Computational Science and Engineering using Python
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Lecture – 13
Gaussian Quadrature Continued

So, Gaussian quadrature is what I was working out. So, these are method to integrate. So, we did one method call Newton codes. So, given n points in fact, they were equispaced point and we get quite accurate result and the order error was either s to power n and or n plus 1 and we divided that part like.

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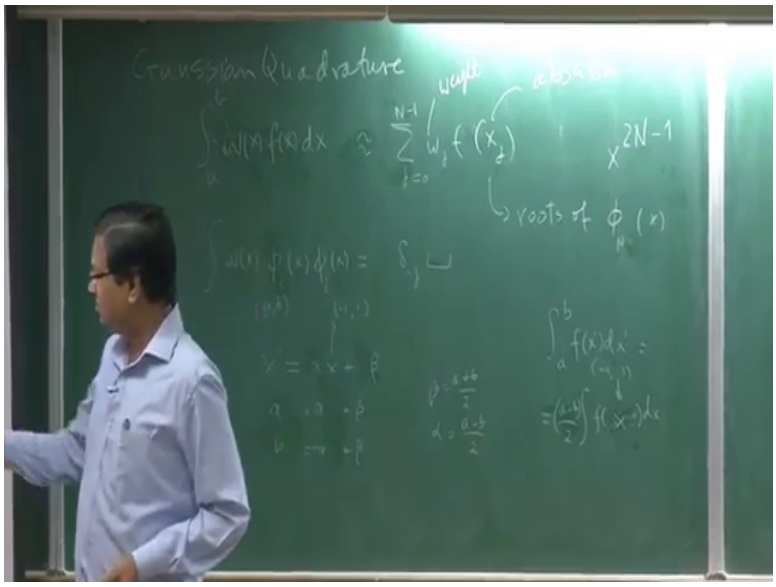

So, examples were trapezoid rule Simpson rule. So, that exercise has been done. So, these are another one which is more accurate. So, if you recall. So, we have integral. So, how did we do it f x d x a to b, I think specify what is a and b that comes from the choice of your polynomial. So, we expand this you know. So, sorry I had to w x f x it will become clear today y w x is important. So, this is approximate of course, j w j f x j.

So, you have to choose points the abscesses and this call weight. So, we choose your abscesses properly then you can get a very good answer. So, if I have n points 0 to N minus 1 in this scheme you can get agreed up to polynomial which is ordered highest power is 2 N minus 1. So, suppose I want to integrate something which is good for cubic

polynomial a x cube x squared x and 1 then how many points you are need an another number of points another number of point i just need to.

So, you see power of this algorithm. So, for this is the standard integration routine which is used in practice we do not use Newton codes in general I mean if you look at the pythons spring will Gaussian quadrature is available. So, I show you how to use it in python. So, what are exists? Exists a roots of which polynomial. So, I expand in terms of polynomials and the polynomials follow this property l x l j of (Refer Time: 02:54) than this phi i use phi, phi i x phi j of x they are also own performance. So, delta i j and need not be there could be a factor. So, this is the factor here need not be 1.

So, depends on the polynomial and w x is not equal to 1 necessary I am sometime it is 1 only generate it is 1, but it need not be all right. So, you choose this polynomials and x j's are roots of which polynomial phi n plus 1. So, this will I n roots. So, I will I will just do some exercise. In fact, we did that for Legendre polynomial sorry let us see I have those nodes let us start looking at those your nodes. So, these are Legendre polynomials.

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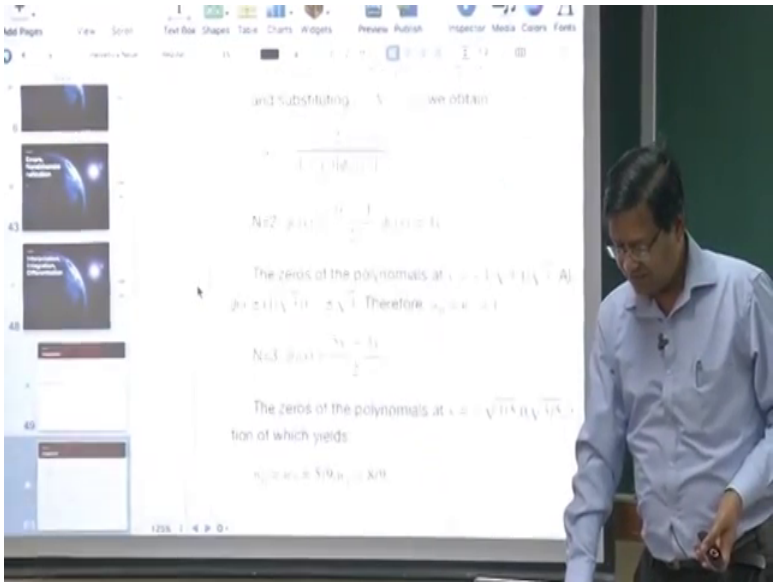

