Biomathematics

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Lecture No # 35

Statistical Thermodynamics of Biological Systems Part – II

Hello, welcome to this lecture on biomathematics. We have been discussing statistical thermodynamics, and its application to biological systems. We discussed about energy, entropy, and we briefly mentioned something about free energy. So, and we said that energy is basically, the energy is that we see that that we know, like spring the pulling spring elastic energy to pull it like a spring pulling or wanderwaals energy or electrostatic energy. So, we know energy that we we knew about energy well before, and yesterday we learnt a bit about entropy, and we said that entropy can be quantified by saying that entropy defining it as, entropy is a quantity proportional to the number of possible states.

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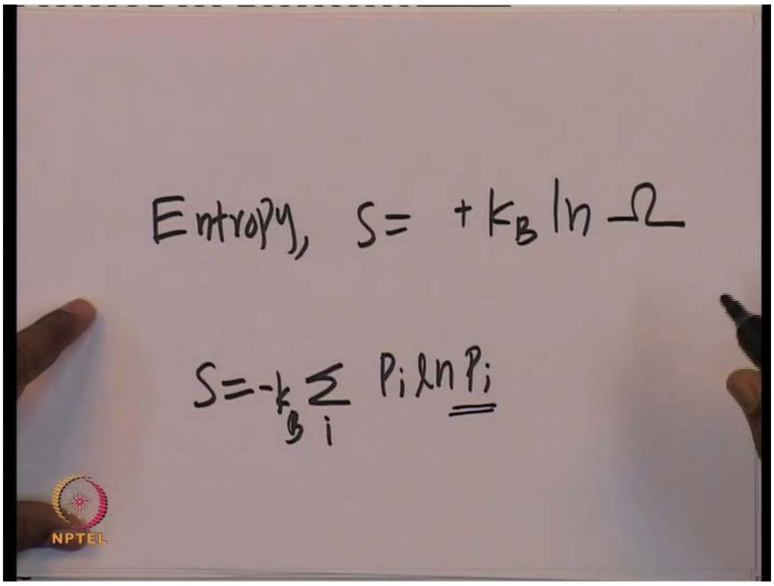

Entropy, $S = +k_B \ln \Omega$

$$S = -k_B \sum_i P_i \ln \underline{\underline{P_i}}$$

So, one and we could count, if we could count the number of states, and we call it omega; we defined entropy as, so, we said that entropy, S is K B log omega, and this is when all states are equally possible or we also wrote an expression minus K B sum over i p i log p i. So, we we told where p i is a probability to be in a particular state i, then you can ask the question, what is the probability to be in a particular state i, we will discuss this today, but this is, we know that, if you know this or this, we can calculate entropy according to this formula, now, let us think a bit about probability to be in a state and so on and so forth.

So, let us today, we will discuss two quantities. So, the the title of lecture is basically statistical thermodynamics of biological systems part 2 and we will talk about some quantity called partition function and free energy. So, we talked about free energy already, now, we will talk a new quantity called partition function. Before talking that, let us let us understand that, we we said that the importance of free energy, we briefly mentioned that any system eventually will go to a state of equilibrium and we defined something called equilibrium and when something is in equilibrium, we can say that our system is in equilibrium, when the free energy has a minimum.

So, if the free energy, if you compute the free energy of the system and if the free energy is minimum, if some some places some places might, you might have studied that, the change in free energy delta g has to be 0, when delta g is 0 or the free energy g itself is minimum or the change in free energy is 0, at that point we can call this as equilibrium. So, we yesterday mentioned F as free energy, some places you have the in biology very often, you might have seen this notation G, in the coming lectures, we will discuss, what is the difference between G and F? So, you might have heard Helmholtz free energy, Gibbs free energy and so on and so forth. So, we will discuss, what is the difference between all these terms, but the concept of free energy is in generally it is true.

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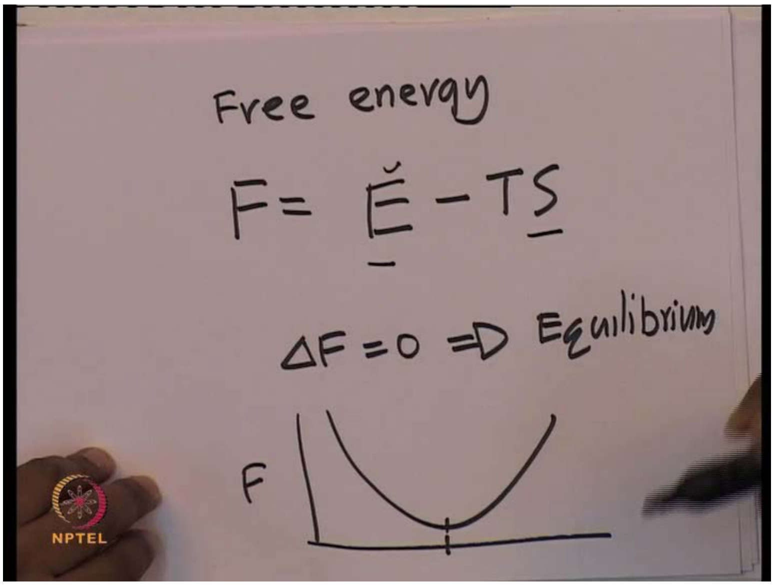

Free energy

$F = \underline{\check{E}} - T\underline{S}$

$\Delta F = 0 \Rightarrow$ Equilibrium

So, we said that the concept of free energy. Yesterday, when we discussed, we said that, free energy is nothing but, we use the notation F, the free energy. So, this is free energy and this is the interaction energy that we know this is like coulomb energy or spring energy depending on the system, this is the energy that we, the potential energy or the interaction energy minus temperature types entropy. So, the free and whenever F is minimum or delta F is 0, we will give you will give lead to equilibrium equilibrium. So, this is the definition of equilibrium.

A system is in equilibrium, when the free energy is minimum or the change in free energy is 0 or we told that, if you plot free energy as a function of any parameter and for whatever that parameter value, you will have this minimum and this is the point where the system was in equilibrium and we will discuss about this equilibrium in detail, but this is this is the importance of free energy by knowing the free energy, we can know whether the system is in equilibrium or not by calculating either delta F or delta G.

So, we will discuss that, but the point you all, want to all of you want, I want all of you to note is that the free energy is the quantity that determines whether the system is in equilibrium or not has energy and entropy. So, it is not enough to just know energy, you have to know also entropy, so that, the combination of energy and entropy is what decides free energy and the free energy is what decides many other things. We will see that free energy decides, many of the properties that we measure, when we do an experimental measurement, all the measurable quantities that we discussed basically will be determined by the free energy.

So, if we know the free energy, we can know many other quantity, we can we can guess, we can understand, we can learn many things about many of the quantities. So, we have two quantities, energy and entropy and a combination of both is required to understand about the system. Now, there is a new quantity which I will discuss, which is called the partition function.

