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Phase field modeling;
the materials science,
mathematics and
computational aspects

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Module No.13
Lecture No.54
Optimization of
functional I

Welcome we are trying to look at the optimization of a functional and let us consider a functional which is like this.

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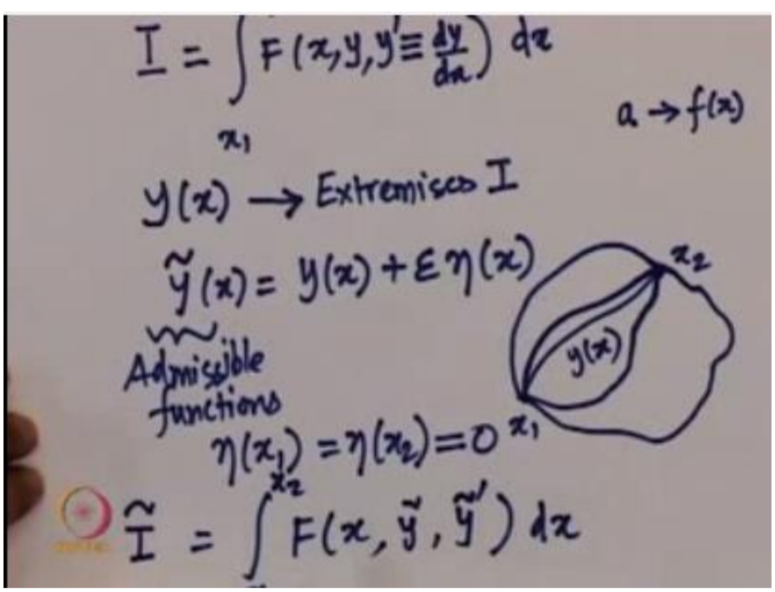

I= integral x1 to x2 F(x, y, y'= dy/dx) dx this is the function which I want to optimize, which I want to extreme. Now like usual in mathematics, we know if we have a function which is dependent on one variable how to extreme, we know what is the necessary conditions. So I mean we are going to oppose this problem in the same fashion, so that we can actually also solve this problem.

For doing that in the case of a function where we are trying to find out where the extreme of point is, we first assume that there is a point A where the function actually achieves extreme. In this case I am going to assume that there is some Y(x) which is a curve or a function or path whatever you want to call, for which this is Y(x) which extremises I, now I am going to assume. This is equivalent assuming that A is the point where F(x) had a extreme.

So like that I am going to assume that Y(x) is the point where if you choose that path this I is going to be extreme. So that is the first thing, now like we said that about A you have to choose points X within an admissible range, I am going to define an admissible set of functions which I will look at the find out to how to organize this. How do I define that admissible functions, I define them at Y tilde of x as nothing, but Y(x)+∑ η(x), so these are admissible functions.

So I am going to choose some function which are admissible function, how do I define they are the extremizing function plus some scalar parameter ∑ multiplying some other function η(x). So what is that we are saying, suppose I am in the X, Y space then Y(x) is a curve like that, so this is Y(x). And this is point X1 and this is point X2 by this I am choosing different function, so I am choosing functions like this.

So each one is by εη but all of this η are going through points x_1 and x_2 which means $\eta(x_1)$ and $\eta(x_2)$ right so the so called variations right how different are these from y(x) they are not different so I am going to assume that they are 0 η are functions such that because they become 0 irrespective ε we use they are your going get $y(x_1)$ and $y(x_2)$ at those points that is that touch is and now ε by choosing different ε you will two different functions.

So this is and I am also going to assume that η and y's are differentiable as many number of times as you would lead them to differentiate so let us assume that that's I given, now let us consider the varied functional what is the varied functional let me call it as some I~ is the functional which I consider between the same x_1 and x_2 with F(x) does not change $\tilde{y}$ and $\tilde{y}'$ dx now when ε becomes 0 the admissible function actually becomes the extremizing functional.

So ε= 0 is the place where my admissible function actually reduces to the extremizing function okay. So let us remember that so we write this F(x) y´ $\tilde{y}$ and $\tilde{y}'$ which I~ and let us look at what happens to this I~ okay so I~.

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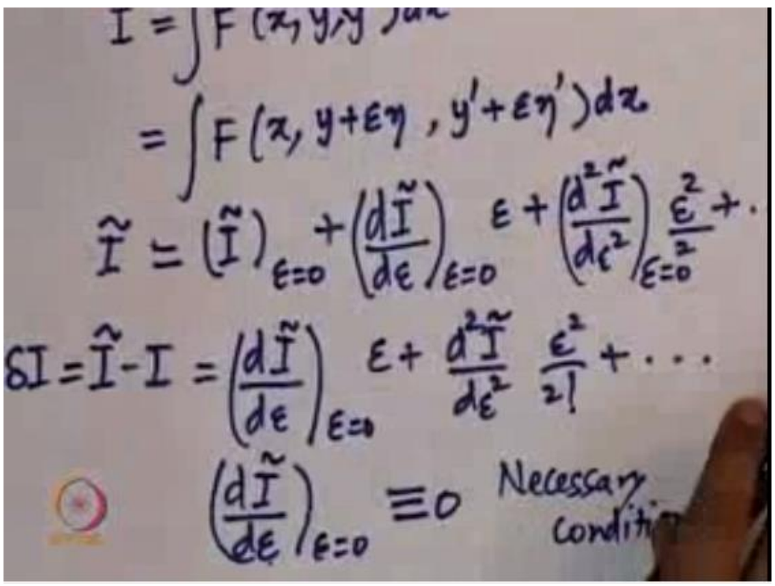

