Computational Physics
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Lecture – 39
Differential Equation For Quantum Mechanical Problems: Numerov Algorithm
Part 04

So, now when one tries to write a code so, one needs to give some minimum amount of information or some amount of input.

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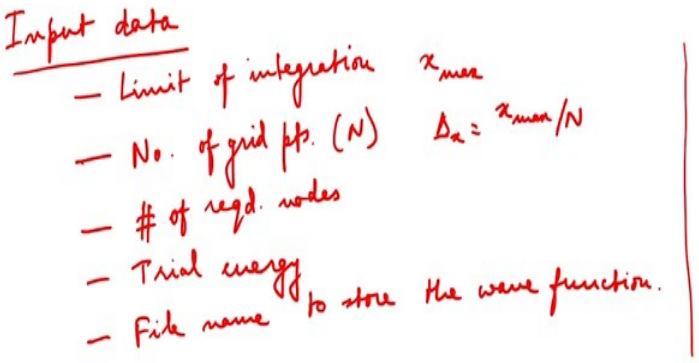

So, the input data that one will need to put in here for this to convert to a code. So, what do we want? The first thing you need to know is what is the limit of integration? So, in general for this particular case your x can go from minus infinity to plus infinity, but that is not possible to do numerically. So, I need to give some maximum value up to which I want to do the integration, some maximum value of x which I call as x max.

Then what we also need to do is to tell the code how many grid points one needs to use. Because, that determines how the value of delta x and also the accuracy of your calculation. So, delta x; will then be given by x max by N, where N is the number of grid points. Then you need to tell code which particular solution you are looking for or the number of nodes of required nodes.

So, do you need a solution with 0 nodes, do you need a solution with 1 nodes, do you need a solution with 2 nodes? You need to give initial guess of energy, a trial energy and you also need to give a file name to store the wave function. So, this is what you need to have in the program, I mean you need to give as input when you write the program.

So, if you just use so whatever we have learned so far and try to write a program we will see how . I will show you an example program and there we will see the problem of the asymptotic behavior which is not till now been taken care of. But before we go there may be I will just show you the program and the result.

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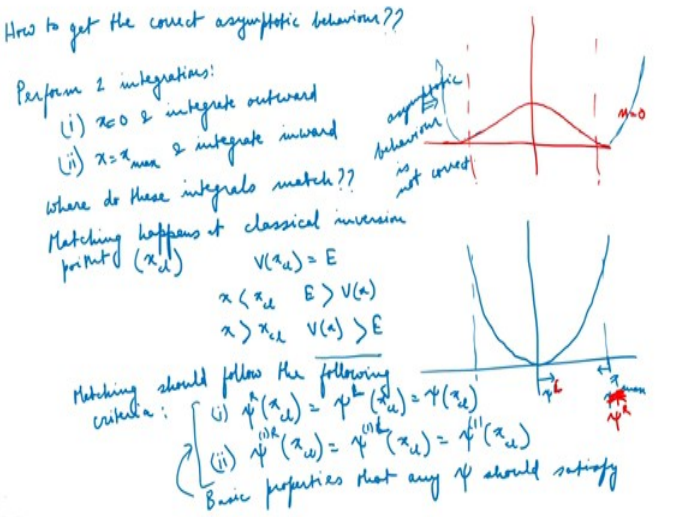

So, what we saw is that, the asymptotic behavior of my wave function is not coming correct. What I mean by that is, suppose this is my limits of integration for my harmonic oscillator. So, ideally for say for M equals to 0; ideally what I would expect is something like this a very symmetric wave function which gradually decays to 0.

But what you actually got from the code is, this part is fine, but then after a certain point it starts going up both this side and this side. So, in other words my asymptotic behavior is not correct. So, the question is how to get the correct asymptotic behavior? So, to achieve this what we will do is, we will perform two integrations. So, far we have been performing just one integration starting from x equals to 0 to x max.

Now, we will perform two integrations, the first integration will be starting from x equals to 0 and integrate outward. And then the second integration will be start from x equals to x max and integrate inward. So, we start from….. so basically, so if this is my potential energy and I am trying to integrate from this limit. So, say this is my x max.