So phi naught, so this is same as what do you get for hydrogen atom spherical harmonics when I will theta part is given by Legendre. So, this is the first 1 0 phi 0 phi 1 phi 2 phi 3 and phi 2 has 2 roots. So, in the third polynomial according to this notation it will be phi n according to this notation. So, let us put follow the same notation. So, phi n has n roots, but I am starting my this indices from 0.

So, it should be clear that this is expansion is done 2 phi n minus 1 in this notation and the root is of the phi n. So, how do this look like? I just, there is a weight of plot them. So, this is there is a function there is a package called spatial. So, using the spatial package which I will just put it share with you. So, using that, it will give you phi of x you do not know need to remember them I mean it is part of python. So, these are the Legendre polynomials I did not plot phi 1 a phi naught, phi naught will be constant this phi 1 phi 2 is this x square minus 1 phi 3 is which one, this 1. So, there are quite a few of them and it is defined from minus 1 to 1. So, cos theta is 0 to cos theta equal to phi.

So, it has vey I mean it has interesting properties using which you can define we can get the weight straight from the function. So, this is the formula for. So, these are comes after bit of algebra. So, these are, weight function can be computed if I have the derivative of phi n at the roots. So, this is the formula, but what is given is table.

So, you do not really need you do not need to calculate first time some bodies done the all the lot of work and you can use this table. So, the table for n equal to 2, so I want accurate up to x squared x cube sorry x cube then I should choose n equal to 2 and here the roots are, so these are abscissas roots are plus minus this number and the weight is 1 this I did not last class, but I am just revising it. So, for if you want 3 abscissas. So, these are 3 roots plus minus will that 2 of them and the weights are given here. So, here I have to multiply appropriate weight with f x j we should pair it appropriately I mean you cannot simply multiply this root with the value of the function here.

So, this table you should know how to use it and you do need to go back and derive from the first principle the weight weight some bodies computed already. So, we can get up to phi. So, these are phi roots phi weights because there are well basically for these 2 values the weights are equal it is the symmetry plus minus symmetry. So, this is good up to which polynomial, so which polynomial. So, I am choosing n equal to phi. So, up to x 1 9, these are the good up to x 4 9. So, it is says very good I mean. So, any polynomial of the x 9 is it works.

So, let us compute a do an example. So, the code I will show you in a minute. So, x squared again get exact value 2 third of course, computed wont write 2 third sink by would write to third, but not numerical python. So, it gives you number which is two-third numerical number for two-third and is exact for n equal to 2. So, for less compute e

to power x. So, let us just do that. So, let us just there is a small code, all right. So, we have to see this with carefully.

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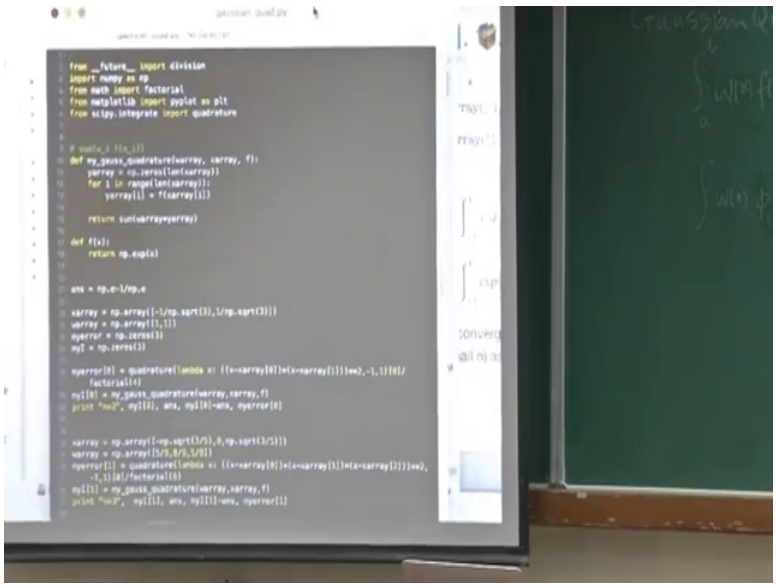