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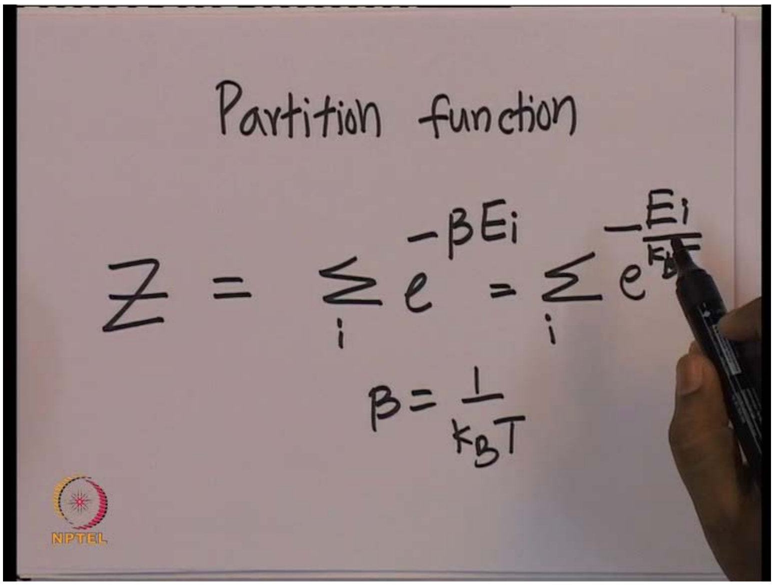

Partition function

$$Z = \sum_i e^{-\beta E_i} = \sum_i e^{-\frac{E_i}{k_B T}}$$

$$\beta = \frac{1}{k_B T}$$

So, this is partition function and this will be denoted by this zed. So, what is zed? So, it turns out that the definition of zed partition function is that, it is sum over all states where beta, I will explain this in a minute. So, if you take exponential of the energy multiplied by beta, beta is basically 1 over K B T or this is, this can be written as e or this can be or this is same as sum over i e power minus E i by K B T. So, if you know the and i is where, if you imagine that the system is in state i and the energy of the system is in state i is E i, you do this, if you know this energy of the system for every state, you exponentiate it, e power minus beta times E i where beta is 1 over K B T, K B is Boltzmann constant, T is temperature.

And if you do this sum, what you get is, this quantity called partition function and this has a relevance, in the sense that, now, there is a relation between partition function and free energy that is what we will go discuss in a minute, but just understand this bit more how to calculate partition function. So, if the, if a system has many states, let us say five states. So, imagine for a moment, imagine that, you have a you have a protein imagine that you have a protein which has three states.

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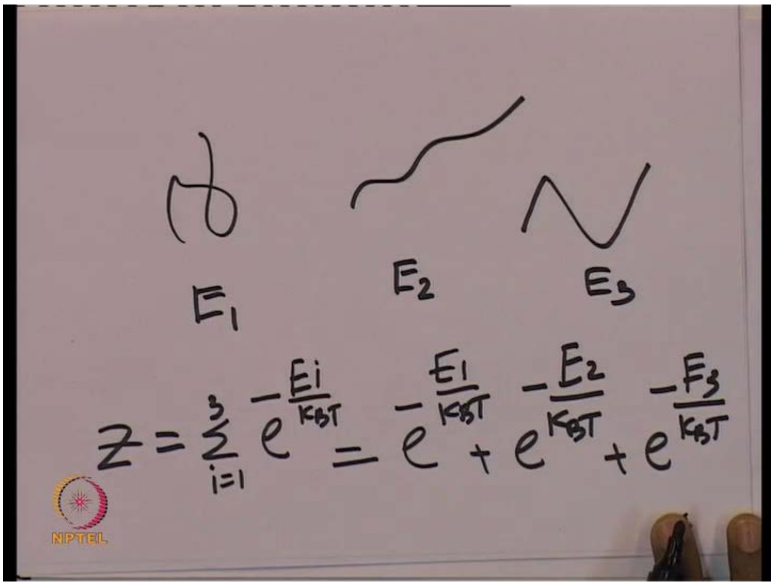

So, imagine that there is a protein which can, this can be one state, this is some other state and let us say this is different state. So, the protein can have three states, let us say and the energy in the state is E 1; energy in this state is E 2 and energy in this state is E 3 then the partition function zed is given by sum over i from 1 to 3, there are three states, so, 1 to 3 e power minus E i by K B T, this is this is the definition of partition function, this means that, e power minus E 1 by K B T plus e power minus E 2 by K B T plus e power minus E 3 by K B T.

So, if you calculate this e power minus E 1 by K B T plus e power minus E 2 by K B T plus e power minus E 3 by K B T, you will get a quantity and that quantity is called partition function and once you know the partition function, we can calculate many quantities, we will discuss that in detail, but this is the definition of partition function, e power minus energy in the state 1 by K B T plus e power minus energy in the state 2 by K B T plus e power minus energy in the state 3 by K B T and if there are more states, you sum like this for many times. So, what we have now, is e power minus beta E by K B T by…

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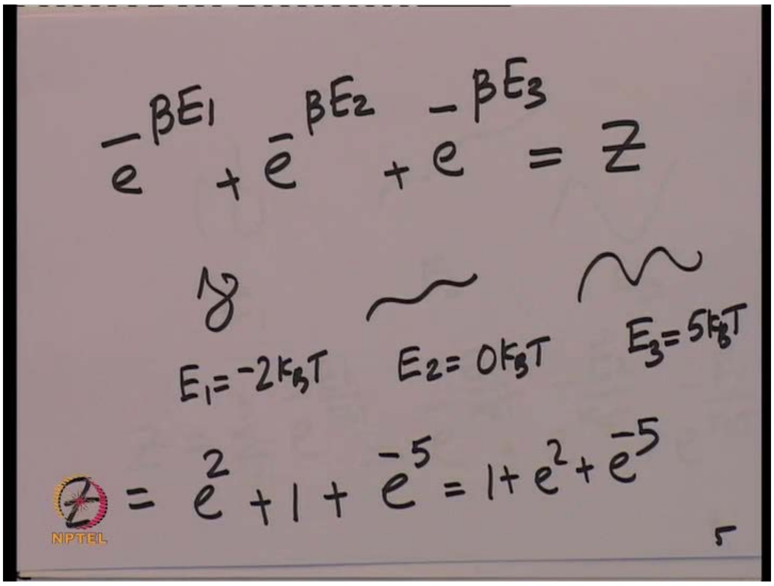

$$e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3} = Z$$

$E_1 = -2k_BT$ $E_2 = 0k_BT$ $E_3 = 5k_BT$

$$Z = e^{2} + 1 + e^{-5} = 1 + e^{2} + e^{-5}$$

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So, let let me write this once more. So, you have protein with three states e power minus, let me write this is beta or beta is 1 over K B T plus e power minus beta E 2 plus e power minus beta E 3, this is our partition function zed. Now, let us say, we said that there is three states for the protein, one is a state like this, one is a straight state and one is a state like this and let us say that, I am saying that the energy of the state one is minus 2 K B T. K B T is a unit of energy, 1 K B T is about ten power minus twenty one joule, we can calculate this K B T is a unit of energy, let us say E 2 is 0 K B T does not cost anything to be like this and let us say E 3 is 5 K B T.

So, these are values, now, let us substitute this. So, now, if you substitute this E 1 as 2 K B T beta is basically 1 over K B T. So, the zed becomes zed is equal to e power minus beta times minus 2 K B T. So, e power minus minus will become to e power 2 and K B T and beta cancels because beta is nothing, but 1 over K B T. So, e power 2 plus, if you substitute E 2 here this will become 0, e power 0 is 1. So, this is 1 plus e power 5, if I substitute will become minus 5. So, this is a number. So, partition function is essentially as a number. So, this is basically 1 plus e power 2 plus e power minus 5.

