Mathematics for Chemistry

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Module - 03
Lecture - 01

Line Integrals and Potential Theory

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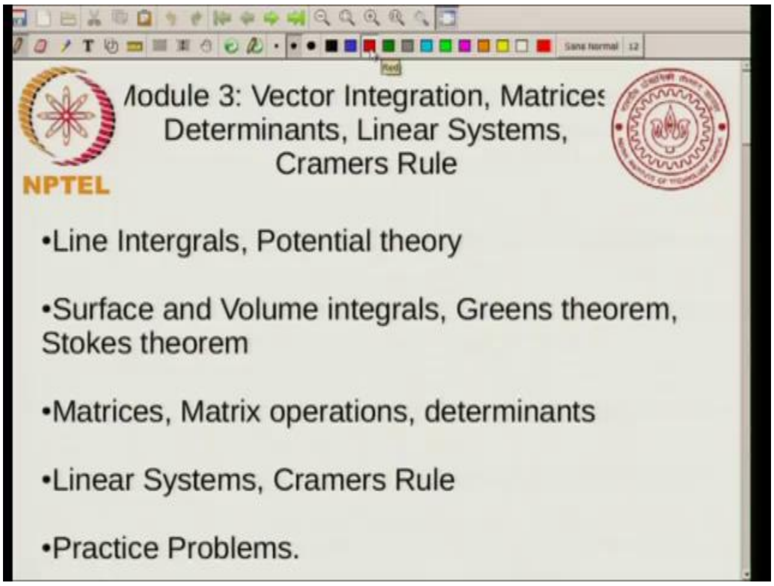

So, now we will start module 3 of this course. In this module, I will be first finishing the part on vectors where I will talk about vector integration. Then we will get to various elementary properties of matrices including determinants, linear systems and Cramer’s rules. So, in the first lecture of this module, I will talk about line integrals and potential theory; then in the second module, I will talk about surface and volume integrals, talk about Greens theorem and show stokes theorem very briefly. And then we will get to then I will start introducing matrices, talk about some basic matrix operations and then a little bit about determinants. Then we will show how to solve a system of linear equations using determinants. What is known as the Cramer’s rule and finally, we will do some practice problems.

So, in this module, there will be 5 lectures and the fifth lecture will just be practice problems. So, let us start. So, today I will be talking mainly about line integrals and potential theory.

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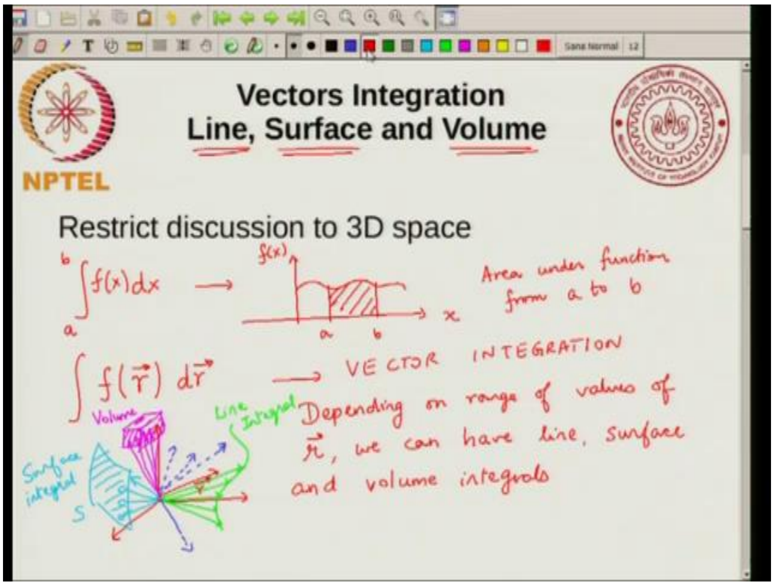

So, this is part of vector integration. And in vector integration, you there are 3 kinds of ways to integrate vectors. Now, let us a step back a little we will restrict this discussion to 3-dimensional space. So, all this talk about line integrals, about surface integrals and volume integrals will be restricted to vectors in a 3-dimensional space. So, let us now what do we want to do? As usually you have done things like integration integrating over some variable from some limit is a to b of some function of x. So, this is something that you are familiar with and the way you are familiar with is that you think you think that this variable, if this variable x is shown like this and f of x is some function when you plot, it looks like this and this is point a and this is point b. Then you know that this integral is nothing but the area under this graph between a and b. So, it is area under the function from a to b, so that is what you mean by this by this integral over a function.