So, something which I probably did not if you said so much, but these are good line to write from feature import division, 2 by 3 will be 0.666 with this otherwise 2 with 3 will give you 0.

So, this is something which I add it that now we have to taking e to the power x and I will take the range from minus 1 to 1. So, that is natural for Legendre for I of course, change it change marine. So, how to change the range? So, let us take a small d 2 if I want to do the integral from a to b using Legendre only general is defining only from minus 1 to n. So, I make a change the variable. So, I will make a change the variable x prime you will a x plus b. So, I will demand that when x is equal to a let us not a to b a b is already define alpha beta. So, when x is equal to a I get x prime as minus 1. So, x is equal to a gives you minus 1 and x is equal to k z 1. So, I can computer alpha and beta easily. So, if I compute also. So, what is alpha beta? So, let us. So, if I just add. So, that is correct. So, so you can compute this number no means did I do this I think I have probably let us let us just do it here my notation is slightly different in the nodes by change the notation. So, I am choosing x prime. So, I have just. So, let us follow my nodes. So, x prime you see here. So, x prime is minus 1, so x prime is equal to minus 1.

So, when x is equal to a so. In fact, is same and x prime is 1 in this. So, alpha beta will come out to be that alpha and beta alpha beta.

So, my interested to compute this object x prime no which will I am making a slight error know. So, x prime I think this is this beta from problem I believe. So, let us just this should be x prime is this is no, no this is I have written it wrongly here is written wrongly here, so x prime. So, this is written wrong, so this is exactly same as (Refer Time: 11:50). So, x is variable goes from minus 1 to 1 and this goes from a to b this type incorrectly. So, now, I can easily solve for alpha and beta.

So, beta is a plus b by 2 and alpha is a minus b by 2. So, what is integral? Integral a to b f x prime this is what I am want. So, this will be equal to. So, I have to replace d x prime by alpha d x that is a Jacobean. So, this is alpha d x alpha is here a minus b by 2 and this is f x, so x prime. So, I have to compute at x prime which is going to be alpha x (Refer Time: 13:00) beta, but if you computed those corresponding values, but x will be going from. So, this will be lying between, so this will be from minus 1 to 1. So, where I mean you have to you have to map it, you have to map it appropriately here, so we can always do it for any interval, but l s focus write down on minus 1 to 1 for e to the power x.

So, this is the code. So, my function is written here. So, I am going to use that function and I will define what it w array and x array. So, w array is the weight and x array is the abscesses array of abscesses, you straight forward. So, I compute y which is this function as for. So, first set it is to 0 with size number of abscesses and I compute y r a is f of x I and then sum it up. So, this is going to give me the integral. So, that is the answer. So, for this my real answer which is from exact answer is e minus 1 by e right integral of e to the power x is ok.

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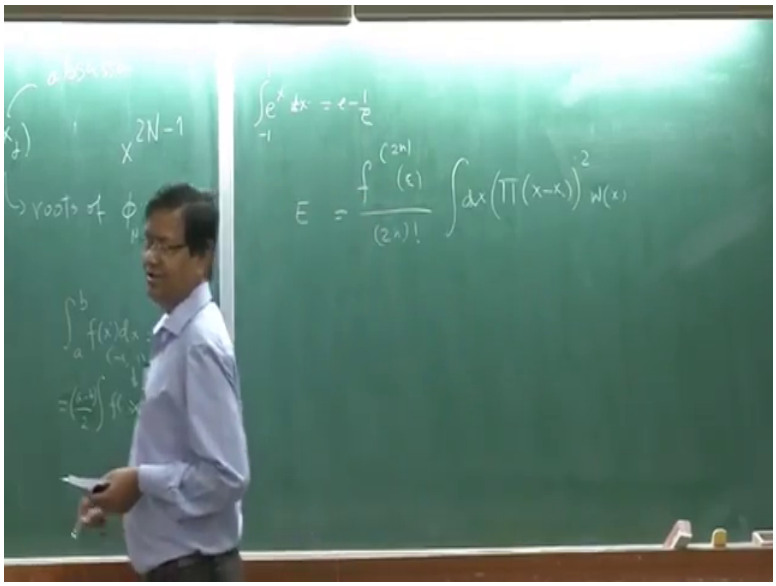