So, you know E is a number. So, you can take a calculator and calculate e power 2 and e power minus 5, you will get some numbers, e power 2, you will get something like very close to nine something like eight point something, you might get around eight, e power minus 5, you will get a very small number. So, this answer will be some some number around nine or ten something like something like that number, you will get. So, this is this is the rough answer you will get. So, z is essentially a number. So, what is the use of knowing z, it turns out that the free energy is nothing, but the log of partition function.

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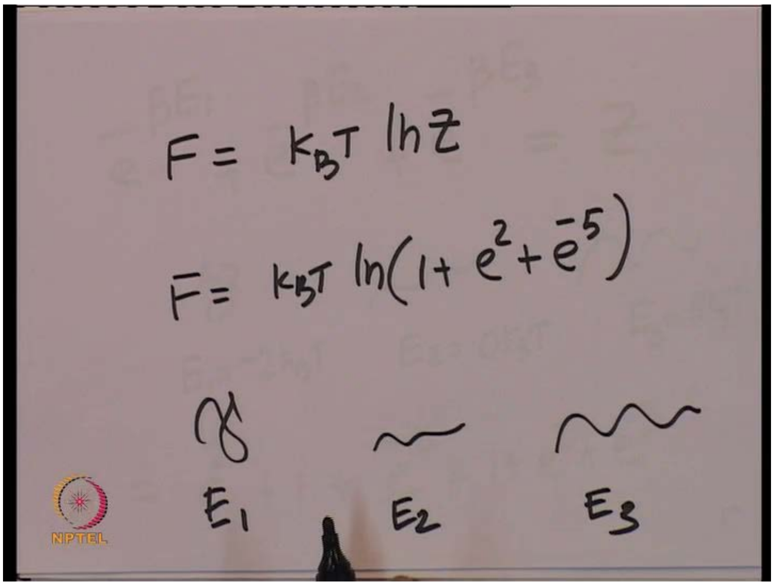

$$F = k_B T \ln z$$

$$F = k_B T \ln(1 + e^{2} + e^{-5})$$

So, it turns out that free energy F is K B T log z. So, if you know the partition function z, you can find the log of it and multiply with K B T and you will get free energy. So, z is a number, log of the z will be some other number and you multiply with K B T, you get unit of energy. So, the if you know the partition function, it is easy to calculate free energy. So, if you know all the states here, you can take the log of this and so, in this case, 1 plus e power 2 plus e power minus 5. So, if you have the free energy of this system is K B T log of 1 plus e power 2 plus e power minus 5.

So, this will be the free energy of that system of protein having three states like this. We said that this is E 1, energy E 1; this is energy E 2 and this is energy E 3 and sum over e power minus beta E 1 plus e power minus beta E 2 plus e power minus beta E 3 gave us this and then you multiply and you take a log and multiply with this, so, you get this. So, once we understand the partition function, once we can calculate the partition function, calculating free energy is easy, we do not need to calculate entropy separately because we are summing over all possible states already here, sum over i. So, we are summing over all possible states and multiplying with e power minus beta e.

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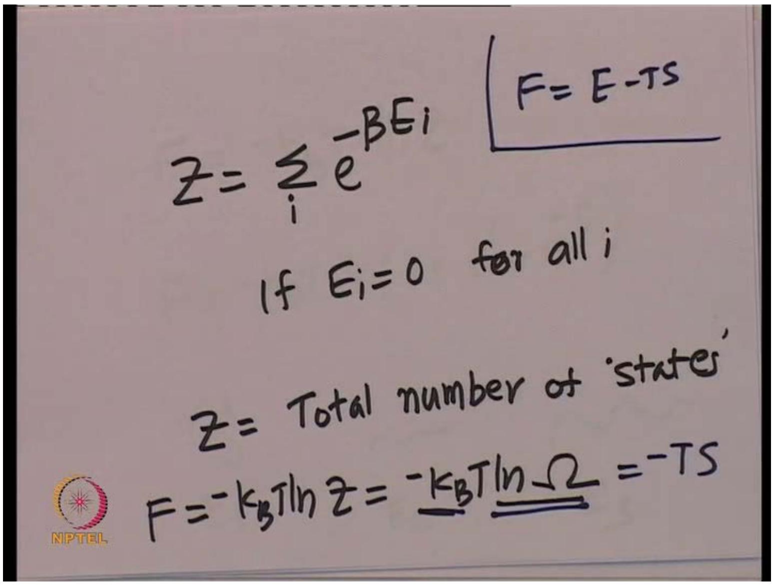

$$\boxed{F = E - TS}$$

$$Z = \sum_i e^{-\beta E_i}$$

If $E_i = 0$ for all i

$Z =$ Total number of 'states'

$$F = -k_B T \ln Z = -\underline{k_B} T \underline{\underline{\ln \Omega}} = -TS$$

So, now, let us imagine that, so, let us look at the definition once more. So, we saw, we said that Zed is sum over i e power minus beta E i, if E i is 0 for all i, this will be sum over i, this will be like just just like zed will be like total number of states (No audio from 15:35 to 15:41). So, zed will be just total number of states because i is equal 1 to n e power 0. So, this will be like e power 0 plus e power 0 plus e power 0 n times where there are n states. So, then a free energy will be K B T log zed which will be K B T log, the number of states omega.

So, that that tells us that there there has to be minus. So, actually there is a minus sign minus K B T log zed. So, this will become K B T minus log omega and we know that K B log omega is nothing, but entropy. So, this part, this K B log omega is entropy. So, this is basically T times entropy. So, this will become minus T S. So, when energy is 0, the free energy has to be minus T S because we know that, F is E minus T S, we learnt that, F is E minus T S. So, if when E is 0, the energy, free energy has to be minus T S. and we got minus T S. So, just just one thing is that, we have to just say that free energy has a minus sign here.

So, with this, we we understand how to calculate free energy and we understand that this is nothing, but the same as this. So, we can calculate it both way either we can calculate this way or we can calculate this way and you will get the same answer. So, we know two ways to calculate free energy now. And now, what is the use of, we will

will take some real example and calculate it also and then we will also calculate, what what is the use of knowing all this.

Now, one more thing related to partition function, we have to know. Now, i said that when the system is in equilibrium, the free energy of the system will be it is lowest, the minimum value. So, then then you can call it an equilibrium, that is a stable when this is this is the system will be in a very stable equilibrium .Now, let us think of we will we will discuss an example, but before that, the modern view is that, the system for example, a protein in principle can go to all possible configurations.

So, you can find the protein in all possible configurations, but the probability of finding it in the equilibrium configuration will be much higher than in the other configurations.

So, the view in statistical thermodynamics is probabilistic, we do not say the system will always in one place, we will say that the probability of finding a protein in a given state is this much. So, we can only talk in terms of probabilities because the system in principle, if you wait infinitely long enough, if you put a protein and then wait millions and millions of years or if you can wait infinitely long, the protein can take any conformation it wants, it can take all possible conformation that is the view of statistical thermodynamics.

So, and that therefore, but the probability of taking certain conformations will be very very very small, it can be as small as a very close to 0; that means, you will you will hardly see it, you may not even see it or you might have to wait infinite time to see it. So, we, now, we have to ask the question, how do we know, that what is the probability of finding a system in a particular state, let us say state one or state two or state three . So, we talked about certain proteins.

