Advanced Mathematical Methods for Chemistry

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Module - 01
Lecture - 04
Vector Integration - Line, Surface and Volume Integrals

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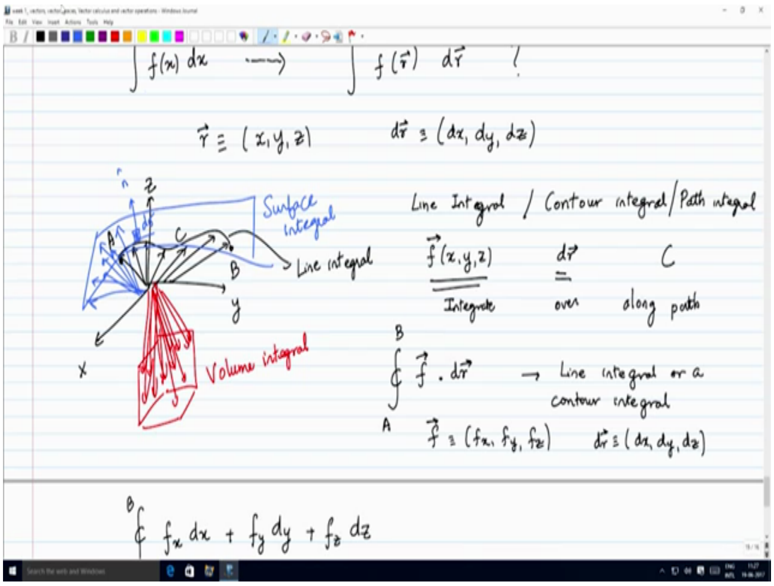

So, the next topic that we want to do in vectors refers to vector integration and here we will talk about 3 kinds of integrals that are commonly seen whenever dealing with vectors these are line surface and volume integrals. And I will I will go these briefly there are lot of interesting relations involving that relate these integrals to each other, but I will not we will not be discussing that. I will just give you the definitions of these 3 ways of doing integrals and you will see that in lot of your courses you will you be using some of these integrations.

So, here what we want to do is we want to do an integral see it is typically we do an integral of a function over a variable this is what you do this is the usual integration of a function of a single variable.

Now, what we want to do today is try to see is there a way to define integral of maybe a function of a vector over a vector how can you define such quantities. It turns out that there are different ways to do it and as we said that your r again we are restricting to 3 dimensional space. So, r is has 3 components x y and z. So, your d r will have will have 3 components d x, d y and d z and, so when you do this integration over d r you can do it in different ways you can do things called line integrals where you actually integrate along a certain line you can a do a surface integral where you integrate over the vector the vector can be anywhere on a surface or you integrate do a volume integral where your vector can be over an entire volume region.

So, the basic idea is the following. So, suppose you have you have x y z and your r is some vector that points anywhere. So, if you have a r vector now when you integrate r vector you can either; you can either integrate along a line. So, you take all possible r values along this line that would be something like a line integral. So, you integrate the function along this line that would be a line integral or you could or you could take r and integrate over an area. So, you take all possible values of r that can be in this area. So, so r can be anywhere here it can be here here here here here here and so on. So, that would be integral over an area or you could integrate over a volume. So, so or you could take something like this you could take some region and you say that r can be anywhere in this region.

So, these are the 3 kinds of integrals that you will see. So, this would be a volume integral this would be a surface integral and this would be a line integral. So, what I want to say is that your integral of this function you can look at all these kinds of integrals and what I will try to do is to give you certain definitions of these integrals. Now it turns out that there are many ways to define some of these integrals. So, you know based on the context these integrals are defined in different ways I will just show you certain definitions and you can easily do the other derivations.

So, let us start with the line integral. Line integral is also sometimes referred to as a contour integral or a path integral. So, here what we have is some function of x y z and let us for convenience take this as a vector field, and then you want to integrate it over a path. So, you want to integrate it over the vector, so integrate you want to integrate this function over this variable and the change of this variable goes along some path c.

So, this is what you are going to do and the line integral is defined in the following ways, so you can define the line integral as f dot d r along path C. So, what is this path represent? So, this path could have an initial point and a final point. So, this path can go from A to B along the path C. So, the path is C. So, then I would write this in the following ways. So, what I could write it is slightly differently I could write from A to B along path C, you could go from A to B along another path that would be a different line integral. So, this is an example of a line integral or a contour integral.