So, now I choose buying weights. So, with 2 points I am putting my exact values minus 1 by root 3 and 1 by root 3 these are abscesses and our weights are 1 1 so, I also created array called my error which has 3 values and my integral. So, I is going on become clear. So, I am go do for n equal to 2 n equal to 3 and n equal to 4. So, I am going to compute with 3 different points theta set up points is a clear. So, n equal to 2 n equal to 3 and n equal to 4, number of points. So, that is why I have created my error with 3 entries. So, you just look at this line my. So, my answer is my quadrature w array and x array and f, weight x array and f. So, this is my answer.

So, how much is the error? So, 1 error is my I minus answer, but I want to an estimate also from the formula I did not write the error estimate. So, error estimate formula if you yeah I am sure you do not remembers I 2 n zeta. So, w x I need a integral of this, so this product. So, this is the error, but it will. So, zeta I do not know. So, I can get only a bound. So, what I am I compute here is this is order 1 right exponential e to the power the derivative of exponential is same. So, this is bound with well it is bounded from. So, we have compute this object.

So, this is a nice feature for python. So, I need to for quadrature this is the formula, this is the function quadrature. So, quadrature requires arguments which are, actually if you my see this here. So, quadrature this is this function, function and the limits. So, lower limit and upper limit. So, these going to give you the answer of course, it reduces goes in

quadrature. So, I do not know what n is it using it will choose appropriately, but I mean it told it is if you look at the literature it will tell you what I (Refer Time: 17:47) using and so on, but I am not worried about it, it gives me a good answer. But suppose, so f is defined for me is e to the power x, but I say well I do not know really defined somewhere else, but I want to just use it in line in the function itself.

So, the idea is called lambda function. So, this is useful construct. So, from here from here till here, here to here is the function definition and these are the limits minus 1 to 1 and the answer is in 0. So, quadrature gives you. So, the first one is the answer second 1 gives you the error and so on it gives you more values. So, what is lambda function? So, I do not know need to get f function entered here otherwise I have to write this function all these guys I have to write like this. So, it will do in short. So, it is written here x minus x 0 x minus x 1 square. So, is that clear what it is doing is integrating quadrature is integrating is integrating pi x minus x 0 x minus x 1 whole square.

So, this line which is a very compact line this part of the line is doing this integral. So, I did not need to define the function f otherwise I have to define another something like here def f prime will be this function. So, lambda function is useful. So, I just want to tell you that you really do not know define I need to do carry this function know I mean I right now is part of the line itself. I have to define divided by factorial 2 n. So, n is 2, so factorial 4. So, this is this object without this. So, it gives a bound it does not really give the error because zeta I do not know, but it gives you some kind of bound.

So, I also print that. So, this is for n equal to 2 is that clear to everyone. So, the few lines it does it. If I want n equal to 3 then I to give you 3 abscesses and 3 abscesses are here minus square root 3 by phi 0 or square root 3 by phi and these are the weights 3 weight. So, this is from the table has number values, but this I know I computed them. So, I know this values and again quadrature error will be, but it is x minus x 0 x 1 x 1 x 1 is x 2. So, it has one more factor there is one more factor whether 3 points and my Gaussian quadrature value is here my I 1. So, I print again n for n equal to 3. Now, n equal to 4 now I put the numerical values not this is from the internet the problem with my table is I do not put that many digits. So, these has some 15 digits. So, double precision, yes accurate is possible and you will find this from the net.

So, but you can use my table as well I mean that is there will give you reasonably good answer. So, this is a abscesses these are weights and I do the same thing. So, I get 3 answers and 3 errors. So, let us plot them. So, we can plot them. So, it turns out, so if I just plot them, but I does some more work. So, let us plot it first, but this, this what we got are this is the 3 lines my answer is here well the correct answer is probably this one my error is here and so, these are some from that column.

