Mathematics for Chemistry
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Module - 03
Lecture - 05
Practice Problems

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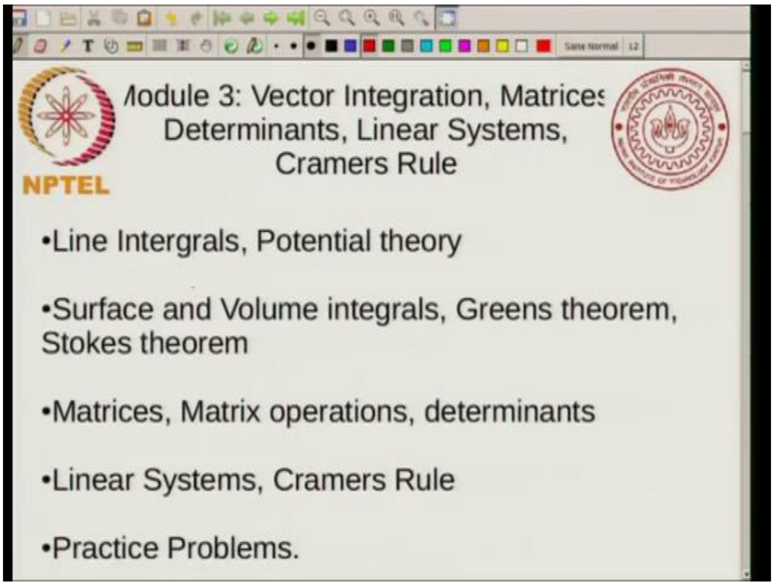

Today, we will be finishing module 3, and as is typically done we will be doing some practice problems. Now, in module 3, we talked about basically about vector integration and then we talked about some basic operations involving matrices and determinants. In these practice problems, I will be focusing on vector integration and matrix operations and determinants and all will be part of the module 4 also. So, there will take up practice problems on the matrix operations and determinants.

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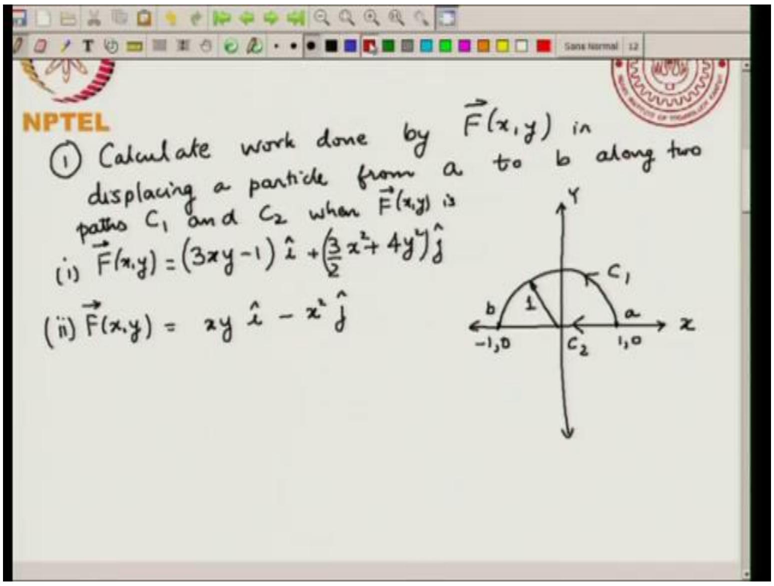

So, I will just write down a few problems that I will work out today. So, the first problem has to do will deal with line integrals. So, what you have to do is to calculate work done by F of x, y. So, the F of x, y is a force in displacing particle from a to b along 2 paths: c 1 and c 2, which will be shown in the figure, I will just show you the paths, the paths are shown here. So, this is the x-axis, this is the y-axis. And you have a point 1, 0 and the point b is minus 1, 0. And you have 2 paths going from a to b the paths c 1 is, this is c 1 and the path c 2 goes right along the x-axis from a to b. So, this is point a, this is point b.

