Computational Physics

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Lecture – 38
Differential Equation for Quantum Mechanical Problems: Numerov Algorithm
Part 03

So, now, what we will do is, we will take an example.

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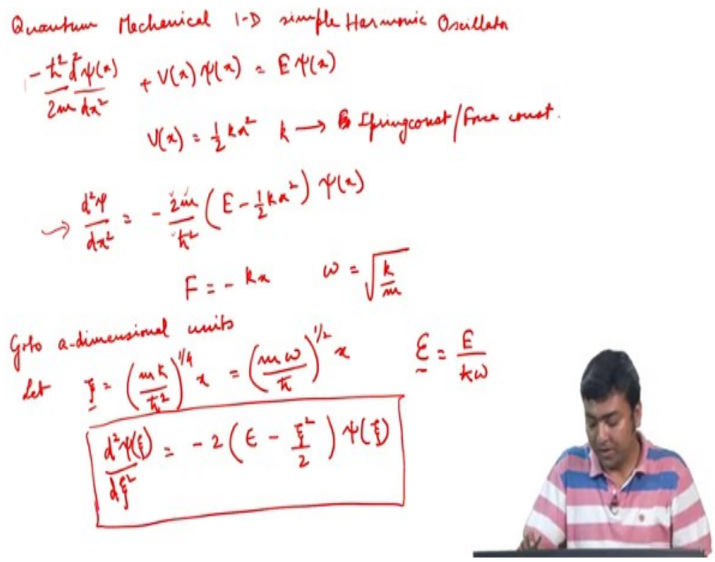

So, the example that we are going to take will be the quantum mechanical one-dimensional harmonic oscillator, simple harmonic oscillator. So, for this, the reason I have chosen this system is because for this particular case, one knows the; one can solve the equations and then one can find out the eigenvalues and the eigenfunctions analytically also.

So, just as a reminder, so in this case your Schrodinger equation will look like this. So, minus h cut square by twice m, d 2 dx 2 psi x plus V x psi x equals to E psi x. So, here my V x in this case is equal to half k x square. So, where k x square is the, k is the spring constant, it is also called the force constant.

So, if we shift this part and this part on to the right hand side of my equation. So, what I will end up with is the following d 2 psi dx 2 is equal to minus twice m by h cut square, E minus half k x square psi x. And we know that, for case of a harmonic, I mean a system exhibits harmonic motion with simple harmonic motion when it has a restoring force. So, basically if force will be equal to minus k x and the frequency with which it oscillates that is given by root over k by m. Now, when trying to do the Numerov algorithm, so what we will not carry on along all these different variables. So what we will do is, we will do some transformation.

So, we will go to a dimensional system or a dimensional units. To achieve that the transformation which we define some new variables; so the first one is zeta which is equal to m k by h cut square to the power one by fourth x and if I plug in the value of k here, so what I will get is m omega by h cut to the power half x.

And we also define epsilon, which is equal to E by h cut omega so, this is my unit of energy which is epsilon and so, if I plug in this zeta and epsilon into this particular equation here. So, this equation gets modified in the following way in terms of zeta and epsilon. So, my Schrodinger equation now becomes d 2 psi d zeta 2 equals to minus 2 epsilon minus zeta square by 2, psi zeta. So, unlike x, psi is now a function of zeta. So, this is what we are going to solve numerically using the Numerov method.