So, my answer, so we can just check which one is the answer fine. So, I have plot the error now error looks like this, for different n 2 3 4.

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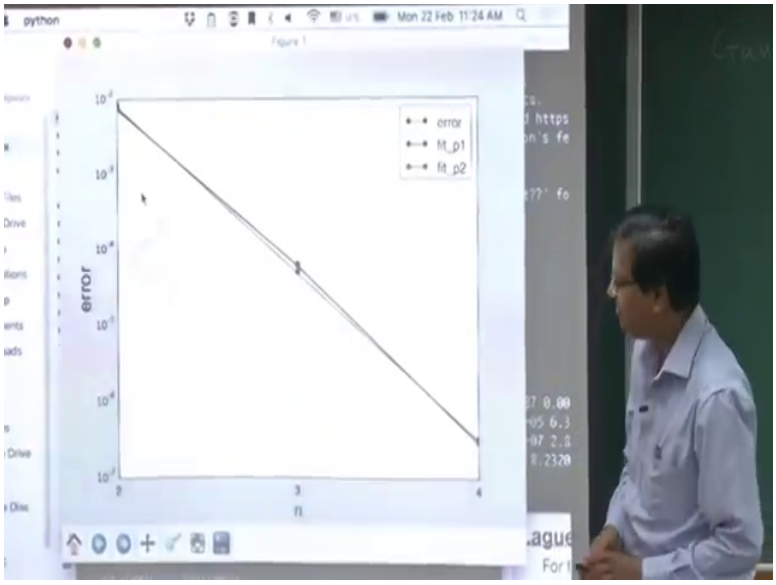

Now I have plotted it works k, what plot? Is a semi log plot; so this is linear and this is log. Why did a full plot semi log? If you do not plot semi log then it looks it falls like that I am no do it just from the same time, but similar it looks linear right. So, I want linearism you get this one very important point I hope it is a (Refer Time: 23:29) some class human beings are very good at identifying linear this is somehow it is in our psychology, non linear physics from we cannot solve non-linear equations we have with lot of difficulty when linear you can see a line is a is linear. So, linear is very easy to identify had it been line which is going down. So, if the line was going down.

Like this you know it is a power law or it is exponential is says it is just not easy to identify or is 1 over x square 1 over x cube, but it is straight line it is straight line easy to

identity. So, always go for a straight line. So, this looks like a straight line, but I want to fit is a really straight line or is it is there some correction to the straight line.

So, python has a very nice function called poly fit. So, polynomial fits. So, what should I poly fit. So, n is 1 access 1 variable. So, fit you know, you must have done this linear regression right y equal to a x plus b given data x i is y i's you can you can linear effect. So, python does that within the scene. So, we do not have to time to get that part, but less I am assume that I have set of x i's and set of y i's. So, I have 3 points and I want to fit a line with that. With 3 points I can do best is quadratic nothing beyond it, with 2 points you can fit a line and with 3 points you can you can have 1 more variable. So, I would try both y equal to a x plus b. So, it is written like this p is p 0 x plus p 1. So, this is my polynomial.

So, 0 will be with the highest power or the second one will be p 0 x squared plus p 1 x plus p 2 I cannot fit any because I have 3 unknowns and I have only 3 points. So, best I could do is this I am mean I assume to any other higher polynomials you have more points and your choice. So, python will has a function no need to worry right now how it is obtained, but if you want to read you can read the literature. So, so it is a poly fit, but I want to in log scale. So, I create a log my error log of my error. So, this is my y coordinate x coordinate is the x n. So, I am fitting log of y with n and I expect it will be linear.

So, first is with one point with the first order polynomial. So, that will be this highest power. So, it tells you the highest power this is one means highest power this is with power 2. So, that is why its power 2 this exactly same as y what I wrote there is that clear yes. So, poly fit will give you quadratic equation here in terms of n and linear equation here. So, I fit both of them this is trivial plot function. So, that 2 lines here as the 2 lines here. So, poly fit p 1 is the red line and poly fit 2 which is quadratic really divides vary by small amount which goes through of course, this point is a green line.