Now, what do we have here, we have a function, but it is not a function of a scalar rather it is a function of a vector. So, f of r and what we have to do is what we are thinking of is something like an integral over a vector. So, what we want to think, this is a general idea of vector integration, this is the general idea of vector integration that we want to do some sort of integral over a vector. And how do you put the limit is how do you define this and as we are discussing that we will come to a line, surface and volume integrals very naturally.

So, it turns out that you can think of different ways to integrate now you could have an integral just over a line. So, in this case, your vector is something that points in 3 dimensions. So, your r space, your r is a vector in 3 dimensions. And now you are integrating a function of vector over various values of r. So, now this r can point in several different direction for example, can point this way, it can point this way, it can point this way it can go in this direction. So, all these are various possibilities for this vector r. And now what do you mean by integrating over a vector that means, you have to integrate over a range of values of r.

Now, there are different ways to do it. So, if you integrate over a range of values of r, if you say your r can be anywhere in some region, then you can have a volume integral. If you say your r has to be restricted to one line, then you get a line integral. So, what I want to emphasize is that depending on a range of values of r, we can have line, surface and volume integrals. So, depending on the range of values of r, you can have line, surface and volume integrals.

So, for example, if I say that my r should be along r whatever your r is it should point along it should be along this line. So, basically if you have r restricted to this line then your r can be this, this, this, this, these are the allowed values of r. So, these green vectors or the allowed values of r that touch the line. We imagine that your allowing values of r to only take these values, and you are doing an integral similar to what we did in the scalar case then you would get something called a line integral. On the other hand, suppose you say that in 3D space, I have a surface, I have some surface; I will just call the surface S. And if my r, r can point to anywhere in that surface any point on the surface then I will get a surface integral. So, this would be something like a line integral and this would be something like a surface integral.

I have not told you how to do the integrals yet we will come to that, but just to motivate that depending on what are the allowed values of r so what you put in this limit is you will get a line or a surface integral. Now, you could also have a case where you take some 3D region, and you have some volume and your r can point to anywhere inside this volume, it can point to anywhere inside this volume, then you will get a volume integral. So, you can get a line integral, a surface integral or a volume integral in this way. And we will talk about this in today's lecture and the next lecture.

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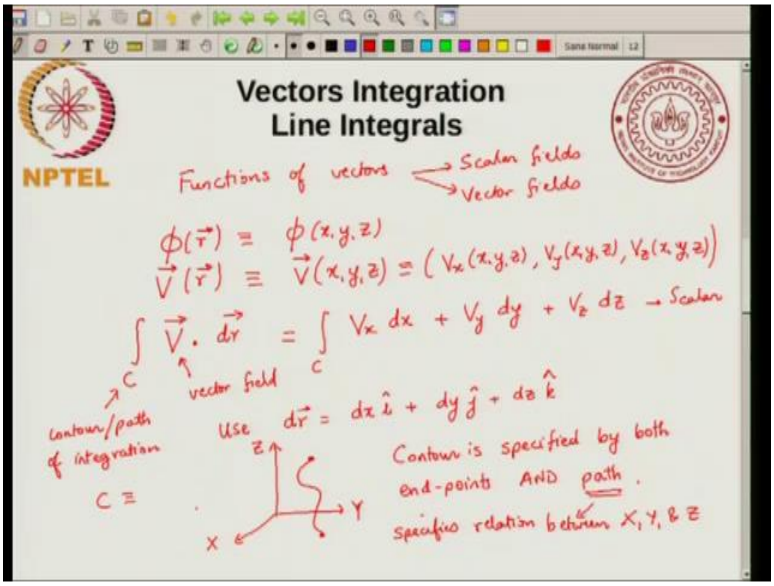

So, now let us get to line integrals. Now, it turns out that that there is not just one-way of defining line integrals, there are a few different ways of defining. And ultimately, we will stick to only one of them, but basically see as I said when we talk about functions of vectors, we talked about 2 kinds of functions one was what are called as scalar fields and the others were vector fields. So, a scalar field is for example, you can have phi of x of r which is equivalent to phi of x, y, z that is a scalar field. And now how would you do an integral involving phi of x, y, z, we will come to that. You could also have something like a vector field V of r, which has various components I mean each of the it will have 3 components and each of the components will be will be a function of x, y, z. So, this will have V x of x, y z v y of x, y, z and v z of x, y, z.