So, what I will do is, I will start one integration from x equals to 0 and move outward. I will start another integration from x equals to x max and move inward. So, this tells me that at some point these two must match. So, now, the question is where do these integrals match? So, to match the integral what we will do is, we will choose the classical point of inversion.

So, the matching happens at, the classical inversion point which I am calling as x cl. What does one mean by this? What one means by this is that, at this value at V x cl my energies are same. So, and for x less than x cl my E is greater than V and for x greater than x cl my V is greater than E. So, here we are going to the classically forbidden regime.

So, this is our natural choice and how do we match it? So, we match it in two ways, matching should follow the following criteria. So, we will use two properties of the wave function. The one property is that at the classical point of inversion. So, if I call this psi R and if at psi L so, at so the psi R at x classical should be equal to this psi left at its classical is equal to psi x classical.

So, that means, my wave function is continuous. And the second condition is we also need to satisfy that the derivative. The first derivative of my wave function is also continuous that is my psi 1 R at x cl is equal to psi 1 R this will be L psi 1 L at x cl equals to psi 1 at x cl 0. So, these are the two basic properties, which any wave function should satisfy.

This we learned from our first class in quantum mechanics. So just to summarize, how we do the matching? The matching is done by making sure that the wave function and its first derivative is continuous at the classical point of inversion.

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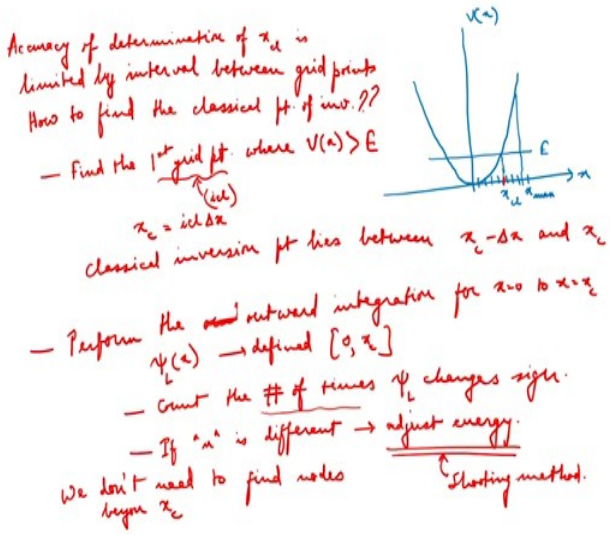

So, far so good, but then there is another problem here. So, if you realize I mean, we are doing a grid method, which is not an analytical method. So, that means? So, I am just drawing it. So, suppose this is this should be symmetric though its not very symmetric here. Suppose this is the particular energy eigen value which I am looking at and this is my exact so, this is my x classical.

But this is the exact value, but in the calculation what we are doing is. In reality what we are doing is, that this x so say from x to and this is my x max this we are dividing it into small grids. So, as a result what might happen is as you see here that this is my exact maybe I use another color pen. So, this is my exact point of this classical inversion which is happening, but that point does not lie on my grid.

So, either I have a point before that or a point after that. So, the accuracy in this case of determination of x cl is limited. If I have a smaller and smaller grid point, then the probability of this x cl I mean one having one of the grid points exactly at x cl increases; and that what it means is that the accuracy of determination of x cl is limited by interval between grid points.

So, in this case, so basically the question is now how to find out the classical point of inversion? So, to do that what we do is, we find the first grid point where V x is greater than E. So, we call this particular grid point as icl, the index i give as icl. So, once we find that grid point. So, my that particular point the x value will be given by icl delta x.

So, then what I know is that, my exact classical inversion. So, my classical inversion point that is where my quantum and classical the energy eigen value and the potential becomes same that inversion point lies between x c minus delta x and x c. So, once I find this classical inversion point, so, the next step will be, I perform the outward integration from x equals to 0 to x equals to x c.

So, which I am calling as psi L x which is defined between 0 to xc. Just let me make sure that, the nomenclatures of I am using the same ok. So, this will be R; so, let me just cut it. So, it will be psi R and this will be psi L not what is L psi L and the invert is psi L. So, while performing this equation this outward integration what I should also do is, count the number of times my psi L change sign.