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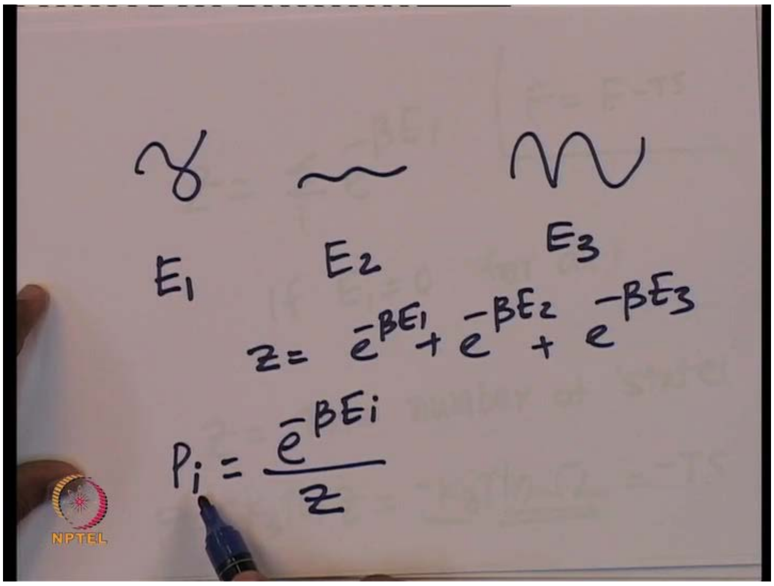

E_1 E_2 E_3

$$Z = e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3}$$

$$P_i = \frac{e^{-\beta E_i}}{Z}$$

So, we said that imagine that the protein has conformations like this, three conformations, conformation one, conformation two, conformation three and this is an energy E 1; this is energy E 2 and this is an energy E 3 and we said, how to calculate zed which is e power minus beta E 1 plus e power minus beta E 2 plus e power minus beta E 3 . Now, you can ask the question what is the probability, that you will find the system in this state and the answer is the probability of finding a system in state i is e power minus beta energy of that divided by the partition function. So, if you know the partition function and if you know energy of a state, we can know, what is the probability of finding the system in a given state i. So, we can ask the question there are three states here, we can ask the question what is the probability of finding the system in state one, state two and state three.

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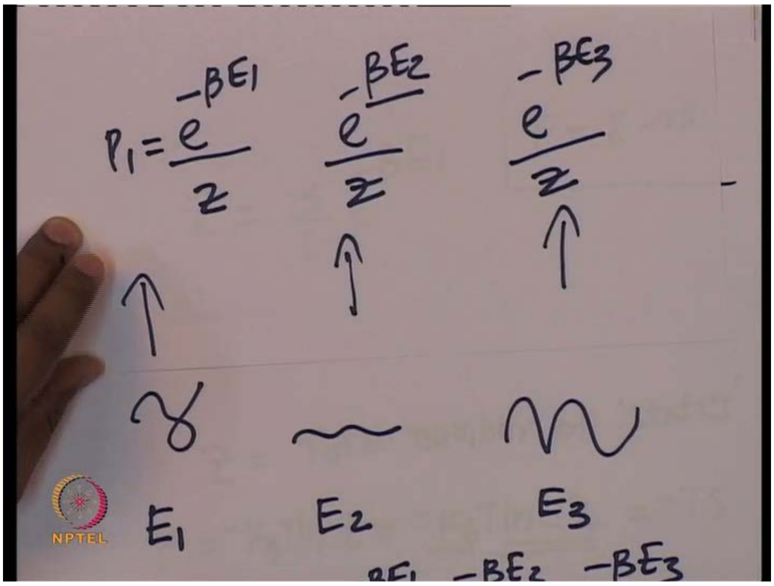

So, the probability of finding the system in state one let me call this P 1, probability of finding the system in this particular state which has an energy E 1 is nothing but e power minus beta E 1 divided by z. So, this is the probability of finding the system in this particular state, what is the probability of finding the system in this state which has an energy E 2 and the probability the finding there is, e power minus beta E 2 by E 2 divided by z and this probability of finding here is e power minus beta E 3 divided by z.

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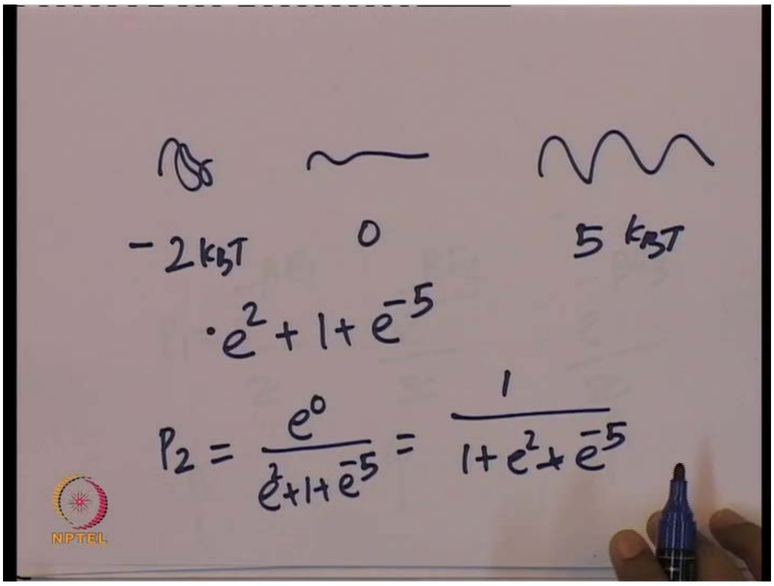

So, we now have some values for z here, we said that the z can be calculated, we we put some values, we said that, the three states, the curved state, straight state and curly state like this this has energy, we said 2 K B T, 0 K B T and sorry this is minus 2 K B T, 0 K B T and 5 K B T these are the energies of this state and we said that the partition function will turn out to be e power 2 plus 1 plus e power minus 5, this e power minus 2 minus minus 2 will be 2, plus 1, minus 5.

So, now probability of finding in this particular state let us say, probability of finding in this particular state, in the middle state p 2 will be e power 0 divided by e power 2 plus 1 plus e power minus 5; that means, e power 0 is 1, so, 1 by 1 plus e power 2 plus e power minus 5, this is p 2. Similarly, you can calculate p 1 and p 3 and if you check, if you do this. So, similarly, you can calculate p 1 and p 3 lets quickly calculate this.

