Computational Physics
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Lecture – 37
Differential Equation for Quantum Mechanical Problems: Numerov Algorithm
Part 02

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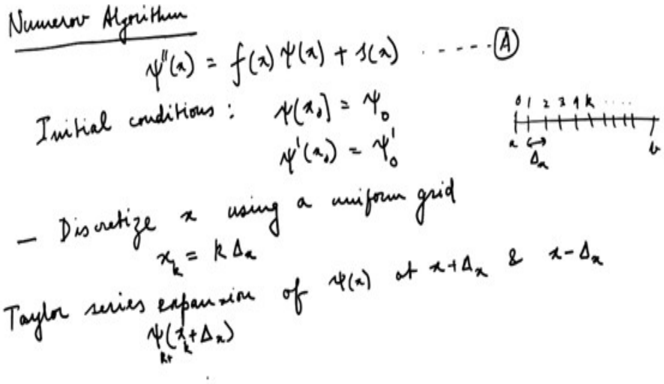

So, now what we will see is, we will look into the Numerov Algorithm. So, the Numerov algorithm is typically used to solve second order differential functions of this form, psi double prime x equals to f x psi x plus s x. So, this is one a general second order differential equation form, which is typically used by solving the Numerov algorithm. Now, since we are trying to solve a second order differential equation, so what we will be needing is two boundary conditions. So, let us put the two boundary(initial) conditions, we will be needing two initial conditions, sorry. So, my initial conditions are, so first of all psi at x 0 is equal to psi 0 and the first derivative of psi at x 0 is equal to psi prime 0.

So, this is what we had we want to solve and we want to solve it for a complete range of x. So, what we need to do is, we need to discretize x in using a uniform grid. So, the next step will be to discretize x and in this case we will be using a uniform grid. So, what I can do is, what it means is basically x at a point k at the k th point of my grid. So, suppose this is my integration range, say from a to b. So what I do is, I divide it into a certain number of grids. So, this is my 0, this is 1 2 3 4 this is k and then it goes on so on and so forth.

So, now x at k is given by my k delta x, where delta x is the width of this particular grid. So, in many physics problem and also in this type of mathematical problem, so what we you this type of trying to convert a mathematical problem to a numerical one, what we often use is the Taylor series expansion of my function and this is precisely what we are going to use again here. So, what we do is, we do Taylor series expansion of psi x at x plus delta x and x minus delta x. So, my psi x plus, so that is say at k plus 1 ok, let me just write it more carefully.

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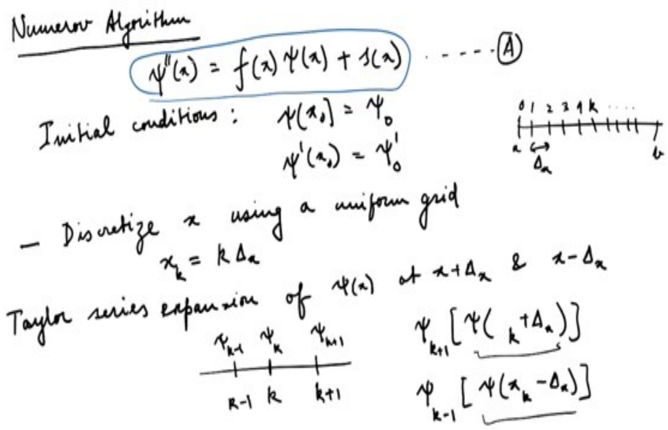

So, basically what I am doing is the idea is, this is my k, this is my k minus 1 and this is my k plus 1. So, I know the wave function here as psi k and this is psi k plus 1 and this is psi k minus 1. So, what I am going to do is, I am going to write psi k plus 1 as psi x k plus delta x and psi k minus 1 psi x k minus delta x and this stuff here this I will do a Taylor series expansion about x k. So, what I will get is the following thing.