Now notice I had a vector field f and I took a dot product with this vector differential d r. So, now when I do this, when I take I can expand this out. So, if my f has components f x, f y and f z and my d r has components d x, d y, d z then you can clearly see that this integrand for the line integral has the components.

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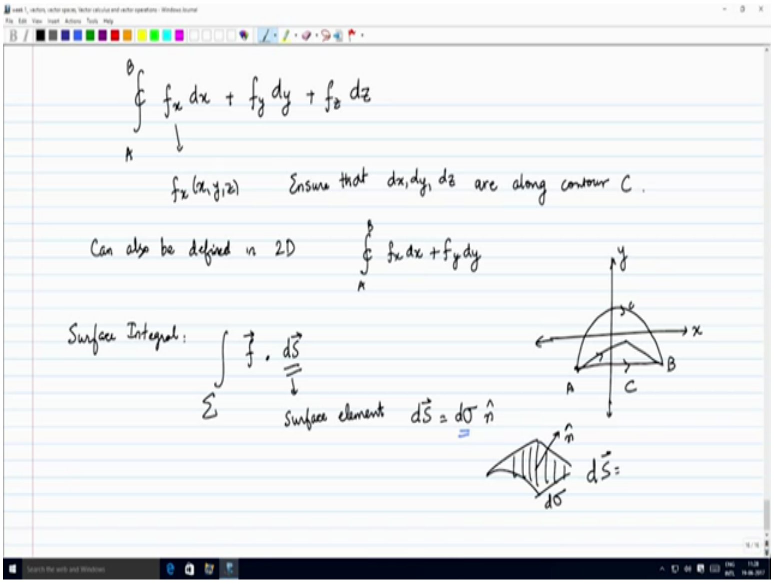

So, I can write this integral a to b f x d x plus f y d y plus f z d z and since f was a vector field f x, f y and f z are all components of x are all functions of f x y and z. So, each of these, f x is a function of x y z, f y is also a function of x y z, f z is also a function of x y z.

So, all these are functions of x y z and so, all you are doing is you are taking you are doing this integral you are integrating over d x, along this contour then you are integrating this function over d y along the again along this contour and then you are integrating this over these are again along this contour. Now it looks easy to write, but in practice it is actually a little tricky to implement because you have to ensure that d x, d y and d z are along contour. So, a differential change in are you cannot take arbitrary differential change in r you have to ensure that these 3 of r they follow the contour C and we will see examples of this.

So, will see how to do this in practice, but basically this is something you have to ensure when you are doing line integrals you can I mean line integrals can also be defined in 2D in 2 d. So, in 2D you could have integral from a to b along contour c f x d x plus f y d y and this is something that is that is a little easier to at least at least in 2D it is easy to show the path show the contour C. So, if you have this x y plane in 2D and if you have a point A and you could have a point B and you could have your contour C might be might be might be might be some sort of path that goes from A to B.

So, you could just have a contour that looks like this, this is my contour going from A to B you could also have other contours going from A to B you could have something that looks like this another contour you could have something that looks like this. So, there are different contours that you can have going from A to B, but you can show this and you can show it nicely in this 2 dimensional space. So, let us take a, let us go into the others other kinds of integrals that you can do and then and then we will come back to some issues with this line integral some interesting aspects of this line integrals. So, the other integral that we talked about is what we call the surface integral.

So, here what you do is you define you take integral and let say you take f some vector field now you dot it over, now I will just write it as d S vector this is a this is called a surface element and this integral is over some surface I will just call it sigma. So, what you are doing here is you define something called a surface element. So, d s is basically your surface area d sigma which is a scalar dotted times the normal. So, the idea is whenever you have, if you have some sort of surface like this then you can define a normal to the surface. So, this is my very very small element d S. So, d is equal to d sigma which is this infinitesimal area times this normal element.

So, the idea is your, you if you go back to what we had shown the way, we had shown the surface integral. So, you have a large you are you are integrating over the region. So, you break it into a small differential elements such that and each one has a normal and you have this d sigma. So, that is the differential surface element and so your d S is nothing, but d sigma into n, n is the normal to the surface is at that point.