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Define $f_k = -2\left(\epsilon - \frac{\zeta^2}{2}\right)$

$$\psi_{k+1} - 2\psi_k + \psi_{k-1} = \Delta_x^2 f_k \psi_k + \frac{1}{12}\Delta_x^2\left[f_{k+1}\psi_{k+1} - 2f_k\psi_k + f_{k-1}\psi_{k-1}\right] + \cdots$$

$$\Rightarrow \psi_{k+1}\left[1 - \frac{\Delta_x^2}{12} f_{k+1}\right] = 2\psi_k + \Delta_x^2 f_k \psi_k - \frac{1}{6}\Delta_x^2 f_k \psi_k - \psi_{k-1}\left[1 - \frac{\Delta_x^2}{12} f_{k-1}\right]$$

Let $y_k = \left[1 - \frac{\Delta_x^2}{12} f_k\right]$ $\Rightarrow f_k = \frac{12 - 12y_k}{\Delta_x^2}$

$$\psi_{k+1} y_{k+1} = \cancel{2\psi_k}\ \psi_k\left[2 + \frac{5}{6}\Delta_x^2 \cdot \frac{12 - 12y_k}{\Delta_x^2}\right] - \psi_{k-1} y_{k-1}$$

$$= \psi_k\left[12 - 10y_k\right] - \psi_{k-1} y_{k-1}$$

$$\boxed{\psi_{k+1} = \frac{\psi_k\left[12 - 10y_k\right] - \psi_{k-1} y_{k-1}}{y_{k+1}}}$$

So, as before what we do is, we now define my f k as equal to minus twice epsilon minus zeta square by 2. And then, we use the Numerov step. So, what we do is now, we have now psi k plus 1 minus twice psi k plus psi k minus 1, this is equal to del x square f k psi k plus 1 by 12 del x square f k plus 1 psi k plus 1 minus twice f k psi k plus f k minus 1 psi k minus 1. And then, I am then I have the sixth order terms which I am not writing down explicitly.

So, now, what I am interested to know is psi k plus 1. So, what I will do is, I will club all the terms in containing psi k plus 1 on the right hand side equation and bring it to the left hand side. And if I do the algebra what I will get is, psi keep this equation above equation I can rewrite in the following form, psi k plus 1 into 1 into grad x square by 12 f k plus 1 equals to twice psi k plus grad x square f k psi k minus 1 by 6 grad x square f k psi k minus psi k minus 1 into 1 minus grad x square by 12 f k minus 1.

So, just to simplify the notations further what we will do is the following. So, what we will assume is that, we will define another variable which we call as y k and we will choose y k equals to 1 minus grad x square by 12 f k. So, if I choose this variable then I can rewrite my f k in terms of y k which becomes 12 minus 12 f k, equals to 12 minus 12 y k by grad x square.

So, I will plug in this new y k and f k in terms of y k in this equation. And what I will get is the following. So, I get psi k plus 1, now this term here in this equation is nothing but my y k. So, or in this case it is y k plus 1 so, psi k plus 1 y k plus 1, that is my left hand side. This equals to twice psi k.

So, now here what I will do is I will club this psi k terms together. So, what I will club this psi k terms together and including this one here and I will put in the value of f k. So, what I will get is psi k into 2 plus 5 by 6 grad x square and f k is 12 minus 12 y k by del x square minus psi k minus 1 y k minus 1. And if I do some algebra, so these two cancels out and this 6, I can cancel out into 2. So, what I will get is, the right hand side becomes psi k into 12 minus 10; so 5 into 2 10 plus 2 12 and then 5 minor into 2 10 y k, this minus psi k minus 1 y k minus 1.

So, therefore, the value of the wave function at the k plus 1th grid is given by, psi k plus 1 equals 2 psi k 12 minus 10 y k minus psi k minus 1 y k minus 1 by y k plus 1. So, this is the expression which I will be using when I will be doing the Numerov algorithm. So, this is what the Numerov algorithm part is and this is how it goes, so this, so as again as I said before, it is a second order differential equation to solve. So, I will be; I need to... in order to find out the wave function at psi k plus 1, I need to know the wave function at psi k and at psi k minus 1.

So, this goes in; so, this part basically what it did is, it has discretized your system and has given you a way to get numerically get the solution. Now, so far, I mean this is common for whether when you try to solve this type of a differential equation, whether it is for a classical system or it is for a quantum system.