Now, if this if the number of times my psi L change sign equal to the desired number of nodes. Then it tells me that this solution is correct if not that is if n is different, we need to do is add just energy. So, we need to adjust the energy using the same shooting method that we described before. Another thing to keep in mind is that, in all the cases your wave function will not have any nodes beyond the classical point of inversion.

Because, beyond the classical point of inversion that is in the region, the presence of the particle is classically forbidden. What if the wave function should behave as an exponentially decaying wave function there we know oscillations in the wave function. So, therefore, we do not find nodes beyond xc. So, this is about the outward integration. So, once you are sure that your outward integration is correct, that is once you know that at the number of nodes match.

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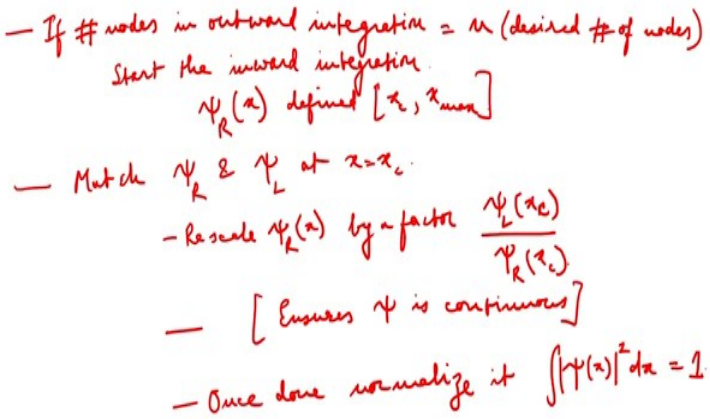

Basically what it means is if number of nodes in outward integration, is equal to n; which is my desired number of nodes. What I do is I start the inward integration, which I define as psi R x and which is defined in xc x max. Now, once I have done the two integrations from 0 to x c and from x max to x c then what I need to do is, now match the wave functions that is match my psi R and psi L at x equals to x c.

So, how do I match it? So, as before my wave functions should be continuous. And to do that, what I do is I rescale my psi R; that is the value of the outward integration by a factor which is equal to psi L the ratio of psi L and psi R at xc. Once its done, so, what this does is, ensures psi is continuous. So, once this is done, we need to normalize it that is my mod psi x square dx the integral over the whole range of x should be equal to 1.

So, this goes the matching of the wave function. Now, if you remember we also need to match. So, we have satisfied the first matching condition that the wave function is continuous.

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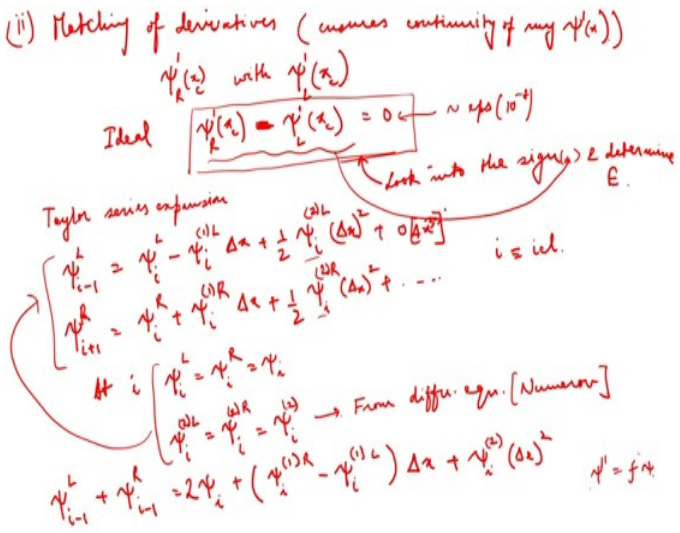

Now, we need to satisfy the second matching condition that is the matching of the derivatives. So, ensures continuity of my derivatives over the range. So, that basically means matching psi R at xc with psi prime L at xc. So, the ideal scenario is that my psi R prime at x c is equal to that or we can write it minus psi prime L at xc is equal to 0.

But this is only correct or you will get this condition only when you are you have reached the correct energy eigen value. Otherwise you will not get it this condition will never be satisfied. So, and so to do that what one needs to do is, basically again go back and apply the Taylor series expansion till you get this condition is matched. So, for the numerical case this should be of the order of this epsa which is ten to the power minus eight, this difference ok.