So, red is as good. So, linear is a very good approximation. So, what can I claim I am not do any mathematical theory, but I can say that error decreases by how much in this scheme error decreases exponentially. So, these are log log plot, so I can claim from here that my error function is e to the power n can I claim it alpha. So, since it is a I (Refer Time: 27:43) it is exponential so my function is e to the power minus alpha n. And what

is alpha? Alpha is, so I can get what is alpha. So, I just a p p 1 I think. So, p 1 is minus. So, first 1 is p 0 is the slope. So, p 0 is minus 5 p 1 also will be p 2 also will be similar p 2 is my variable I stored them, so minus 3.16

So, this is the linear, linear coefficient of linear plot. So, I cannot really put my I mean I want bit on this number minus 5, but is linear we minus 3 minus 4. So, I can claim definitely that error goes down linearly. So, this is about Legendre polynomial. So, I can use Legendre polynomials to do Gaussian quadrature. If I want from not minus 1 to 1, but some other some other points then I use this scheme to get my answer. I have to compute this function it the scale values ok.

Now, this is about a Legendre polynomial, but we can do more. So, let us just use the slide only I mean I am no write this functions.

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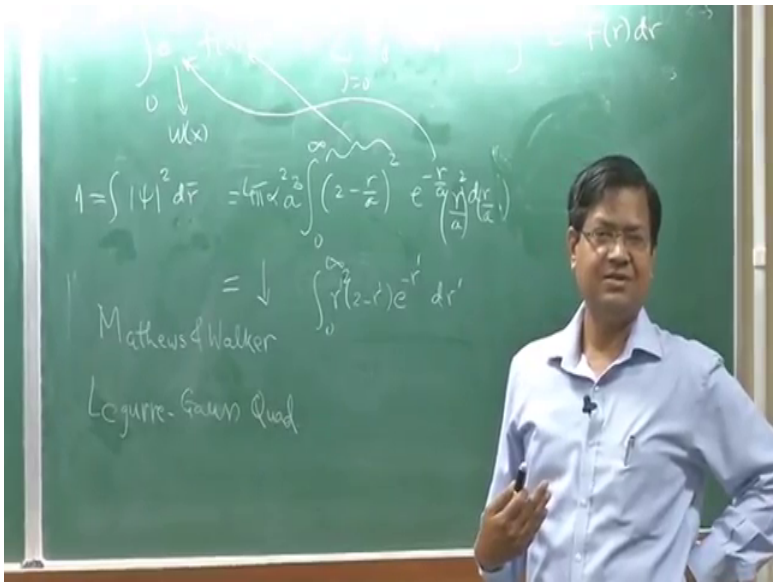

So, we encounter this can have integrals now I want to integrate this integral. So, of course, is no idea no good idea to use a Legendre for this because infinity is coming in here. So, can you make a guess what basis function should I use or what polynomial should I use Laguerre polynomial which is done for hydrogen atom. So, hydrogen atom if you recall less than e to the power minus r like this. So, Laguerre polynomial is a good choice and it has very interesting set of properties.

So, is exactly same scheme, but my weight function these now you can see that here weight is not is equal to 1 and this approximated as w j f x j. So, my weights will be completed from Laguerre, Laguerre polynomial and my x j is will come from the 0s of the Laguerre appropriate Laguerre polynomial. Now the derivation some bodies done with already we do not need to compute this, but given n I will give x j's and I will give w j's. So, I have put down some nodes. In fact, those polynomials I am very well I am not afraid, but there very kind of is quite I want to use about clumpsy, but like this lot of algebra. How many of you like them? Nobody likes them, but they are very powerful that much I can say. So, you should know how do use them and I am very comfortable with them because I do not remember all those recurrence relation. So, we can get this is formula for the weight this formula for the weight. So, given the Laguerre polynomial I can compute the what is the weight and also the abscesses are obtain by the 0s and 0s of course, how to compute 0s I am not told you I am not sure whether alter time, but there methods you compute 0s of a function ok.

Newton was one of the person who give raise there is scheme. So, there are several schemes who compute 0s, but let us assume that some bodies done it already. So, these are the, this is the table. So, one thing is to know how to use them there is something which I would wanted to learn from this discussion. So, this is my 2 abscesses for n equal to 2 and these are the weight. So, now, there not there is no symmetry there is no. In fact, minus 12 is do not even exist r is always positive. So, will the n equal to 3 then this thing this is. So, this is one home work. So, solve for hydrogen atom. So, hydrogen atom you are the way function. So, some regular from different department, but I quantum mechanics you done it already, but you do not need really go back to your quantum book if you do not want to if you want to of course, go back in look at is more useful.