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$$\psi(x_{k+1}) = \psi(x_k + \Delta_x) = \psi(x_k) + \sum_{n=1}^{\infty} \frac{(\Delta_x)^n}{n!} \psi^{(n)}(x_k) \quad \cdots\cdots (1)$$

n^{th} derivative of ψ

$$\psi(x_{k-1}) = \psi(x_k - \Delta_x) = \psi(x_k) + \sum_{n=1}^{\infty} (-1)^n \frac{(\Delta_x)^n}{n!} \psi^{(n)}(x_k) \quad \cdots (2)$$

(1) + (2)

$$\psi(x_{k+1}) + \psi(x_{k-1}) = 2\psi(x_k) + (\Delta_x)^2 \psi^{(2)}(x_k) + \frac{1}{12}(\Delta_x)^4 \psi^{(4)}(x_k) + O(\Delta_x)^6 \quad \cdots (3)$$

$$\underbrace{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}_{\delta^2 \psi(x_k)} = (\Delta_x)^2 \psi^{(2)}(x_k) + \frac{1}{12}(\Delta_x)^4 \psi^{(4)}(x_k) + O(\Delta_x)^6$$

So, my psi at x k plus 1 this is nothing, but psi at x k plus delta x, which is equal to psi k this notation I will come to later, this short form let me write it in the full form first, psi at x k plus this following series expansion then equals to 1 to infinity, delta x to the power n by n factorial psi n x k, this is my say call this as equation 1.

So, just note one thing that when I write in this fashion, this means the nth derivative and not psi to the power n. So, that I mean I just wanted to make it clear, so that there is no confusion later. In the similar way what we can do is, we can write psi at x k minus 1 that is psi at x k minus delta x this will be same except with slight changes, so the first term is psi x k and then we have under summation n equals to 1 to infinity. Now the additional term which we have is, minus 1 to the power n and then the rest are again same delta x to the power n by n factorial psi n x k, this is my equation 2.

Now what I will do is, I will add 1 and 2. So, I will add 1 plus 2, so what I will get is psi x k plus 1 plus psi x k minus 1, this will be equal to, so I will add this term plus this term so I will get 2 psi x k and then if I look into these terms, so the terms are same the only difference here is for odd values of n. So, for example, n equals to 1 this term in this second equation, this will be negative while the same term in the first equation will be positive, so it will be canceled out. So, what will be left are only the terms, so this will be true for all the odd values of n.

So, when I add up equation 1 and equation 2, the terms will get cancelled and we will be left only with the terms with even values of n and so, if I collect them, so what I will get is the following. So, what I will have is, the delta x square psi 2 x k, again remember here psi 2 is the second derivative of psi plus 1 by 12 delta x to the power 4 psi 4 x k plus order delta x to the power 6. So this, I call as equation 3. So, I am neglecting the(higher order terms), I am keeping till the fourth order term and I am neglecting the other terms in the expansion.

So, the next step what I will do is, I will pick this psi x and I will bring it to the left hand side. So, if I do that what I land up with is, psi x k plus 1 minus twice psi x k plus psi x k minus 1, this will be equal to delta x whole square psi second derivative of psi at x k plus 1 by 12 delta x to the power 4, fourth derivative of psi at x k plus some order delta x to the power 6 terms.

So, this is what you get and if you look at the expression in the left hand side; this part here so this reminds me of one thing, so this part is nothing, but my delta 2 psi of x k right, this is the central difference formula which we always use. So, using this, so what we can do is we can rewrite this equation in the following way.

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$$\delta^2 \psi(x_k) = \Delta_x^2 \psi^{(2)}(x_k) + \frac{1}{12}\Delta_x^4 \psi^{(4)}(x_k) + O(\Delta_x)^6 \quad \cdots\cdots (3)$$

Write $\psi^{(4)}(x_k)$ as central difference of $\psi^{(2)}(x_k)$

$$\psi^{(2)}(x_k+\Delta_x) = \psi^{(2)}(x_k) + \cancel{(\Delta_x)\psi^{(3)}(x_k)} + \frac{(\Delta_x)^2}{2}\psi^{(4)}(x_k) + \cdots$$

$$\psi^{(2)}(x_k-\Delta_x) = \psi^{2}(x_k) - \cancel{(\Delta_x)\psi^{(3)}(x_k)} + \frac{(\Delta_x)^2}{2}\psi^{(4)}(x_k) + \cdots$$

$$\psi^{(2)}(x_k+\Delta_x) + \psi^{(2)}(x_k-\Delta_x) = 2\psi^{(2)}(x_k) + (\Delta_x)^2\psi^{(4)}(x_k) + \cdots$$

$$\boxed{(\Delta_x)^2\psi^{(4)}(x_k) = \delta\,\psi^{(2)}(x_k)} \quad \cdots\cdots (4)$$

So, what we have is, on the left hand side of this of the equation in the previous slide, so what instead of having that three terms, we write it as psi x k this equals to delta x square psi 2 x k plus 1 by 12 delta x to the power 4 psi 4 x k plus order delta x to the power 6.