So, how to do that? To do that, what we do is we again apply Taylor series expansion. So, now, what we are going to do is, we are going to look into the sign of this difference. So, basically the sign of this quantity here and determine E. So, if I do the Taylor series expansion of my left wave function that is psi L i minus 1, this is equal to psi i L minus psi 1 L i delta x plus half psi 2 L i delta x square plus I have third order term here.

Similarly my the right hand psi R i plus 1 is equal to psi i right plus, the first derivative of the right hand at i del x plus half psi i second derivative of right to del x square plus the third order term. Now, here you note one thing that I have just written as the short form of my icl that all this is happening in front of inversion.

Now, from the previous part what we have seen is that, at i my psi i left equals to psi i right because I am already ensured the continuity of my wave function this is equal to psi i. So, we put that in to this particular so we put this values of psi L and psi R and psi i into this wave function. Also you should note that, the second thing is again at i the second derivative L i is equal to the second derivative of the right hand side i which I am writing as psi 2 i.

The reason for this is, this comes from the this is my from my differential equation right based on the Numerov algorithm ok. So, what we do is now, we plug in these two things into these two equations and we take the difference we will just add up these two equations. So, we plug in so, here instead of psi L i I will put psi L i psi R i I will put psi R i. And again these two are also same and then if we add what I get is the following.

So, psi i minus 1 L plus psi R i minus 1 this equals to psi i both are same I am reading so, I will get 2. Then I will get plus psi i 1 R minus psi i 1 L into delta x plus again these two are same. So, its just twice this so, that will be psi i second derivative delta x whole square and then we have the (Refer Time: 22:33).

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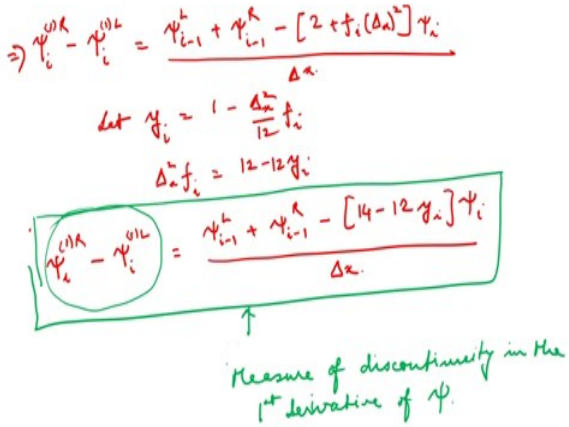

So, if I simplify this. So, what I will get is now psi so what I want is to compute the difference between the derivatives of my wave function from the output integration. And from the inward integration add the inversion classical inversion point so, that will be

given from this equation. So, 1 R minus psi 1 L at i this is equal to psi i minus 1 L plus psi i minus 1 R minus 2 plus f i delta x square.

So, how do I get fi? I get fi because the this is from the Schrodinger equation itself. So, I have my Schrodinger equation psi double dash equals 2 f psi. So, from there I have just put in I plugged in the value of psi double dash into this one divided by delta x.

Now, if I let us assume y i equals to 1 minus as this is as before we have done the similar assumption before. So, what I get is, delta x square, f i equals to 12 minus 12 y i. So, if I plug this thing here. So, at the end of the day what I get is the difference between the first derivative of my inward and outward integration. This is given by psi i minus 1 L plus psi i minus 1 R minus 14 minus 12 y i psi i divided by delta x.

So, this thing so this particular equation this basically what it does is it. So, its a measure of discontinuity in the first derivative of my psi. So, now, looking into this the sign of this particular quantity I can judge whether my energy has been I mean the my initial guess of energy is higher than the actual one or the initial guess of energy is lower than the actual one. Accordingly I changed my racketing region and then I 0 down to the correct value of energy.