So, what you have to do is to calculate the work done. And there are 2 forms of the forces when F of x, y is, so in the first case, I take F of x, y is equal to 3 x y minus 1 into i hat plus 3 by 2 x square plus 4 y square into j hat. And in the second case, the force is given by x y times i minus x square times j. So, this is the statement of the problem. And I just wanted to you know understand what we are trying to do in this problem. So, the problem is you are taking this particle from a to b, and you are taking it along 2 different paths, this is c 1 which is along a circle of unit radius, and c 2 which goes right along the x-axis. So, just to emphasize this radius equal to 1, so there are 2 possible paths going from a to b, and I am giving 2 possible forces. So, for each force you calculate the work done along each path, work done when the particle is moved along each path. To solve this, let us take the first force.

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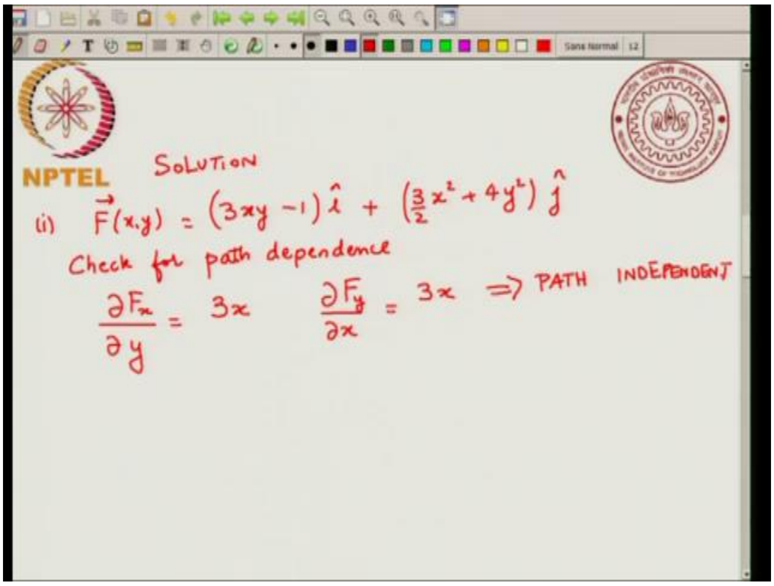

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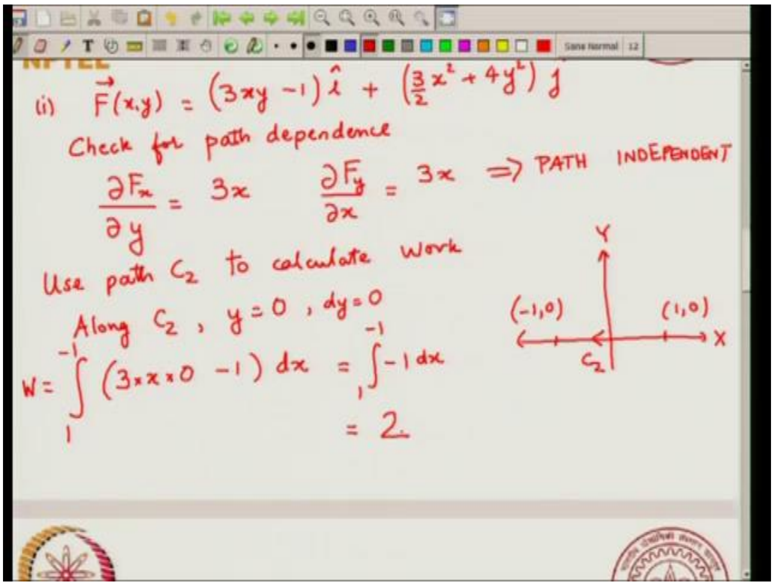

So, the solution I will write it in red. Solution, so F, so the first case F is equal to 3 x y minus 1 times i plus 3 by 2 square plus 4 y square into j. So, the first term 3 x y minus 1 is the x component of the force; and the second term 3 x square plus 3 by 2 x square plus 4 y square is the y component of the force, so that is that is just what we had here. Now, the first thing you can do is to check for path dependence, path dependence. And to do that you take the derivative, you take the derivative of the x component of the force with respect to y. So, dou F x by dou y is equal to. So, the x component of the force is 3 x y minus 1, so the derivative with respect to y will just be 3 x. Then you do the derivative of the y component of the force with respect to x, and when you take the differential again you get a derivative of 3 x.