Now, if you look at these expressions, so what is unknown here is this thing, this term we do not know what is the fourth derivative of my wave function. So, to evaluate it what we will do is, we will again use the trick of the central difference. So, what we will do is, we will write this fourth derivative of x k as central difference of second derivative of x k. So, and once we, so how do we do that.

So, we do it in the following way, again we use the help of terror expansion. So, we write psi 2 x k at delta x plus delta x k, that is k plus 1 this we write as psi 2 x k plus delta x psi 3 and x k plus delta x square by 2 psi for at x k plus other higher order terms and similarly we write psi 2 at x k minus delta x, that is at k minus 1th point of my grid as psi 2 x k.

Now, the first term will be again a negative one, delta x psi 3 x k plus delta x by sorry, it will not be whole square, so delta x square by 2 psi 4 x k. Now if we add these two terms, so if we add these two equations. So, what we will get is, psi 2 x k plus delta x plus psi 2 x k minus delta x, this equals to twice, so we have one here and one here, twice psi 2 x k, these two terms cancels out if I add them plus and here I get again to twice the same term. So, what I will get is delta x square psi, fourth derivative of psi x k plus other higher order terms.

So, what we do as before, what we will be doing is next step will be, we can bring this down to this side and what we will have as a result is delta x square psi fourth derivative of psi k x k is given by delta 2 psi 2 x k. And what we will do next is, once we know this expression this term, this thing, so this we will plug into this particular equation and let us see what we get. So, I can what I can do is, I can call this as my equation 4 and this as my equation 3 prime.

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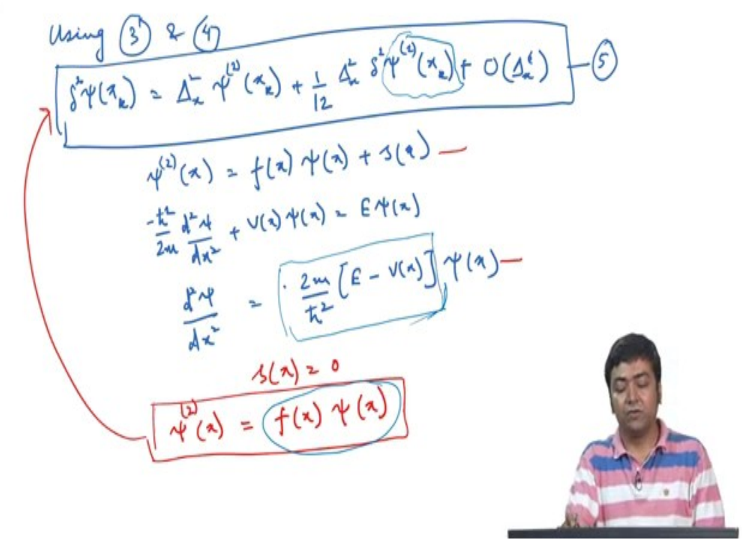

So, the next step will be, so using 3 prime and 4 what we get is the following thing. So, that is del 2 psi x k, this is equal to del x square psi second derivative of psi at x k plus 1 by 12 delta x square del 2 psi 2 x k plus my order del x to the power 6. So, this is what I get and I call this as equation 5.

Now if you go back and, so and just to recollect we started off with this, (which) is my differential equations, right. So, this is the differential equation which I am solving at present. So, this differential equation gives me the second derivative of psi x. So, we will use the fact here. So, coming back to here, what we have is as per the differential equation, my second derivative of x is given by f x psi x plus s x. But now we bring in a Schrodinger equation, a Schrodinger equation what we have is minus h square by twice m d 2 psi d x 2 plus v x psi x equals to E psi x.

So, once we and if we do some simplification what we will land up is, minus twice m by h cut square E minus v x psi x. So, now, if we compare this equation, this one and this one, so what we find is that my s x equals to 0 in case of the Schrodinger equation. So, for the rest part of the derivation of the numerical algorithm, what we will do is that, we will basically we will be looking for solution of this form, where my psi the second derivative of psi x is equal to f x psi x. So, this is the solution we are looking for, this is the differential equation which we are trying to solve and then we will use it here at this particular point.