So, now there are some popular ways to define these line integrals. And you know based on what your application is you use the appropriate one. So, one example one way of defining the line integral is to just do an integral over a c, I will come to what c is, c is a contour of integration contour or path of integration. And you can have something like a V a vector field dotted into dr. Now, notice that since r is a vector dr will also be a vector. And what we did is we took a vector field, this is a vector field, and you dot the vector field into dr, because the vector field has various components, you dot these with way with the various components of dr. So, this is the typical line integral that will be talking about.

So, if you want, I can expand this out. So, use dr equal to dx i plus dy j plus dz k. So, this is the differential element in r. And if you have these as the components of the vector I can write this as integral over c, c is a contour. And what I will have is V x dx plus V y dy plus V z dz. So, what you can write is you can write it as the sum of 3 integrals each of them is an integral over a single variable each of them is integral over a scalar. So, you have V x dx, V y dy and V z dz.

So, this is the typical line integral that we will be using. There are other line integrals where instead of a dot, you put a cross, or you have a scalar field here, which I would not be talking about in this course, but you might come across those sometimes when you are reading various other books. But for this course, we will just talk about this type of line integral. Now, notice that since V is a vector dr is a vector v dot dr is a scalar, so this is integral of a scalar. So, what you get finally is a scalar, so this is a scalar. In other words, what you will get is a number, this integral if you integrate over a contour and you put various limit is then you will get a number.

Now, what is the contour? Contour has 2 things contour. So, what you mean by this contour is some path. So, if you take this as my space. So, if I take this as x, y, z this is some path it has some initial point and some final point, but the contour is not just specified by the initial and final points, it is also specified by the path. So, contour is specified by both end points and path. This is a very important thing. When you are saying a line integral, it is not enough just to specify what are the limit is you have to specify the path. And we will come to this in a bit, and we will see when we actually do some examples of line integrals, we will come to this. So, this is the definition of the line integral. Now, where is the path enter? So, the path actually specifies relation between x, y and z between the coordinate. So, between this x, y and z the contour actually specifies this relation.

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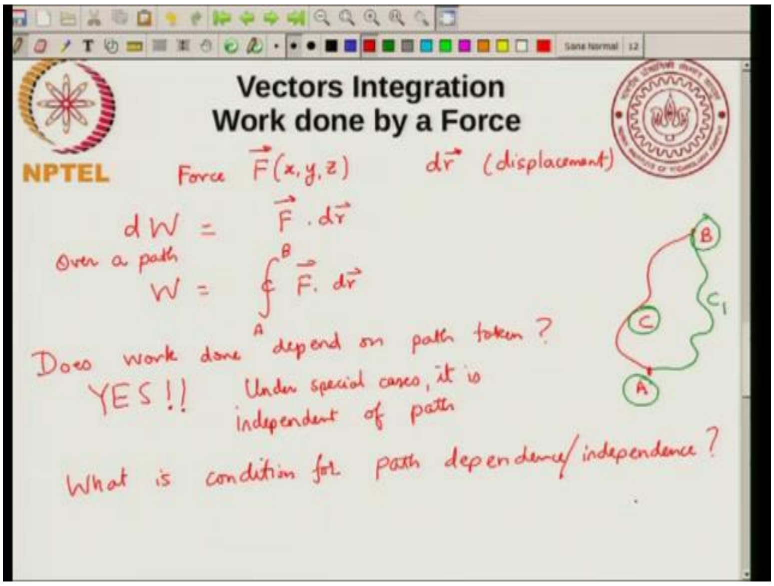

Now, we will come to the most popular example of vector integration is to calculate the work done by a force, and this is where we use the idea of line integrals. So, we will do this and we will take an example of calculating the work done by a force. What is it. So, the idea is that suppose you have a force F; F is a vector field, it is a function of x, y, z. And due to this force you displace a particle you imagine that you have a particle that is moved by this force, then what is the work done. Then work; so if you displace it by some small amount dr, so this is displacement. So, if you if you just move the particle a small distance dr then the work done is given by F dot dr, it is a dot product.

And if you do a if you do over a path, so if you displace the particle some distance over some path a let say you go from point A to point B then the work done over some contour will call this contour C. Then the work done is equal to integral over the contour C from A to B F dot dr. So, it is just a line integral. I have just explicitly specified the end points A and B. So, this is where this is the most common application of vector integration that you will see in the chemistry. There are also many such examples in different areas of chemistry and also in engineering and other disciplines.

Now, this if you look at this, if you look at this picture right here, so you have A, you have B, and you have this path. So, now this immediately raises questions that suppose I go from A to B - this way, now if I go to from A to B by a different path by go this way, is the work the same or different. So, if I go through some path C 1 is the work same or different. So, does work depend on path take? And the answer is yes, in general yes. Under some special conditions, you will have path independents, but in general yes it depends on path.