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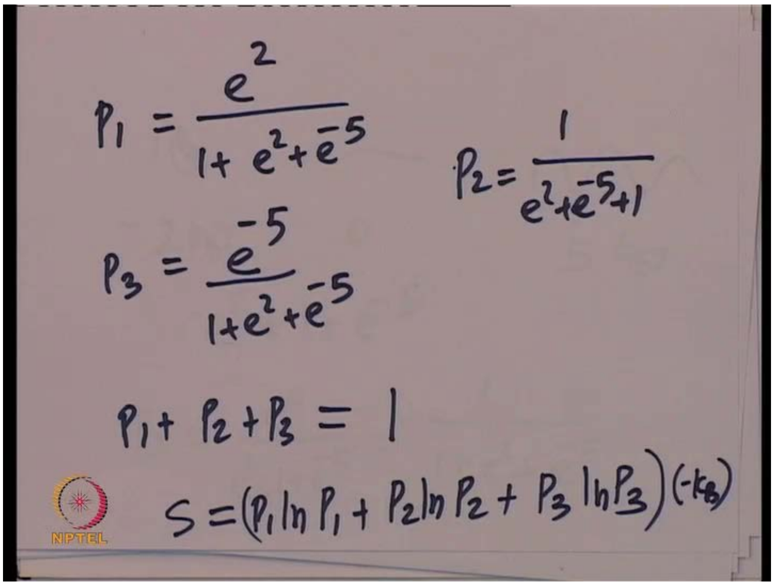

$$P_1 = \frac{e^{2}}{1+e^{2}+e^{-5}} \qquad P_2 = \frac{1}{e^{2}+e^{-5}+1}$$

$$P_3 = \frac{e^{-5}}{1+e^{2}+e^{-5}}$$

$$P_1 + P_2 + P_3 = 1$$

$$S = (P_1 \ln P_1 + P_2 \ln P_2 + P_3 \ln P_3)(-k_B)$$

So, you you can do this and you can see that, you will see that p 1 is basically e power 2 divided by 1 plus e power 2 plus e power minus 5 and p 3 will be e power minus 5 divided by 1 plus e power 2 plus e power minus 5 and we will see that p 1 plus p 2 plus p 3, the total probability, this is the probability of finding in any of these three states, the total probability of finding is 1. So, we know this p 1, p 2 and you can see p 3, p 2 we wrote, which is e power 0 which is 1 1 by e power 2 plus e power minus 5 plus 1. So, the denominator is same in all this and the sum of numerator will give you, 1 plus e power minus 5 plus e power 2 and this will become 1. So, you can see that, if you know partition function, you can calculate the probability of finding the system in any state i and from that, you will you will get the total probability.

So, now here, you know this probable. So, you know how to calculate p i and from this you know, once you know p i, you will also know, you might remember the formula for entropy which is p i log p i. So, the entropy of this system, if you want to calculate. So, look at this here. So, you have this system we know p 1, we know p 2 and we know p 3, p 1, p 2, p 3 and if you want to calculate entropy is easy, entropy of this system is p 1 log p 1 plus p 2 log p 2 plus p 3 log p 3 .

So, we know p 1, we know p 2, we know p 3, if you add this and multiply with minus K B, you will get entropy. So, minus K B log minus K B, p 1 log p 1 plus p 2 log p 2 plus p 3 log p 3, this will be the entropy. So, now we understand, how to calculate various things, we know how to calculate partition function, from partition function we know how to calculate free energy we know how to calculate free energy, if we know the entropy and we know the how to calculate entropy, if you know, if you the system if the system had different states and if all the states had different energies, we just saw that in this particular way, we could calculate entropy.

So, now our aim is, we we yesterday calculated the entropy of a simple protein which had no particular energy. Now, we will think of one very famous model which can describe for example, the conformations of D N A. So, there is, this is an important questions in biophysics in general people have been wondering that, if you have a piece of D N A in water, what will be the conformation of D N A, what will be the most preferred conformation of the D N A.

So, it turns out that, it depends on the length of the D N A, if the D N A is very short or very large, it will have various conformations, but using the idea of statistical thermodynamics we can compute, we can calculate, what will be the most preferred conformation of a D N A of a given length L. Now, this has a very popular simple model called worm like chain model of a DN A and we will briefly discuss that and we see, how to calculate the partition function for this D N A and we will see what we can learn from the partition function later.

So, today right now, we will discuss calculating a partition function of a piece of D N A and you know that, once you know the partition function we can also also calculate, what is the probability of the D N A shape being in particular shape and this has some importance because like various context in biology, it turns out that for a various gene expression for a promotion for a when various proteins repress or promote gene expression.

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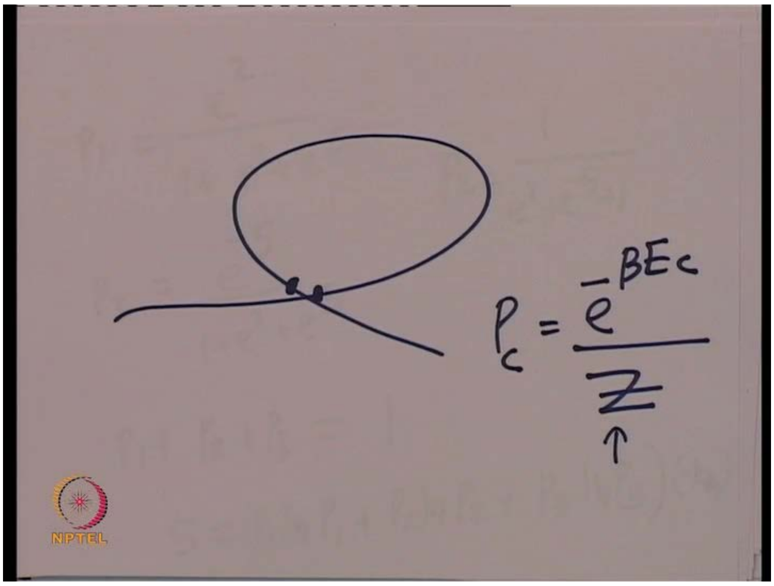

The d N A typically forms a loop like this. So, this end of the D N A and this end of the two parts of the D N A has to come together for such that certain either gene expression or gene repression will take place depending upon the context. So, you can ask the question, if you have a length D N A of length L, what is the probability that two parts of the D N A will come together and the probability will be given by probability will have to have this particular configuration c will be given by e power minus beta energy of that configuration divided by the partition function.

So, this will be the probability here to have this particular configuration. So, energy of that configuration divided by the partition function. So, if you know, how to calculate partition function, you can calculate the probability that the D N A has a particular confor conformation. So, now, we will discuss how to calculate partition function for the D N A in a given model.

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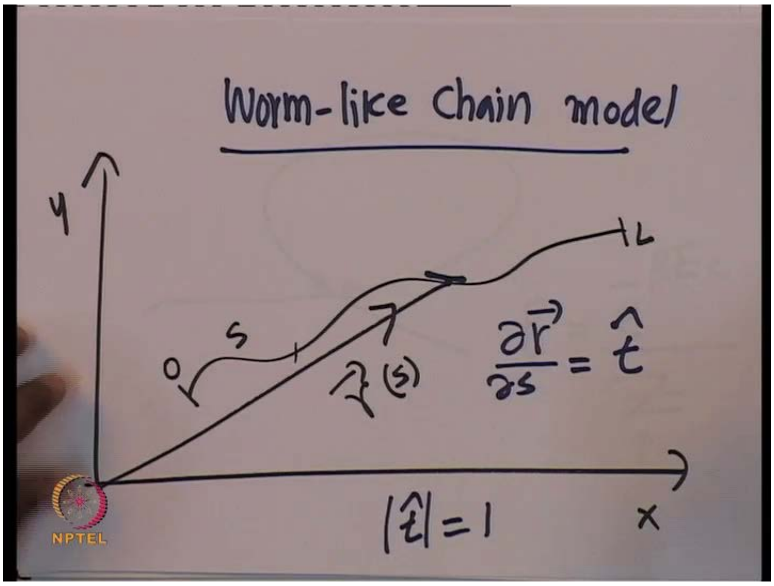

So, the simplest model for the D N A, you might have some of you might have heard of this called worm-like chain model worm-like chain model. So, this is a good model for double standard conformations of double standard of D N A. So, the assumption here is that, D N A can be thought of as a line for simplicity which represents basically the central line across the double stand, you would not consider the complete double stand, it is to understand what conformation it will take, it is enough to think of D N A as a line.