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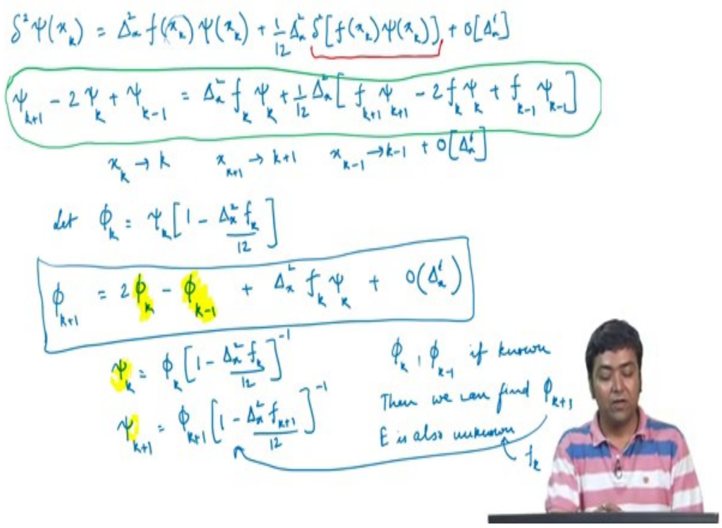

So, what we get is the following equation, del 2 psi at x k equals to grad del x square f at x k psi x k plus 1 by 12 del x square del 2 f at x k psi at x k plus order del x to the power 6. So, what I have done is, basically here instead of, so this psi 2 here I have, that is the second derivative of the psi, I have plucked in this value f x psi x which I get from the differential equation, which is my original differential equation.

So, once I do that, then what we get is the following. So, now psi k plus 1 minus twice psi k plus psi k minus 1, this is equal to now del x square f k. So, I am, now what I am doing is, I am now getting rid to make it simple, I am now getting rid of this dependence or the functional dependence on x k and I am just, so when I write f as a suffix k it means f is a function of x k at the gate point of my grid and then psi k plus 1 by 12 grad x square. So, here for this part, that is this one. So, for this part what I will do now is, I will use the second central difference formula for the second derivative.

So, this my, I am writing in this form, that is f of k plus 1 psi k plus 1 minus twice f of k psi k plus f of k minus 1 psi k minus 1, then I have this term also the order delta x to the power 6. So, just to write what I have done is, I have replaced in this equation x k as k, x k plus 1 as k plus 1 and x k minus 1 as k minus 1. So, this is what I did here, I have just shortened the summation, now let us try to simplify this still further. So, let us define another variable which is phi k as the product of psi k into 1 minus del x square f k by 12.

So, if I do that, what now this whole equation this particular equation, the equation which I am marking with this green line, so this equation I will rewrite this equation in terms of phi k. So, what I will have is, if I am not doing the detailed algebra, I am just writing the final result, so what I will have is phi k plus 1 equals to twice phi k minus phi k minus 1 plus del x square f k psi k plus order del x to the power 6. So, using this where in this, we can get psi k equals to phi k into 1 minus grad x square f k by 12 to the power minus 1. And similarly where psi k plus 1 what I have done is I replaced it by phi k plus 1 1 minus grad x square f k plus 1 by 12 to the power minus 1.

So this is my equation. So, what this equation tells me is that, if I know the value of phi k, if phi k and phi k minus 1 if known, then we can find phi k plus 1 and once we know phi k plus 1, then by putting it in this equation in this one, we can find psi k plus 1 also. So, this method, it is our; it is a very elegant method and it is also much more elegant than the Runge Kutta method, which you have learnt about earlier.

So, once we get this, so what is also known unknown is our E is also unknown. If you remember as I was talking earlier, so not only the wave function is unknown in this equation, the E is also unknown and this is involved through the f k function. So, this is my f k function just for your reminder. So, this is the f k function. So, the E enters to the equations through this particular f k function.

So, now we will, this is how the Numerov algorithm is derived and basically, since it is a second order differential equation as you can see from the equation itself, it depends on two starting initial conditions. So, we need to know phi k and we need to know phi k minus 1; these are the two things we need to know to find out the equation that the next value of the wave function phi or in terms of wave function we need to know psi k and psi k minus 1. So, this one and this, and similarly psi k minus 1 also and then we can from there we can find psi k plus 1.