Then is equal to $\int F(x, \tilde{y}, \tilde{y}')$ dx but we know $\tilde{y}$ and $\tilde{y}'$ are nothing but F(x, y + $\varepsilon\eta$, y´ that is nothing $\tilde{y}'$ nothing but $\varepsilon\eta'$) then dx so now let us look at this I~ if I look at I~ ad some quantity so which is I~ at ε = 0 that is the for the optimizing function I~ that will become I itself + dI~ / dε where ε= 0 times ε + d^2I~/ dε^2at ε=0 ε^2/ 2+ etc what is this is nothing but the Taylor series explanation for this because now depended only this ε so in terms of εi call actually Taylor expand fro I~ now I~ when ε = 0 is nothing but so I~ - I which is nothing but what is known as the variation of I is equal to dI~ / dε at ε=0 ε + d^2 I~ / dε^2 ε^2/2!+….

Now we know that the necessary condition for an extreme M to be achieved is that $d\tilde{I}/d\varepsilon$ at $\varepsilon = 0$ should be 0 $d\tilde{I}/d\varepsilon$ at $\varepsilon = 0$ should be 0 so this is the necessary condition, so what did we do? We took the functional we varied it a little bit and the variation was defined completely in terms of a scalar parameter so we could go back to some f(x) one parameter function.

For which we know what is a necessary condition for optimization and now we are implementing that necessary condition on this functional, so what is $d\tilde{I}/d\varepsilon$ at $\varepsilon = 0$ for this function, so let us write that down.

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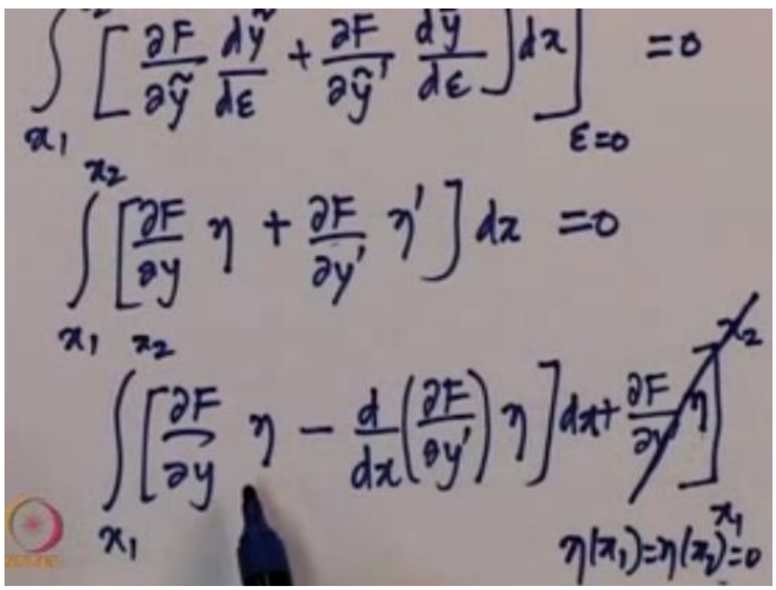

So that is nothing but integral x1 to x2 $[\partial F/ \partial\tilde{y} /d \varepsilon + \partial F/\partial\tilde{y}' \partial\tilde{y}'/\partial \varepsilon]$ dx all of it is evaluated at $\varepsilon = 0$ that is equal to 0 so this is what we have formed as the condition, now when $\varepsilon = 0$ you can see that $\tilde{y}$ will become y itself and so you will get integral x1, x2 $\partial F/ \partial y$ and because ε is 0 $\partial\tilde{y}$ /d ε which will become just η similarly $\tilde{y}'$ will become when ε is 0 $\partial F/ \partial y'$ and this will be η' dx that should be equal to 0 right, so we have implemented the condition that ε should be equal to 0 at the for the extreme I mean this has to be evaluated at $\varepsilon = 0$ and that used to be this one, now η' is nothing but d η/dx.

So I can do an integration by parts and that gets me to the point x1, x2 $\partial F/ \partial y$ and η, if I take d. dx and put it here on top on in front of this so I get $d/xd(\partial F/ \partial y')$ times η integral dx there is an extra term so it is vdx so it will be vu dv which will be uv evaluated at the extreme points –vdu so that is how we got this, so there is that other term so which is δF, so $+\delta F/\delta y'$ and η which is evaluated at the points x_1 and x_2, so this is the excess term that is coming because of the integration by parts.