So, since both these are equal you conclude that this is path independent. So, what you would expect is that the work done in going along paths c 1 should be the same as the work done and going along path c 2. So, for this particular force, so for the first force the work done in going along path c 1 and work done on going along path c 2 will be the same. So, what we saw is that the work done for the first force for the first case of the force the work done does not depend on which path you take. And for convenience, I will calculate this work using path c 2.

So, what do we know about path c 2. So, use path c 2 to calculate work. So, once again just let us remind ourselves you have x and you have y, x and y, and you have this point 1, 0, and you have this point here minus 1, 0, and the path c 2 goes along the x-axis this way. So, along c 2, y equal to 0. So, I can write integral or work is equal to integral from and x goes from. So, x goes from 1 to minus 1 then so d y is also 0. So, the only term that will contribute will be the x component. Now, I will get 3 x y minus 1 dx, but since y equal to 0. So, I have 3 into x into 0 minus 1 dx.

So, remember d y is 0. So, I do not have any term involving d y. So, then I just get minus 1 dx this is equal to integral minus 1 dx from 1 to minus 1. So, we are going from 1 to minus 1 and x, so x is going from 1 to minus 1. So, this is equal to 2, so that solves the first path. And you know you can verify it is a little more tedious, but you can verify that even if you take path c 1, you will get the same answer, but I would not do that here, but in the second case of the force, we will we will look at path c 1.

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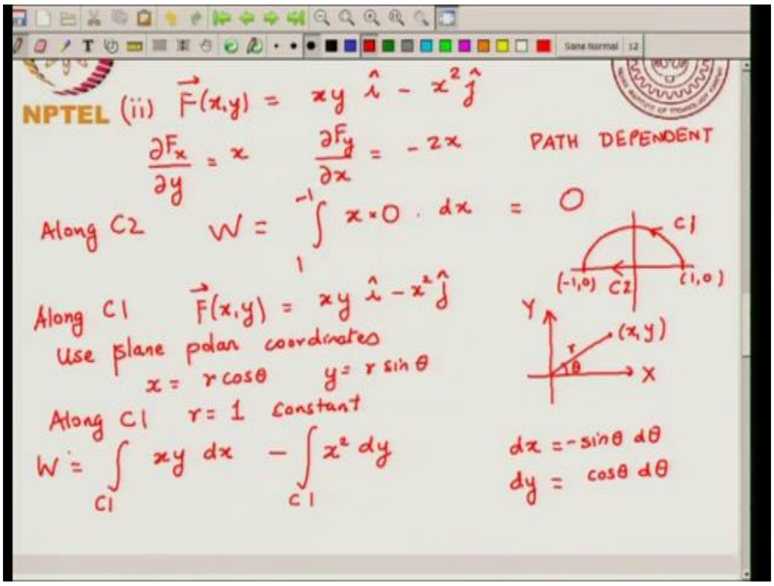

So, let us look at the second case. So, in the second case, we have the force given by minus x square j. Now you calculate dou F x by dou y, so if you take the derivative of this, this first term with respect to y you just get x and dou F y by dou x, this is equal to minus 2 x. So, clearly these 2 are not equal. So, this is path dependent. So, now let us use the along path c 2 to work done is equal to integral, again you will have 1 to minus 1 and you just have the x component times dx. But if you look at the x component, so you have x into now y y is 0 as we saw in the last in the earlier part of the problem and you have dx. So, the work done is 0. So, along this path c 2, you do not do any work and just to remind you have c 2 is the path going from 1, 0 to minus 1, 0 along the axis; c 1 is the path going along the circle, so the work done along path c 2 equal to 0.