So, given the way function I only do the radial part I am not worried about the theta and phi part because I give you only m equal to 0 and l equal to 0 two quantum numbers are 0 0s the what is equal to azimuthal quantum number and?

Student: Magnetic.

Magnetic quantum number. So, they are set to 0 in fact, the home work is here. So, these are this is one of the hydrogen wave function. So, this is my f of r or if I want mod

square then I had to square them, but it is again f of r. So, you clear on with it and now actually f of r want be there, sorry f of r will be, what is f of r. So, let us say I want to compute mod size square d x. So, just to do the exercise I am interested in mod psi squared d vector r integral 0 to. So, over whole volume I am right now I cannot put the limits. So, let us, they are factors in front a is the more radius ok. So, the factor is in front let us call it alpha a squared inside will be the 1 r dependent is 2 minus r by a whole squared exponential minus r by a. So, I square it, so r by a. So, this d r integral is volume integral.

Student: 4 5.

D r and so this is the d cos theta d phi. So, I had d phi and d, d cos d phi. So, this gives you since there is no theta dependence and phi dependence this gives you 4 pi 2 coming from here and 2 pi coming from here. So, I have to do this integral. So, somebody I told me that you can use this formulas.

So, this will correspond to that and f x will correspond to this. So, I have to compute this function at the abscesses. So, you are basically left with bear integral with 4 pi coming outside now my strong recommendation is get rid of a. So, how will get rid of a. So, r by a is equal to r prime. So, I divide by a multiplied by a. So, a will come out of here. So, a comes out here now this is a number 0 to infinity this has no a dependence right. So, this is. So, I can write this is 0 to infinity 2 minus r prime the exponential minus r prime d r prime.

This is more convenient if you use this formulas first you will get number you will not get a length dimension in the mathematical formulas. So, exponential of 1 one is the number is not if it is not 1 centimeter is that. So, in all the maths formulas we have exponential takes only a number exponential does not take 1 centimeter you always a dividing my some unit. So, this is the what you should compute from here, so this I will leave it as an exercise you must do it and you should get an answer 1 for this now this a looks like the mod size where as a dimension of a is a correct. So, this should be number 1. So, this a must cancel with something. So, where does it cancel with?

Student: (Refer Time: 37:02).

So, alpha a squared has very rightly. So, f 3 by 2.

Student: a to the power r squared.

R squared yes. So, we made a mistake. So, r square d r it is not r d r, so this is r squared d r so. In fact, I should get it out put a cube outside because I have to divide by r by a whole. So, now, this guys cancel dimensions. So, this is another way to check whether I am doing it correctly or not. So, I need to compute this object r prime squared. So, that is how you. So, this is the very standard stuff, but is a always a good idea to get rid of quantities with dimension. So, this is the very nice book in math methods you are aware of this is Mathews and Walker, this Mathews right. So, Mathews and Walker math methods he does quite a bit of integrals quite nice discussion on that.

Now, this for hydrogen atom now we can do the similar exercise for oscillator. So, oscillator what does the corresponding formula looks like l e g u e r r e, so Leguerre Gauss quadrature. Now for hydrogen atom I get the formulas of this sort. So, I just choose something which has weight function like that. So, these weight function. In fact, if you look at Hermite's polynomial the orthogonal relation is e to the power minus x squared h n of x this is goes from minus infinity to plus infinity and this is the factor in front which I do not remember. So, these are orthogonal relationship for Hermite's polynomial and these appropriate.

So, my function f of x should be expanded with this, somebody may say why not expand this, but is not a good choice to expand it to my x squared minus infinity to plus infinity that has very high order polynomials. So, you should, you want to good answer then my f of s you see it is really for this case. So, for hydrogen atom also this f of x will be small order polynomial and we will get a very good answer we use f of s as a super position of Hermite's polynomial. So, this object is again same formula w j f x j now my x thesis are 0s of the Hermite's polynomial appropriate Hermite's polynomial and weights are computed again by some bodies it done it already.