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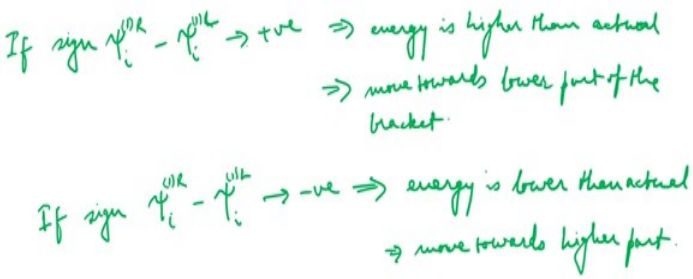

So, the way to do that is, if my sign of psi 1 R at i minus psi 1 R at sorry this will be L at i. If this is positive this is positive, this typically implies that my energy is high. So, what

we need to do as before is, move towards lower part of the bracket. If my if sign of psi 1 R i minus psi 1 L I, if this is negative this imply energy is lower than actual. So, this is higher than actual.

And then what we do is, we move towards higher part of the bracket. And then we repeatedly go on doing this till we reach the convergence. Now, so far so good now, one thing is still left is that now the next question is for. So, we have we know how to or how to set the initial conditions. The two initial conditions for my outward integrations that is, when I am going from x equals to 0 to xc.

But we have not talked about what is the initial….. what should be the initial conditions for the inward integration. That is when we go from x equals to x max towards x equals to xc. So, that is what we I will just briefly describe now.

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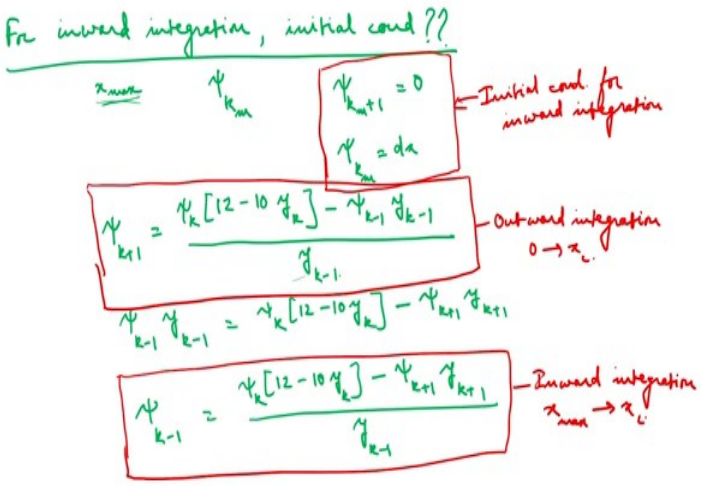

Now, so for inward integration, what are the initial conditions? So, this is what I am going to talk about. So, suppose my I have at x equals to x max if this wave function I call as psi k m ok. So, I need two initial conditions. So, the by definition since this outward integration I am already in the classical leave orbit regime.

And I know that my wave function should decay exponentially and if my x max this one is quite large. So, it is safe to assume that the next point after this x max the wave function is 0. So, the first initial condition I set two is chi psi at x max 1 equals to 0. And

then psi at x max this I said to some small arbitrary value which is I call dx. So, once I know that, so what I do is, I use this equation.

So, earlier what we did is for the output integration we need to know k minus 1 and k and we go to k plus 1. Here what instead we have to go the other way long. So, what we know is k plus 1 we know what is k and we need to find out is k minus 1. So, we need to rewrite my (Refer Time: 29:27) of algorithm in or the numeral equation in a certain way. So, this is my Numerov equation, which I have been using for my outward integration.

So, now what I will do it is, I will rewrite this in terms of yk minus 1. So, what I will do is, I will take this to the left hand side then bring this product to the right hand side and this to the left hand side. So, if I do that, so what I get is psi k minus 1 y k minus 1 this equals to psi k 12 minus 10 yk minus psi k plus 1 y k plus 1. So, therefore, my psi k minus 1 is equal to psi k into 12 minus 10 y k minus psi k plus 1 into y k plus 1 divided by y k minus 1.

So, this is how I will proceed, this is for my inward integration that is from x max to xc. This was for my outward integration that is 0 to xc. And these two are my initial condition for inward integration. So, note that for the initial conditions for the inward integration, we did not need to use the property of the parity of the wave function and so on and so forth.

Because the reason for that is we know that in this case the integration will always lie down to 0. Because for the regime outside where the particle is classically forbidden. There we always know that whatever be your problem the quantum mechanical problem for all bound potentials the wave function should always go to 0. So, this is more general in that sense.