This is the assumption of this model and if each point of this line, you can have a, so, if you have a coordinate, this is x and y. Each point on this D N A can be represented by a vector and this this is 0 and this is the length of the D N A, L and you can think of one parameter called S which is arc length, the length along the contour of the D N A. So, if you, this is S is the parameter, S something that varies from 0 to L. So, if it is here, the S is this much, S is the length from one end to that particular point along the contour.

So, every point at any point S, you can draw a vector r from some coordinate system and at any point, you can also define a tangent vector. So, you can define a tangent vector here, which del r by del s, the derivate of the r at any point, we can define as tangent vector and it turns out that, this is a unit vector. So, the worm-like chain model assumes that the D N A is inextensible, if you apply some force and pull it ,the D N A will not extend, this is an assumption of the model and it turns out that for small forces, typical D N A of typical lengths, they do not show any stretching.

So, based on this fact, it is assumed that D N A will not get stretched. So, worm like chain model assume that, D N A will not stretch. So, somehow… So, this this mod t is 1, this mod of this tangent vector. So, think of what is the what are we saying now, D N A is a line and you can define a vector at every point r and the derivative of this vector is tangent vector. So, at every point, you have a tangent vector, so, if you think of slightly more clearly.

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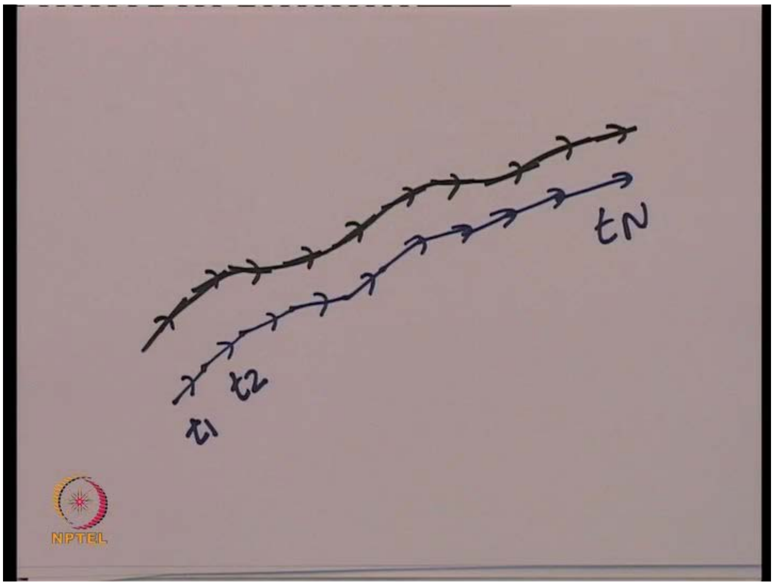

So, you can think of D N A as as set of a line like this, at every point we can define a tangent vector (no audio from 32:14 to 32:20). So, equivalently this could also be thought of as, a set of tangent vectors like this (no audio from 32:30 to 32:34). So, this is the power of mathematics here that, we wanted to describe this idea through some equations. So, and we have a tangent vectors. So, let me call this t 1, t 2, you can call it t 3 up to there are n tangent vectors t N.

So, D N A could be thought of as n tangent vectors. So, each of the tangent vectors could be one base pair long for example, or it could take whatever length you want discretized unit as a tangent vector. So, typically you could think of it as each base pair as tangent vector. So, and many each, there are many many base pairs organized like this. So, D N A could be thought of or any protein in principle could be thought of as, any polymer could be thought of as combination of many sub units. So, in this particular way D N A could also be thought of as a set of tangent vectors t 1.

Now, what is the energy of this system? So, it turns out that D N A does not like to bend D N A like to be in a straight conformation beyond if D N A is very short, it would like to be straight, if D N A is very long, it might be bending. So, to put in this fact that D N A does not like bent, if you want to bend D N A, you have to do some work. So, you have to put some energy to bend the D N A and the energy is depends on how much you bend this tangent vectors.

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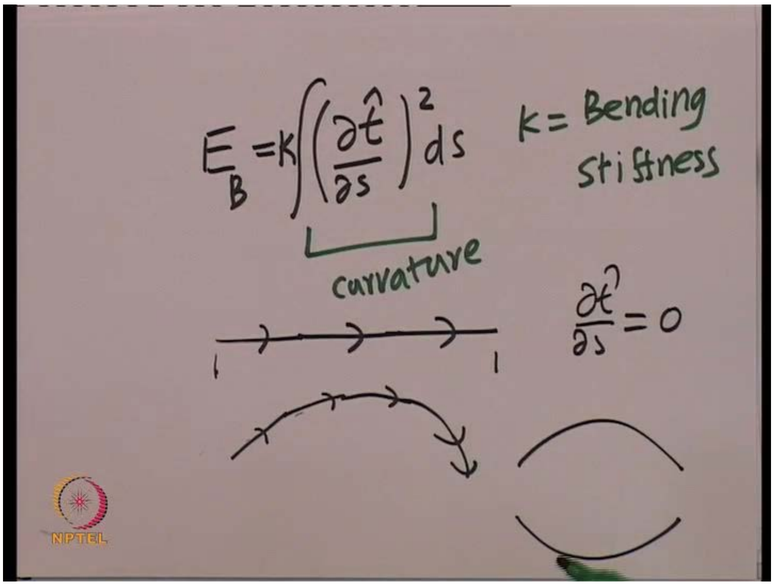

So, it turns out that, this can be the energy can be written as E is equal to del t by del s whole square integral d s with some constant kappa. So, this is the bending energy of D N A, what is the logic behind writing down this equation. So, we want to write down bending energy and the logic behind is that, if the tangent vector changes, if there is no bending or then tangent vectors will be straight then the d t by and this is, s is something varying from here to here. So, if as you go along the s which is this distance, if the tangent vector does not change then del t by del s will be 0.

So, there the bending energy will be 0. On the other hand, if it is bent, the tangent vector would have changed. So, the del t then the tangent vector here is like this, here is like this. So, tangent vector along the contour changes its direction. So, if the tangent vector changes its direction then there is a bending and therefore, the bending has to be proportional to del t by del s, now, why is it square because del t by del s has different sign, if it is like this or like this, but the energy to bend, if you take any filament, if you think of any filament, if you bend this way or this way, it is the same energy, if you assume everything as symmetric. If you bend this way or this way, same energy therefore, the energy should not depend on which way you bend it.

So, therefore, del t by del s has a sign, we do not want the sign to come in the energy. So, we have to the simplest way to put this square. So, del t by del s by whole square and the sum of this bending energy bending this is the curvature, basically we discussed something about curvature earlier in calculus. So, this is curvature and when we discuss, we said we said something about bending energy. So, this is a curvature energy, curvature and curvature sum over curvature and multiply with a constant and this kappa is called bending stiffness bending stiffness, if it is more, the bending stiffness is large for a, this is applicable for many proteins also.

