end up wrong is wrong diverging solutions or wrong diverging wave functions in the classically forbidden region. Although you might would not find anything any problem in the quantum mechanically allowed region.

So, the idea is you should have a code which will sort of take care of both these two aspects associated with the quantum mechanical problem. The first aspect is that you have discrete energy eigenvalues and only certain eigen functions are allowed which are determined by the boundary conditions which we allow to the problem which we are solving and the second fact is that in classically forbidden region the wave function should decay exponentially to 0.

So, the asymptotic behaviour so, this is nothing, but the the second point is the asymptotic behaviour of the wave function; at large values of x how it should behave for a given particular function. So, this behaviour also should come out the code should able to come out with solutions with the correct asymptotic behaviour also. So, both these facts needs to be taken care of when we are trying to solve quantum mechanical problems numerically.

So, with this brief introduction of the issues associated or the additional difficulties associated with solve solving quantum mechanical problems, numerically now what we will do is we will move to the numeral algorithm. So, I will briefly derive the numerical and numeral algorithm for this and then what we will do is we will apply this numeral algorithm to solve the or to find out the eigen values and eigen functions of a same quantum mechanical 1-D simple harmonic oscillator.