So, what about the work done along path c 1? So, now you have to parameterize this path c 1. So, in other words, you have to somehow write this path, so we have we have F of x, y is equal to x y i minus x square j. Now, in this x, y coordinates, this path is not easy to parameterize. So, what you have to do is to go to spherical polar coordinates. So, you use or in this case is actually plane polar coordinate. What is done is you go from x and y to r and theta. So, instead of having a point x, y, you described by r and theta; and you use x equal to r cos theta y equal to r sin theta.

Why does plane polar coordinate cell along c 1 r equal to 1 constant? So, along this path your r does not change at all, so r is fixed at constant. So, the only change is due to theta and what you can do is you can write this integral now. So, you substitute for x, substitute for y, and you also have to consider this. So, if I write W is equal to integral x y dx plus integral or minus in this case, so there is a minus sign there is a minus x square. So, I will put a minus sign, so minus integral x square dy. This is along path c 1. Now, what I can do I can use is that since x is r cos theta and r is fixed I can write d x is equal to sin theta d theta with a minus sign, so minus sin theta d theta and dy is equal to cos theta d theta. So, both dx and dy can be expressed in terms of theta. And similarly, I can express x and y in terms of theta, again r equal to 1, I am taking r equal to 1.

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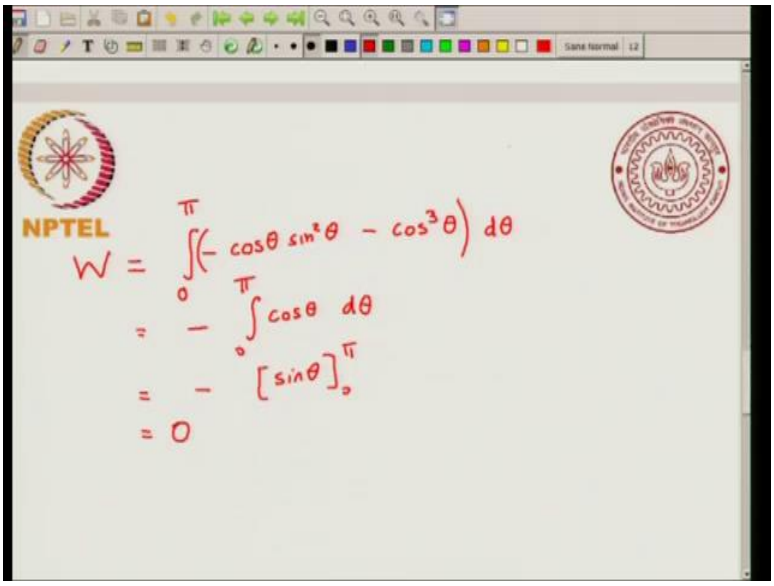

So, I can calculate the work and I will get the expression I will get it as an integral. Now, theta along this path, so if you look at theta here theta goes from 0 to pi theta is defined to go from 0 to pi. So, what you have is integral from 0 to pi, now x times y x times y is nothing, but cos theta times sin theta. So, it is cos theta times sin theta and then and then you have a dx, so you will get another sin theta. So, what you have is minus cos theta sin square theta that comes from here. And the other term minus x square that is x square will give you cos square theta, and dy will give you another cos theta. So, you have minus cos cube theta, the whole thing d theta.

And you can simplify this in this case, in this case by take cos theta outside then I get sin square theta plus cos square theta. So, I get minus integral 0 to pi cos theta d theta. So, what is this value equal to, so this is equal to, so integral of cos theta is sin theta. So, minus sin theta from 0 to pi and this is equal to 0. So, the work done is actually 0. So, what you notice is that you got 0 works along both these path c 1 and c 2, even though your force was actually path dependent. So, the force is path dependent, but for these 2 paths and I emphasized it only these 2 paths that you got the same work done. So, in both these cases the work done was 0, so that completes the first problem.