Now, as I mentioned before for the quantum system there are two more things to do. So, we do not know what is the energy eigenvalue, we need to decide the energy and we need to decide asymptotic, the values of my wave functions at the asymptotic limit correct. So, how do we incorporate that?

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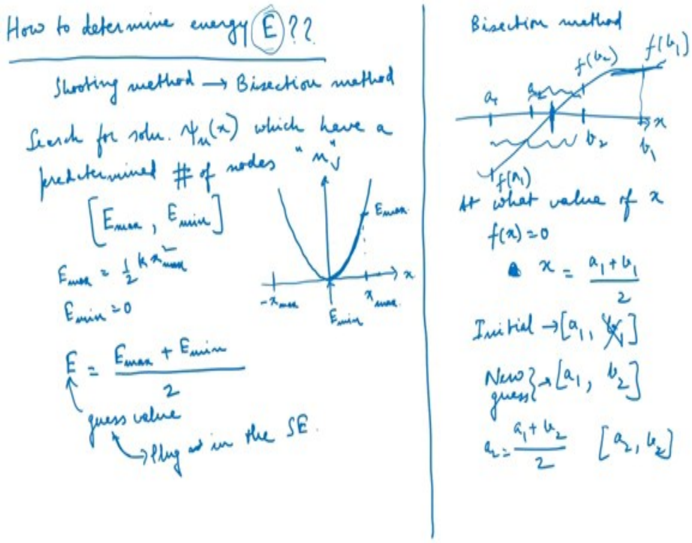

So, first question which we try to answer now is how to determine energy. So, this is done by using something called the shooting method, I will explain what it is. So, this is analogous to the bisection method which some of you may be familiar with, but I will just quickly recap what is done in the bisection method.

So, that it will be very easy to translate the same idea in that will be using to determine the value of E. So, in bisection method what you have is, suppose this is my x axis and I have some function which goes like this. So, basically what I want to find out is the root of the function. That is at what value of x. So, this is a slightly detour so, this is my bisection method. So the question I ask is at what value of x, f x is equal to 0.

So, what is typically done is, you start at from two points say you start from a 1 and you start from say this function goes something like this and you start from another point b 1. So, you note here that your choice of a 1 and b 1 should be such that it brackets the root. And so, what does it mean by bracketing the root? Bracketing the root ones means is that, the sign of the function at a 1 and that is the sign of the value of the function that is f at a 1 and f at b 2 at b 1. These two should be of opposite sign, then only it tells me that, I have somewhere upon a value of x for which the function can be 0.

So, once I choose this start initial guess is a 1 and b 1, what I do is I find a new guess and new value of x which is the midpoint of a 1 and b 1, a 1 plus b 2. Now let us suppose for this case, this is my midpoint so b 2. Then what I do is, I compute the value of the function there f b 2. And then what I do is, I compute the product of f a 1 and f b 2 and f b 2 and f b 1.

So, and what I check is whether which case the product is gives me and returns me a negative value. So, if suppose in this case the product in for this particular case in this schematic diagram, the product of f a 1 and f b 2 will determine my negative value. So, initial guess was a 1 and b 1. So, now, I know that this is the interval within which my function, the root of my function lie so, this upper limit what I do is I replace b 1 with b 2.

So, my new guess is a 1 and b 2. Then what I do is, I again do the bisection method and I find out the midpoint of a 1 and b 2 as the new guess of the root and it comes somewhere here suppose, say I which I call it as a 2. And in this case I see that the interval using the same logic by taking the product of the functions of f a 1 and f a 2 and f a 2 and f b 2, I see that my new interval is this one; that is between a 2 and b 2.

And I keep on repeating doing, I do this repeatedly till I reach I hit this point as the midpoint. So, this is the basic idea of the bisection method and what we are going to do is, we are going to use this same idea to determine the value of the energy E. So, the aim is to search for solutions of psi n which have a predetermined number of nodes. Let us call this number of nodes as n, ok. So, what we do is, we start take initial guess say we take E max and E min as my value. Again, we have to ensure that the E max and E min should lie it should contain the correct eigenvalue E here.