And you will immediately recall when I say this when I talk about path dependent work and you know whether it is you will immediately recall from your thermodynamics courses, you talk about state functions and you talk about transfer functions like heat and work which actually depend on the path taken. So, work is dependent on the path taken. Under some special cases, it is independent of path. And we will come to that a little later, but before that I will come to the example of the path dependence.

So, what we said is that the work dependent a work done by a force, in general, it depends on the path taken, but I said that under some special cases, it is independent of path. So, what is the condition for path dependence, and path independence? So, what is condition for path dependence slash independence? So, the question is when is work path dependent and when is it path independent and again this is something that you might be familiar with from your from your thermodynamics courses.

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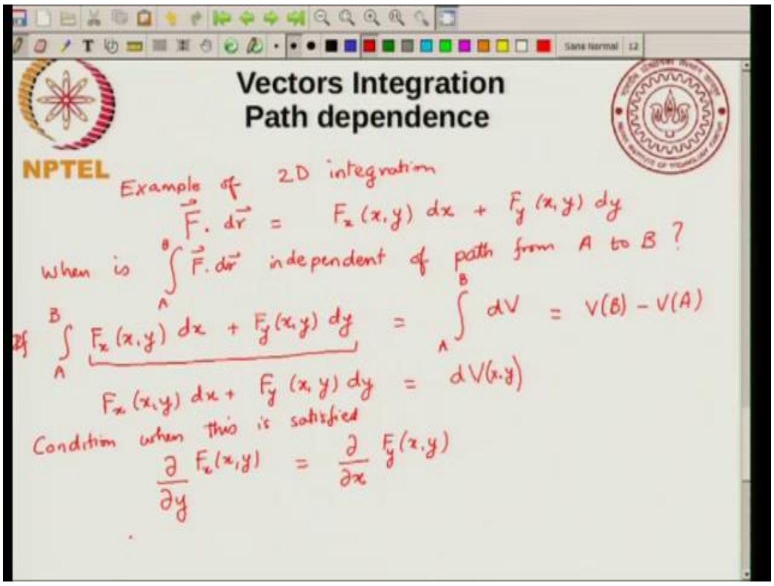

So, let us take again here we will take we take an example of 2D integration. So, I am just making this a little easier by taking a 2D integration. So, for example, if you take F dot dr, now this becomes F x of x, y dx plus F y of x, y dy. And now you want to ask a question when is integral from A to B F dot dr independent of path A to B. So, when is it independent of path from A to B?

Now, now the way you can see this in many ways, but let me motivate it in the following way. Suppose I expand this out, so I have integral A to B. Now, if I write this explicit expression for F, I have F x of x, y dx plus F y of x, y dy. Now, suppose I could write this whole thing this whole thing as. So, suppose I could write this whole thing as as. So, if this is equal to if I could write this whole piece as something like dV, I am choosing the term V, from A to B then integral of dV is just V of B minus V of A, it is independent of path. So, if you could write your integral in this form then it will be path independent.

So, the condition for path independence is that you should be able to write F of x of x, y dx plus F y of x, y dy as dV, V is some field. So, V depends on x, y, z or x, y in this case we do not have z. So, V is a function of x, y. So, if you could write it in that form then it would be path independent. And the condition for this, the condition when this is satisfied is when d partial derivative with respect to y of F of x is equal to partial with derivative with respect to x of F of y of x, y. So, what you do is you take the first F x of x, y you differentiate that with respect to y that should be equal to F y of x, y differentiated with respect to x, and these are partial derivatives. So, this is the condition. So, if you have this condition, then this integral is independent of path and your work becomes independent of path.

So, now this is again a useful condition, you can always check whether work that you calculate is path independent or not using this way. However, let me mention one thing that that when you say, it is independent of path that means, you can take any path any path and you will always get the same answer. Now, there are cases when you know integral might be same for 2 different paths, but it might not be same for other paths. So, even if it is path dependent, you might accidentally get the same work for 2 paths, so that is also possible. But when you have this condition when you satisfy this condition it will be independent for any paths.