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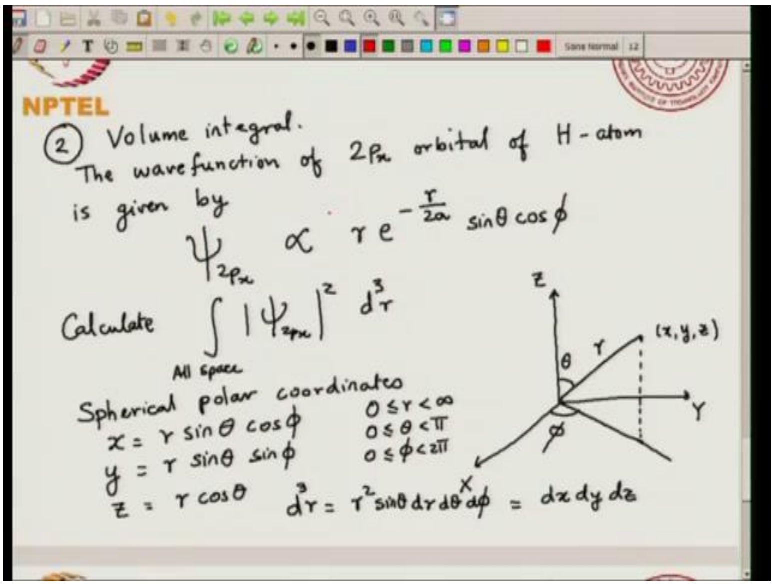

Now, I will do the second problem. So, the second problem that I want to give that involves volume integral. So, this involves a volume integral. So, here provided that the wave function of 2 p x orbital of hydrogen atom is given by psi of 2 p x, this is proportional to r e to the minus r by 2 a into sin theta cos phi. Now, what you are asked to do is to calculate the volume integral, and that volume integral I will just is to calculate psi 2 p x square d cube r, so overall (Refer Time: 18:10). So, you calculate the volume over the entire, if three-dimensional space.

So, I will just give you a little bit of background about this problem. So, I have expressed this wave function in terms of r theta and phi. So, it is already expressed in spherical polar coordinates. So, I will just mention it here. So, we have used spherical polar coordinates. So, what are spherical polar coordinates? So, if you have a coordinate system, where these are the axis x, y, z; then if there is a point x, y, z or the coordinates of that point. So, instead of using x, y, z coordinates you use different coordinates, you use spiracle polar coordinates, so where this is given by r, r is the distance of the point from the origin. And then your theta is the angle that this arm makes with the z-axis, and phi is the angle that a projection of r and to the x, y plane makes with the x-axis. So, these three coordinates, they define what is the usual spherical polar coordinates.

Now, what are the conversions used. So, you can use. So, r theta phi can be expressed in terms of x, y, z as follows. So, I can write x as r sin theta cosine of phi, y is expressed as r sin theta sin of phi, and z is expressed as r cosine theta. So, and the other thing that you need to know for this is that d cube r can be written as r square sin theta dr d theta d phi. So, when you do a volume integral, you have a integral over three variables and you have a. So, this is dr, d theta, d phi. But when you write d cube r d cube r is the same as dx into dy into dz. So, this is equal to dx, dy, dz when you converted to spherical polar coordinates then you do not just write dr, d theta d, phi you have to add this factor of r square sin theta you have to have a multiplicative factor of r square sin theta.

So, with all this information, we can easily go ahead and calculate this integral just little bit more information. So, the range of variables, so I will just, so 0 less than equal to r less than infinity, 0 less than equal to theta less than pi, 0 less than equal to phi less than 2 pi, so these are the ranges of variables. So, if you want to span the entire space these are the allowed values of r theta and phi in this spherical polar coordinates. So, 0 less than r going to infinity as r becomes larger, you go more and more outside, you go more and more further from the origin. So, with this information we can go ahead and calculate this integral.

So, let us calculate integral size square d cube r. And you might recall from your quantum mechanics course that this is what you need to calculate in order to find out the normalization constant for this, for this wave function. So, now we can go ahead we have all the information needed. So, let us just go ahead and calculate that integral.