So, your surface integral is defined in this way this d sigma is usually can be represented in terms of if you are in 2 dimensions you can represent it in terms of d x and d y and you can usually calculate this surface integral. Again you will see some of these when you are dealing in quantum mechanics. Let me mention the third type of integral and this is also something that you see regularly in quantum mechanics that is the following that is a volume integral.

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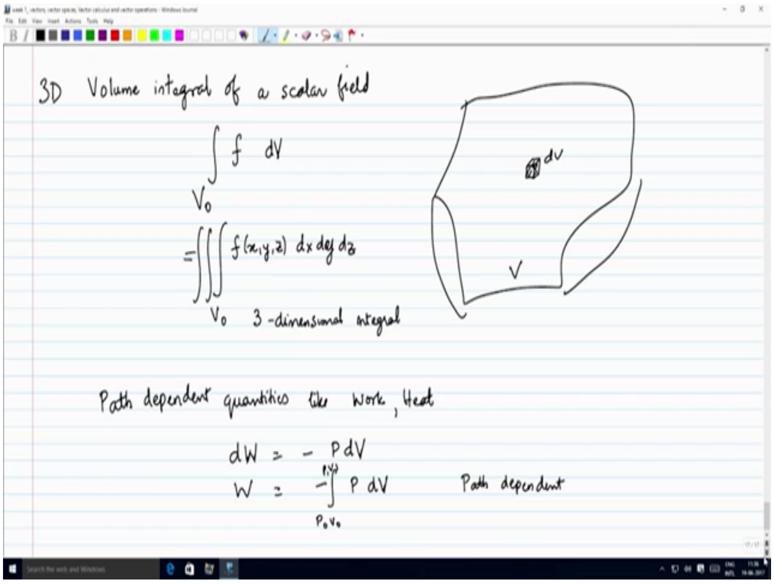

So, here what is done is you take a scalar field and then here we are particularly referring to 3D volume integral of a scalar field. So, we take a scalar field f and you and you multiply it by a differential volume element d V and you integrate over this volume over some region I will just call it V 0. So, this is, so what you are doing is you have you have some sort of infinitesimal volume element d V and you want to integrate over this some volume V. So, you are integrating over some volume this is a 3 dimensional volume region.

So, maybe show it this way and you want to integrate the function over this region. So, what you have is you have is you typically define it for a scalar field. So, the scalar field is this and this is nothing, but your scalar field is a function of x y z and the differential volume element is nothing, but d x, d y, d z and you integrate it over this region. So, this is actually a; this is actually a 3 dimensional integral; that means, you have to take this function integrate it first (Refer Time: 16:18) I mean you have to do 3 integrations and you know your volume region you have to make sure that the boundaries are such that they define the volume V 0 .

So, these are the 3 integrals that you see most often and let us just go back the surface integral.

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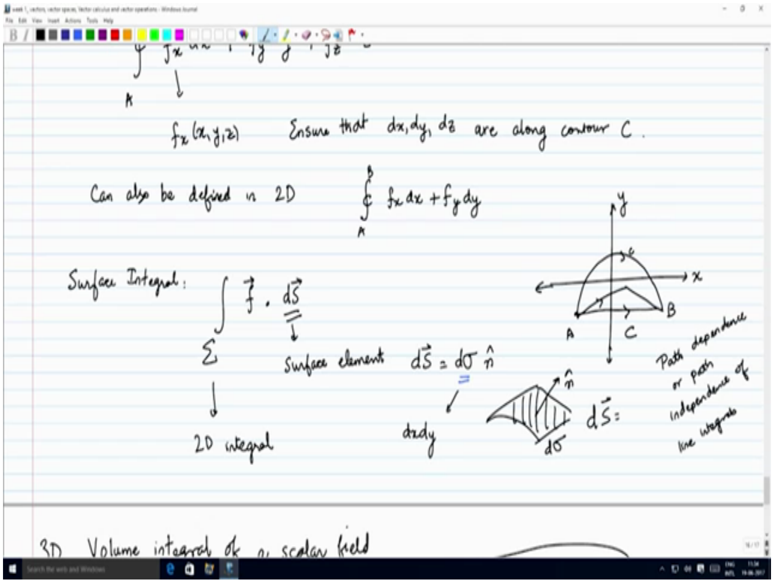

So, this d sigma usually can be written as d x, d y and so you have 2 dimensional integrals. So, this is a 2 dimensional integral. So, we saw that the line integral. So, you can go from point A to point B you can go along different paths, along different contours and in general the line integral is dependent on the path it depends on which path you go through you will not get the same answer, but under certain conditions you get the same answer you get an answer that is independent of path.