Now we assume that η at both x_1 and x_2 is 0 so because of that this goes to 0 because we assume that there is no variation at the points x_1 and x_2 notice that I also choose functions for which $\eta(x_1)\eta(x_2)$ might not be 0 as long as $\delta F/\delta y'$ is 0 at these points I can still satisfy this condition.

So we assume one condition but this is not the only condition in which this term will go to 0, in any7 case you can make it go to 0 either by assuming the variations which are consistent with the end points the η by coming 0 or $\delta F/\delta y'$ becoming 0 at the end points so either way you can do it, you end up with this, so let us write that in a slightly simplified fashion.

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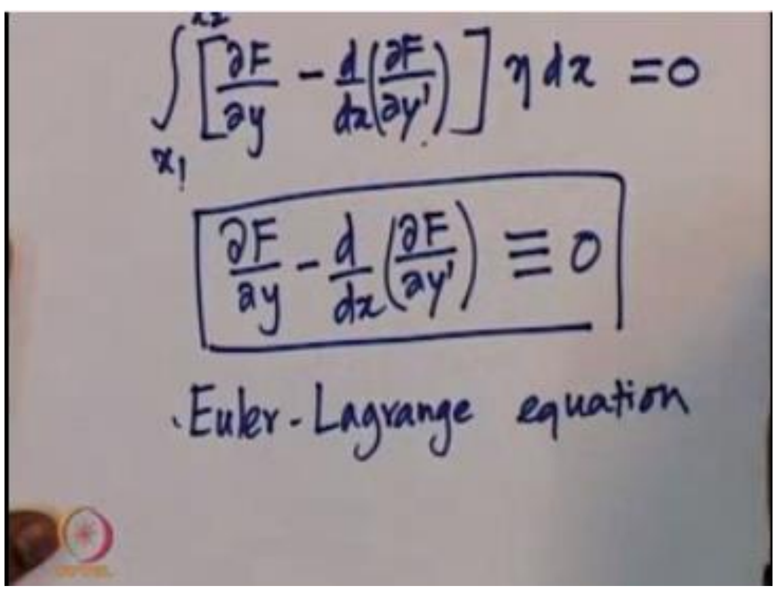

So we get this x_1 to x_2 $[\delta F/\delta y - d/dx(\delta F/\delta y')]$ everything multiplying $\eta dx=0$, now η is an arbitrary function. If you have an integral x_1 to x_2 multiplying some arbitrary function is equal to 0 then it necessarily means that this integral should be 0. Suppose if it is not 0, if it becomes non zero even if at one single point because I have the freedom to choose η arbitrarily I can choose η to be a Δ function, a function which will be only that point will be 0 everywhere else so this integral will become non zero.

So it is not allowed for this integrant to be non zero even at a single point in this domain, it has to be necessarily equal to 0 over their entire domain. This is known as the Euler Lagrange equation, from the derivation it is clear that Euler Lagrange equation is nothing but the necessary condition for a functional to have an extreme why because that so we derived this Euler Lagrange equation we took the functional we demanded that it should have an extreme at some point and we posted as a problem with one single variable so used our usual tailor serous expansionary and we know what is a necessary condition is that necessary condition let to this condition.

So Euler Lagrange equation in the case of functional it is a condition on the variation derivative that it should obey certain equation for that function to have an implement. So this is known as the Euler Lagrange equation of course to prove that the extremer that you have achieved is a minimum or maximum you have to look a the second variation and in general it can be done and it is little bit complicated then not many material science text books I have seen where the second variation is done.

And exception is a excellent text book by Chathorian on structural transformations he does both the first variation and second variation but at most of the cases because the functional that we would write is a physically motivated functional for example it is something like action or it is something like free energy or it is something like an entropy these functional we already know whether they get minimized or maximized right in physically meaningful situation are these functions are going to be free energy for example is always going to be minimized.

So if the problem is post thermo dynamically correctly then that functional automatically if it reach as an extreme I know what type of extreme it is so most of the time we do not worry about the second variation or looking at the next condition which is the sufficiency condition but the necessary condition is the so called Euler Lagrange equation. This is for the function to achieve it is extreme okay.

In most of the physical cases extreme that extreme is basically the equivalent state so this also the condition for example if you are taking a free energy a functional and if you are doing Euler Lagrange equation the solution you get basically tells you that that is he condition for that free energy to be minimized. So at the equal erbium and the free energy is minimized that is what we will achieve in that particular system.

So that is what it means so what we have seen is the definition of the functional how they naturally arise there are many problem in which functional of this type come about and using some tailor serious expansion based ideas about minimization to maximization of single variable functions you can extend it the case of functional and you can derive an expression which tells for a functional to be extreme what is the condition that has to be satisfied that condition is known as the Euler Lagrange equation which is what we have derived in this part.

So this is one of the important pieces apart form look the variant symmetry when we want to look at phase free models okay so this is known as variation calculus so writing functional and taking variation derivative of them is the one of the part of expects of the phase free formulation so we will look at little bit more of details about variations in the next lecture. Thank you.

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