So, depending on the system, if depending on the filament, if it is D N A kappa has a particular value, if the filament you have that you think of is a protein kappa has a different value. So, kappa is a parameter that represent the property of the filament that we are discussing. So, for a D N A kappa has a particular value, we will see what the value is.

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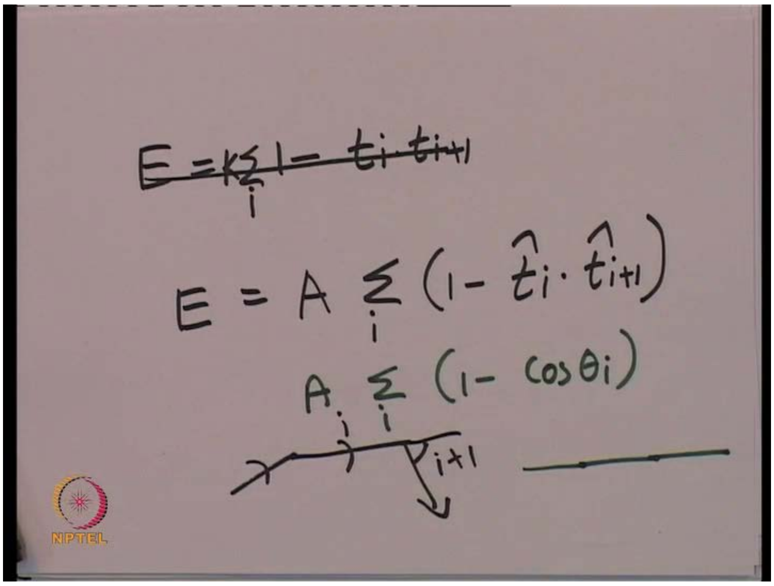

$$~~E = K\sum_i 1 - t_i\, t_{i+1}~~$$

$$E = A \sum_i (1 - \hat{t}_i \cdot \hat{t}_{i+1})$$

$$A \sum_i (1 - \cos\theta_i)$$

So, this is the bending energy and we can convert it turns out that, this can also be written as E is equal to 1 minus t i dot t i plus 1 sum over i and there is a kappa, there is a different kappa, so, let me call this kappa. So, let me call this E is basically some constant A times sum over i 1 minus t i dot t i plus 1. So, it can also be written like this, what does this mean, t i dot t i plus 1, if we have vectors tangent vectors like this, t i dot t i plus 1 is the product between two tangents. If this is i th tangent vector and this is i plus 1 tangent vector, this t i dot t i plus 1 is the cos of the A dot B is A B cos theta, these are unit vectors.

So, t i dot t i plus 1 is basically the cos theta cos of angle between this two. So, it depends on the angle, if the angle is too much, Cos of the angle is too much more the bending energy. So, the bending energy can also be represented in this particular manner or you can call this one minus Cos theta i. So, you can write this also as A into sum over i 1 minus Cos theta i.

The Cos of the angle, if everything is straight Cos theta will be 0 sorry Cos theta will be 0, so, Cos theta will be 1 and 1 minus 1 will be 0. So, the bending energy will be 0, if the filament is straight, the bending energy will be 0, if the filament is bent with there will be some angle. So, there we will have bending energy will have some particular value. So, this is the bending energy of a D N A in worm-like chain of the D N A in the worm like according to worm like chain model. Now, you know the energy, if you know now a particular configuration, we can calculate the energy let us think of some particular configuration of D N A.

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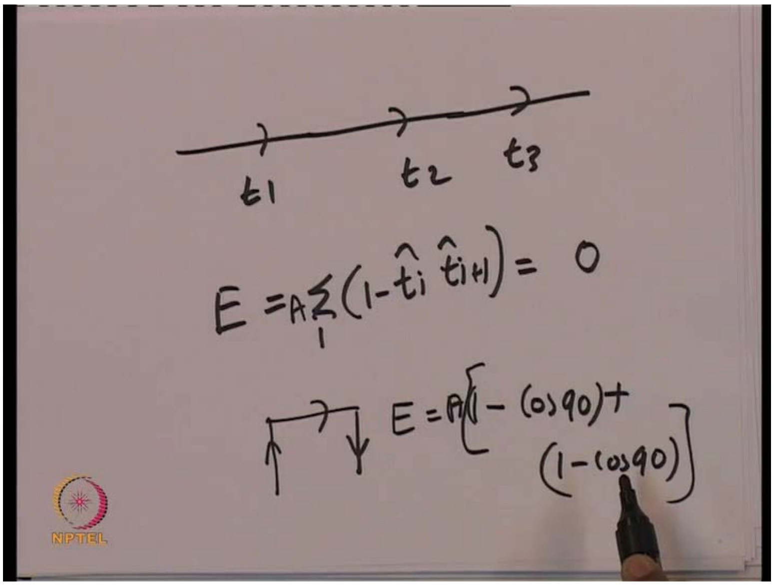

So, let us think of think of D N A which is like this. So, let us think of first, let us think of D N A like this. So, this is t 1, t 2, t 3 and here they are all straight. So, the angle is t 1 dot t 2 is 0. So, it turns out that the Cos theta t 1 dot t 2 is Cos of 0 is 1. So, the energy of this conformation is sum over i 1 minus t i dot t i plus 1 and the t i dot t i plus will become just 1. So, this will become 0. The energy will become 0, if the conformation was let us say, let us imagine some very funny conformations like this.

So, the angle between this is ninety degrees. So, the energy of this, so, there is three tangents and two angles. So, there is energy of this will be 1 minus Cos of 90 and there is there is an a here, a into 1 minus Cos 90 plus this is also 90 degree again, 1 minus Cos 90. So, Cos 90 Cos pi by 2 is basically, so, Cos 0 is 1 Cos pi, so, Cos 90 is 0. So, this is 1 minus Cos 0, Cos 90 is 1. So, this is 1 plus 1 is 2. So, let me write it little more carefully this.

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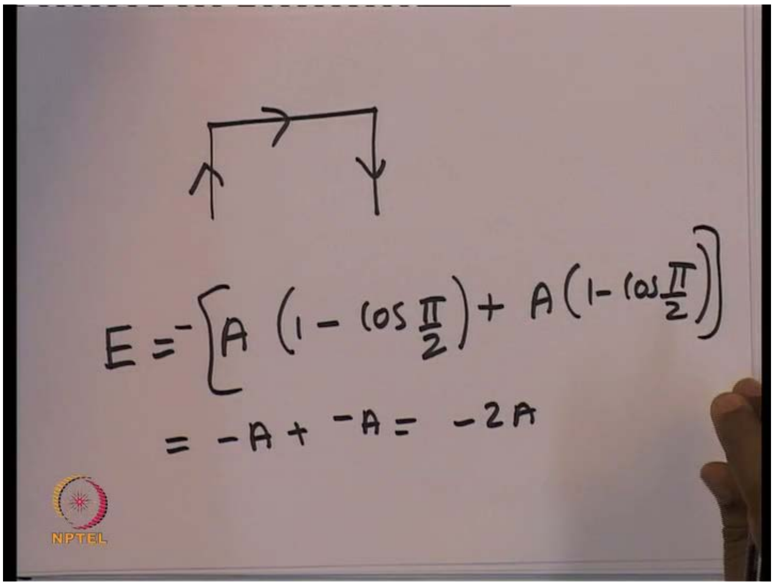

$$E = -\left[A\left(1 - \cos\frac{\pi}{2}\right) + A\left(1 - \cos\frac{\pi}{2}\right)\right]$$

$$= -A + {}^{-}A = -2A$$

So, what we want to calculate is basically energy of this. So, if D N A had this particular shape, the energy here is, the angle here is 90 degrees. So, energy is A into 1 minus Cos, this angle is pi by 2, so, pi by 2 plus A into 1 minus Cos pi by 2 and pi Cos pi by 2 is 0. So, 1 minus Cos pi by 2 is 1. So, there is there is also minus sign here. So, the energy whatever we discussed, the discreet energy that we discussed, has a minus sign, so, minus A into 1 minus t i dot t i plus 1. So, this answer will have a energy which is minus A into plus minus A, so, minus 2 A. So, there is an overall minus sign for the discreet energy.