Now, for the particular case, if I look at it, so this is my harmonic potential. So, this is my v and this is my x. So, and suppose I want to do the integration from minus x, this is it is symmetric I am calling both side as minus x max to plus x max. So, I know that a proper choice of E max and E min will be, my initial guess of E max you can put E min I can put here. Because that is the lowest value of the potential and the initial guess of E min, E max I can put here because I know that my energy eigenvalues will lie between this range. So, that ensures me that there by choosing E max and E min.

So, basically my E max to choose will be half k x max square and my E min I will choose to be 0, because my eigenvalue will definitely lie between these two points. So, once I have chosen this. So, as the first case what I do is I compute the, I choose the my energy the first case of my energy as the midpoint of E max and E min.

So, now I know the value of the energy E; so, this is my guess, this is my guess value. So, this guess value, I what I do is I plug it in the Schrodinger equation for my simple harmonic oscillator and then I solve it.

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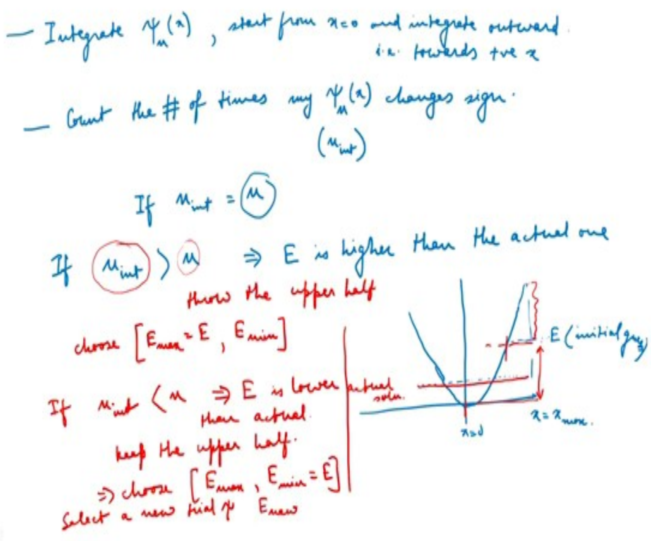

So, what I do is the next step is I integrate psi n at x so, I start from x equals to 0 and integrate outwards, that is towards positive x. So, in while doing this integration I need to do another thing, I also count the number of times my wave function that is psi n x changes sign. Let us, say that this number I am calling it as n int. Now if my n int is equal to n, which is my desired solution with n number of nodes, then I would say that my energy eigenvalue is correct and this is my correct solution.

But more, but this may often and in for all practical purposes you will not get this condition in your very first guess. So, what I need to do. So, it will be so, your n int will be either greater than or either less than the desired number of nodes. So, in that case what I do. So, if my n int is greater than n what it tells me is that, my E which is the guess eigenvalue, this is higher than the actual one.

So, just to remind you, so this is my potential, ok suppose, I am looking for the ground state which is the solution is here. Now I started off from here, so this is my x equals to 0 and this is my x equals to x max. So, half of this is somewhere here. So, this will be my E which is my initial guess. Maybe the actual solution I draw with a different coloured line. So, this is my actual solution, ok.

So, if you remember the other solutions. So, as you go from n equals to 0 to n equals to 1 to n equals to 2. So, what happens is you have more and the number of nodes increases. So, higher the value of the energy is for a solution, more the number of nodes is; so, hence if the number of times the wave function changes sign is greater than the desired number of nodes, that definitely tells me that my energy is higher.

So, what I will I know from this part is that I can neglect this part of my guess. So, my new bounds will now be between this and so, no we are looking for the energy scale, so I neglect this part. So, my new bound will be between this and this. So, this is my new bound, ok. So, what I do is if E is higher than actual one, so throw the upper half and that what that means is, choose my E max is equal to E and the E min changes.