So, this is how we compute for hydrogen atom and, so I just for completeness I can show you that so this is your this is the wave function psi 0.

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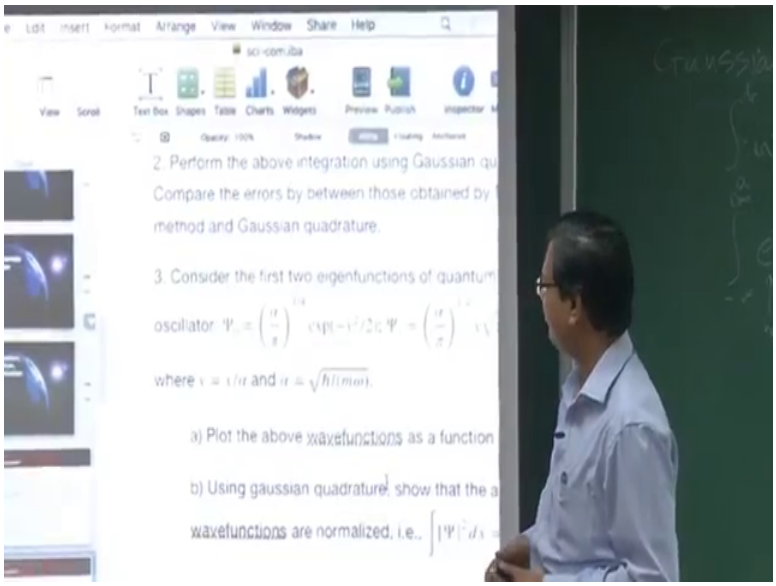

Now it has exponential minus y squared, which is similar to this. So, if I square the wave function and it will get exactly this, but y is already dimension less and y comes as x y alpha and alpha is that quadratic with dimension. So, you can use Hermite's polynomials for integrating hydrogen atom wave function and quantities related to it and, I will leave this part how to do it. So, 0s are given in the table these are the 0s for Hermite's polynomial these are symmetric now again plus minus symmetric. So, for n equal to 2 these are 2 values these are abscesses and weighs 3 values abscesses and weights and like this. So, again you should do for n equal to 2 3 4 and see how the error drops with n.

So, this is for Hermite Gauss. So, I have bit of time so let me also show you how to use the spatial function. So, you have to import from psi phi spatial. So, this is what you may be import special now this one Legendre. So, spatial dot Legendre with n will give you this Legendre polynomial. So, I can just play around with this. So, by this will give you a polynomial it does not it does not give a numerical value and you can compute at any value you like of that problem value. So, let just play around with it how does it give you. So, spatial is my spatial function.

So, let us copy this. So, l e g equal to spatial dot. So, I want second order polynomial phi 2 I will use. So, l e g how does it look like. So, this gives the coefficients. So, it gives you that, so this are the coefficients minus 3 half 0, 3 half where minus half. So, remember about what it was. So, Legendre 2 is 3 by 2 minus. So, what is 3 x squared.

So, it tells you the 3 x square minus 1 by 2. So, you can construct from here. So, 3 x square this is 0 minus.

Student: (Refer Time: 44:27).

Minus half x, sorry minus half minus half no x minus half, so 1.5 x squared minus half. So, we will do for even so Legendre which is 3 it gives you 2 point. So, it is a 5. So, 5 x cube minus 3 x by 2. So, this is what I did here I wanted to plot. So, I need numerical values. So, I put a link space something has happened here. So, I compute y array y legates and plot. So, this will plot all of them in 1 loop. So, I go from 1 to 5 I did not do 0 0s flat. So, 0 is not included in that plot.

So, you can also play around with spherical harmonics. So, this was spherical harmonics part, but it is a nice plot I have committed it, but you can play around it. So, this is my discussion about quadrature. So, I am going to skip. So, there are several ways to integrate. So, their functions which are most complicated I am skipping that part like similar functions how to integrate that I will not do in the course you can also use random numbers for integration that I will do later. And there are some nice iterative procedure to integrate to get accurate answers that also I will not do now. So, next class we will do differentiation and then we quickly go to ODE solvers. So, I want do kind of cover grounds so that you can start your project. So, next class is differentiation of (Refer Time: 46:24).