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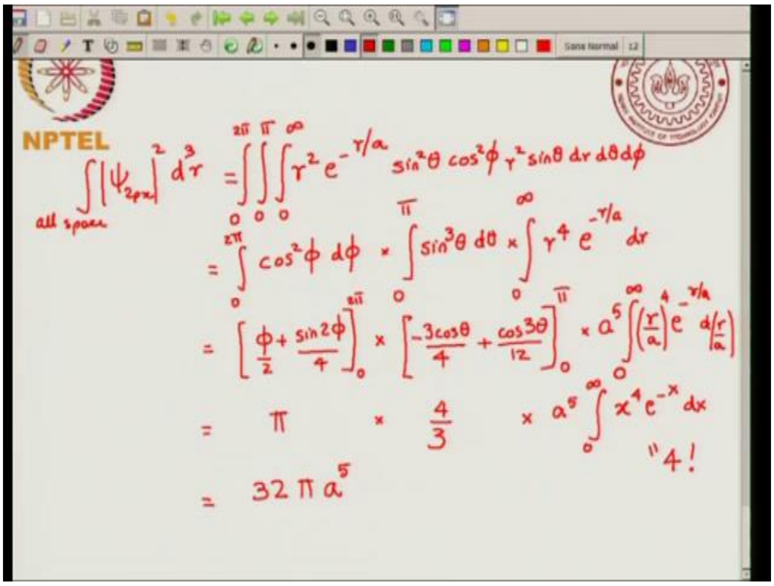

So, what we need to do is integral psi 2 p x square d cube r. So, I will just over all space. So, let us just go and copy it down. So, you have r square e to the minus. So, when you square this, you will get r square e to the minus r by a 0, r bar by a. So, you have r square e to the minus r by a, I will put the limits in a bit. So, r goes from 0 to infinity, theta goes from 0 to pi, and phi goes from 0 to 2 pi. Now, I just substituted one path and then I have a square of this. So, sin square theta cos square phi, so times. And then I had a d cube r I had a d cube r here. So, the d cube r is given by r square sin theta dr, d theta, d phi.

Now what you can do is you can separate the integral into three integrals. So, I will write. So, you have 0 to 2 pi. So, 0 to 2 pi is the range for phi for the variable phi, and the only function of phi is cos square phi. And then this will multiply an integral over theta which goes from 0 to pi, and the now you have a sin square theta into sin theta. So, you have sin cube theta. And finally, you have a integral over r which goes from 0 to infinity and what you have is r square into r square, so that is r to the power 4 and you have e to the minus r by a dr. So, you have to do each of these integrals, you have to do each of these is a simple you know one-dimensional integral, and you can do this easily and calculate the values.

So, if you want to do cos square phi d phi then you replace cos square phi by 1 plus cos 2 phi by 2. So, when you replace this by 1 plus cos 2 phi by 2 then you do the integral you will get integral you will get phi plus sin 2 phi. So, phi by 2 plus sin 2 phi by 4 integral and you put the limits 0 to 2 pi, so that is this first path. The second path the theta path that works out to so sin cube theta, so if you replace sin cube theta in terms of sin theta and sin 3 theta and then you can you can do the integral I will just write the final answer for the integral. So, you get minus 3 cos theta by 4 plus cos 3 theta by 12 integral from 0 to pi.

And then this last integral, I will write it slightly differently, I will take integral now instead of instead of my variable instead of taking my variable as r, I will take my variable as r by a I will just change my variable from just r to r by a, and there is a reason for that. So, I will write this as a raise to 5 times integral r by a raise to 4 e to the minus r by a d of r by a. So, you can see that I have changed the variable of integration from r to r by a, but the limits do not change because when r equal to 0 r by a equal to 0, when r equal to infinity r by a equal to infinity. So, this is my final expression, and you can you can substitute this, this will give you a factor of pi.

This particular expression will give you factor of 4 by 3. And finally, this particular expression is a raise to 5 and then you have an integral that looks like x raise to 4 e to the minus x dx, you have an integral of this from 0 to infinity. And if you look up this is related to something called the gamma function this is a essentially this is an integral representation of a factorial. So, this is equal to 4 factorial. So, finally, what you get you can you can write your expression as, so 4 factorial is 1 into 2 into 3 into 4. So, if I canceled the 3, then I will get 1 into 2 into 4 that is 8, 8 into 4; 32. So, I have 32 pi a raise to 5. So, this is a final expression, and you got this by doing this volume integral. So, we will start module 4 in the next class.

Thank you.