Similarly, if my n int is less than n, so this tells me that my guess energy is low. So, in this case what we do is, we keep the upper half and throw away the lower half. So, what it means is choose so, my E max remains same, but my E min I now replace with the new guess. So, basically the energy window is reducing. So, and once we do this then we get another new trial wave function. So, basically select a new trial psi using this new value, using the new guess of energy.

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- Repeat these steps till
$|E_{max} - E_{min}| < eps \sim 10^{-8}$
convergence criteria.

For -ve x $\Rightarrow \psi_n(-x) = (-1)^n \psi(x)$

If this doesn't apply then one needs to perform the integ. over the whole range.

So, this repeat these steps till the difference between E max and E min is less than some numerical value, a very small numerical value till the mod of the difference between E max and E min is less than some very small numbers; so epsilon typically of the order of 10 to the power minus 8.

So, once it is done, then we get say my solutions have converged. So, this defines the convergence criteria. So, I say my solutions are converged and then the corresponding psi gives me the wave function and the corresponding value of E gives me the energy, eigenvalue. So, now, this goes further. So far, we have integrated from 0 to the positive x. Now, what about the 0 to minus x, the negative x; so in this particular case for this particular example of a simple harmonic oscillator, we do not need to explicitly calculate that. Because what we will do is we will use the property that my wave function sorry my potential is a symmetric potential and what we will do is, we will use the parity operator.

So, for negative x, my wave function psi n at minus x, this becomes minus 1 to the power n psi x. So, if my n is an even number that is say 1 2, sorry 0 2 then I will get a symmetric wave function and if n is odd number then I will get a anti symmetric wave function. If that case is not valid, if this does not apply then one needs to perform the integration over the whole range.

So, this is how one determines E, but then we are still left with one more thing we need to find out, need to know also to start the integrations. So, we need to know what the initial conditions are.

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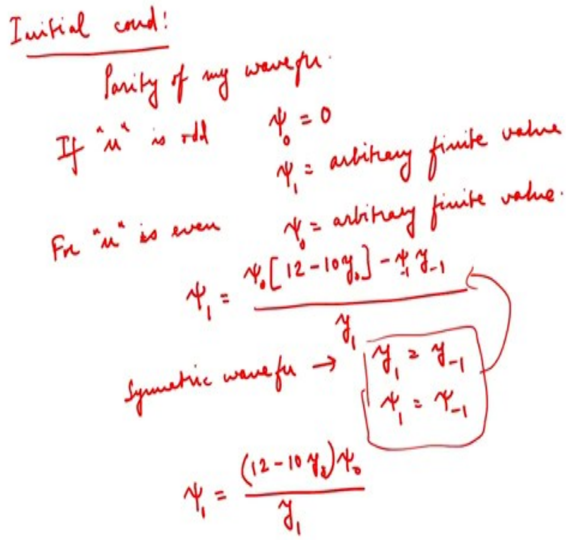

So, now we will decide what my initial conditions are and to decide that or to start with the initial condition what we will use is the parity of my wave function. So, if my n is odd; so, what I know is that, is it has to be antisymmetric and for the function to be antisymmetric in this particular case, it has to go through 0 at the origin. So, what that implies is my psi 0 is equal to 0 and then for my psi 1, I add some arbitrary finite value. On the other hand, for n is even, we know that at psi 0, the wave function has some arbitrary finite value. It would always be nonzero at psi 0, ok.

And, psi 1; so to obtain psi 1, we use the Numerov thing, that is psi 0 12 minus 10, y 0 minus psi 1. This will be psi minus 1, y minus 1 by y 1. Now, we know that for the even fun for even values of n my wave function is symmetric; so what, so for symmetric wave function, what we have, is y at 1 is equal to y at minus 1 and psi at 1 equals to psi at minus 1.

So, if we use these conditions in this equation so, what we will get as the initial guess, the second initial condition psi 1 we will get as 12 minus 10 y 0 psi 0 by y 1. So, this is , how I initialize the wave function.