So, I just want to mention this and you know you can you can easily find out what are the conditions. So, there are conditions for path dependence or path independence of line integrals of line integrals. So, the question is when are these line integrals dependent on the path and when are they independent of path and this will sound familiar to you for those who have taken, who have seen thermodynamics. So, you learn in thermodynamics. So, you learn about path dependent, dependent quantities like work and heat.

So, what we learn in what we do in thermodynamics is that you write your differential work as minus P times d V and now what you do is you to calculate the work done in any process you have to do an integral minus P d V and this integral is over some path it goes from some initial from some initial condition let us say P 0 V 0 to P 1 V 1. So, it goes from some P 0 V 0 to some P 1 V 1. So, you go along some path and this is in general this is path dependent. And there are very sound mathematical reasons why this is path dependent, but basically this work, work is the quantity that is in thermodynamics we say work is a path dependent quantity.

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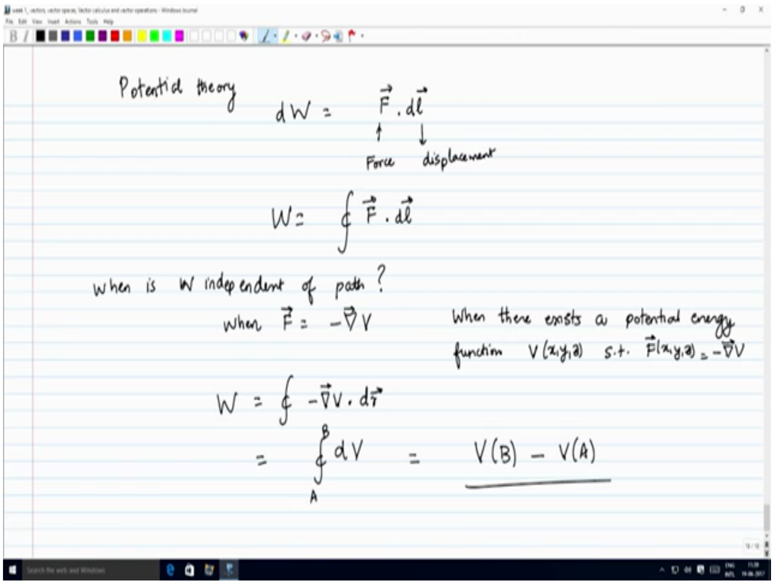

Now, in potential theory, you write your work d W as F dot d you can, so it is some force time some displacement. So, it is a force dotted into displacement. So, this is your force and this is a displacement and again your work done is actually integral F dot d l over some path. So, this is a line integral.

So, work is a line integral and what you have to what you have to; you can ask a question when is this line integral in the independent of path. So, when is W independent of path, now it turns out that you can give a very straightforward answer to this? So, answer is when F is equal to minus gradient of some potential. So, when there exists a potential energy function V of x y z such that F of x y z equal to minus grad V. So, when you can write this then you can write W as a contour integral of minus grad V dot I will just write instead of writing d l I just write it as d r and what we said is that gradient of V dotted into d r is nothing, but the differential change in V going along that path this is nothing, but the V at, if you are going from point A to point B then this is nothing, but the potential at B minus the potential at A, this is clearly this is independent of path.

So, whenever you can write a potential energy function then the work done in going from any point to some other point will be independent of the paths taken and this is a very fundamental idea in all of physics that whenever you can write a potential then you know your force is said to be path independent and this leads to lot of nice relaxations. That means, that means you go from one point to any other point then the then the work whichever way you go the work will always be equal to the difference in the potential energy. So, whenever you can write a potential energy, energy function you know that the work done in instead displacing particles from one point to another will be independent of the path taken.

So, I will stop the discussion on vectors here. So, in the next class I will do some practice problems where you see application of some of these concepts.

Thank you.