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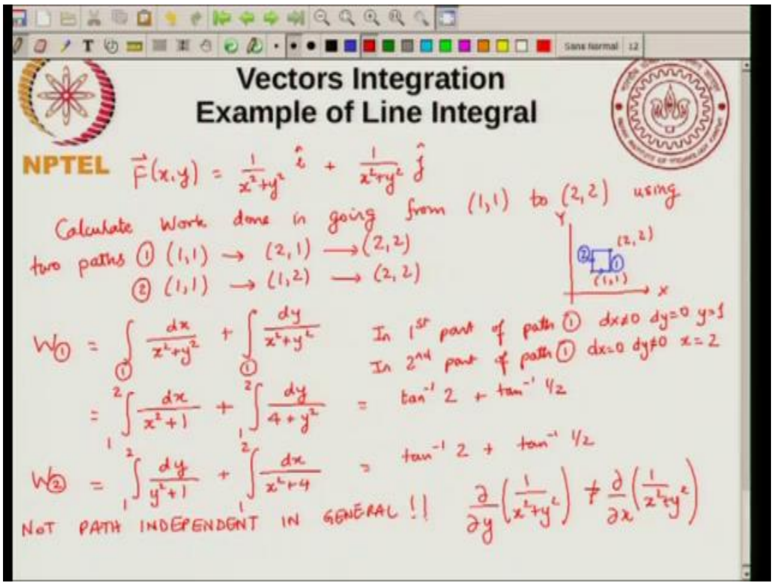

So, let us quickly do one example of a line integral. So, what we are going to do is an example lets calculate the work done. So, if F of x, y is equal to 1 over x square plus y square i plus 1 over x square plus y square j. What is the work being done going from a point from going from, so calculate work done in going from 1, 1 to 2, 2. And we will do we will do using 2 paths. So, the first path you first path is you go from 1, 1 to 2, 1 along the straight line and then you go to 2, 2. And then the second path, so this is the first path, the second path is you go from 1, 1 to 1, 2 and then to 2, 2. So, just it pictorially what you have is you have the x and y you have the points 1, 1. So, this is 1, 1 and here is the point 2, 2.

And you do 2 paths. So, in the first path you go from 1, 1 to this use 2 different colors. So, the first path you go this way. In the second path, you go this way. This is 2; this is one. So, how do you calculate both these works? Now, what you have to do is in either case you will write that the work done. So, let us calculate from path one. So, this is equal to integral now what we will do is you will write you will multiplied this by dr and dr is dx i plus dy j. So, what you will get is you will get dx over x square plus y square plus integral dy over x square plus y square both are over path one, I will just put a one here. So, these are the 2 things.

Now, you have to do both these integrals over path one. Now, if you can see in path one there are 2 parts; in one part only the x changes in the other part only the y changes. So, in the first part of path one, your dy is 0; in the second part of path one dx equal to 0. Not only that in the first part of path one, so in first part of path one dx not equal to 0, dy equal to 0, and y equal to 1; in second part of path one, dx equal to 0, dy not equal to 0, and x is fixed at 2. So, along the entire second part of path one x is fixed at 2. So, this is a information about the contour that you have to use in order to do this integral.

So, when you when you put this condition, you will get, so for the first part of path one dx is not equal to 0, so dy goes out. So, all you have is you have an integral over dx the limit is of x are from 1 to 2, and you have x square and y is set at one, so you have x square plus 1. So, you just get an integral over a single variable and you can do this integral. In the second part, what you have is integral dy, now y goes from 1 to 2, now x is fixed at 2. So, it is 4 plus y square x is equal to 2. And in the second part, dx equal to 0, so that part goes away. So, this is how you would get for the first part. So, you can do both these integrals both these integrals are related to tan inverse. So, this is nothing, but equal to tan inverse, in this case it will be tan inverse of 2; in the second case it will be tan inverse of half. So, it is the sum of sum of these 2 is this.

Now, in the second part, in the in the second part you will get again very similar things. So, but what will happen in that case is that in the first part your dx is 0, only dy is changing. So, what you will get is integral dy over y square plus 1 from 1 to 2 plus dx over x square plus 4 from 1 to 2. And again this is the same, tan inverse of 2 plus tan inverse of half. So, basically it is what you find is that the work is the same for both these paths. And in this case, you can easily look at F of x, y, you can look at both these and you can easily what you do is for these 2 paths you get the same work.

So, but is it is it path independent in general, the answer is not path independent in general. And why did I say it is not path dependent in general, you take d by dy of 1 over x square plus y square that is d by dy of this is not equal to d by dx of this, which is again 1 over x square plus y square, clearly these 2 are not equal. You take a partial derivative of this and partial derivative this, you will get different functions and they are not equal. So, in general it is not path independent, it is just for this special case of these 2 paths that you got path independence.

So, in the next lecture, I will talk about surface and volume integrals.