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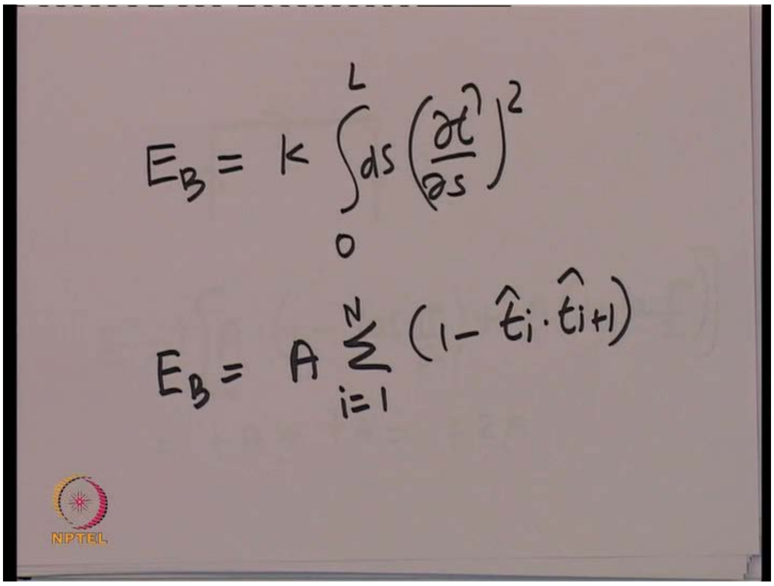

$$E_B = k\int_0^L ds\left(\frac{\partial t}{\partial s}\right)^2$$

$$E_B = A\sum_{i=1}^{N}\left(1 - \hat{t}_i \cdot \hat{t}_{i+1}\right)$$

It turns out that, the bending energy we discussed the bending energy we discussed kappa times integral 0 to L d S del t by del s whole square. If we convert this to a discreet format, you will get E B as A times sum over i is equal to 1 to, so, there is no minus sign, this is correct what i wrote, 1 to n, 1 minus t i dot t i plus 1. So, this is the correct answer. So, this you will get this answer, there is no minus sign here. So, this is plus plus, the answer will be 2 A. So, there is no minus sign here, whatever we discussed is correct. So, A into 1 minus Cos pi by 2 plus A into 1 minus Cos pi by 2, the answer is 2 A.

So, the energy of this system will be 2 A. So, these are the two energies in the discreet worm like chain model, energy bending energy is kappa into d t by d s whole square and here, it is a discreet format there will 1 minus t i dot t i plus 1 where t i is unit vector. So, now, if you know the energy now, we can think of calculating the partition function. So, the partition function is sum over all states e power minus beta E.

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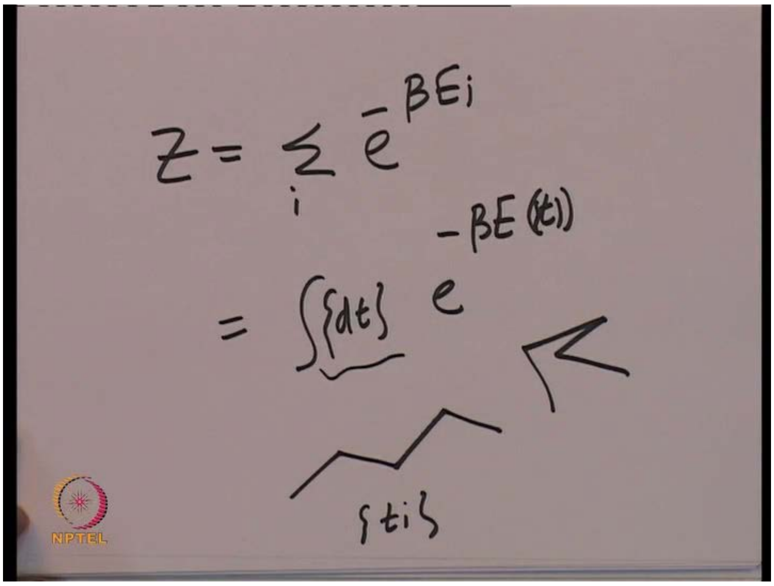

So, we can write the partition function in two ways, Z is sum over i e power minus beta E I, we know E i or you could write in an a continuum fashion, instead of sum you can use integral over all possible conformations, what is I I will explain to you, what is this I mean, e power minus beta E, E will depend on the value. So, now what is this d t means? So, if you have a particular, this is one conformation, this is another conformation. So, one set of t, this is t 1, t 2, t 3, t 4, this is one set of t.

So, this is t i, t 1, t 2, t 3, one set of t will give you one conformation, another set of t’s will give you another set of conformation. So, all possible sum over all possible conformations. So, sum over all possible conformations is, what it is. So, whenever is sum over i, this is sum over all possible conformations and this what, this represents, you have you have to have set of t’s and all possible set of t s will give you and sum over this e power minus beta E and E depends on these t s orientation of t s that is why E wrote E bracket t because E depends on t, you will get this.

So, now how do we do this? So, now, it turns out that, if we can calculate this, we can calculate the partition function and then we can calculate the probability of finding a D N A in a particular state. So, now, let us quickly calculate this in the in the continuum format. So, see see we have to do it. So, let us, so, let me let us understand, what do you mean by all possible conformations. So, when we when we say all possible conformations lets think of a simple example, let us think this as a D N A. So, this is one conformation possible, this is like this. So, we have one base pair, another base pair.

So, we have two base pair, this is one conformation. Now, if you have this, this base pair, if it changes a bit, this is a different conformation, this is a different conformation, this is a different conformation different conformation. So, this is... So, I can go have a set of conformations here itself. So, by varying one this angle, I can vary all possible conform. Now, I can have slightly like this and have all possible conformations. So, I can have when I say all keeping this tangent constant, I can vary this tangent in all possible angles, around all over this in 3 D and all of this is different conformations, this is a different conformation, this is a different conformation, this is a different conformation.

So, when you think of a polymer with two monomers by varying one of it, the monomer all over you will get different then for each of this you can vary this also. So, if you call this as tangent vector one and this as tangent vector two, t 1 and t 2, integral of t 1, the sum of t 1 over all possible angles will give you and will give you all possible conformations, you integrate over you sum over all possible angles keeping the other one fixed then keeping this one fixed you sum over all possible angles here then that will give you another set of conformations and for each of this, you have all possible angles for this.

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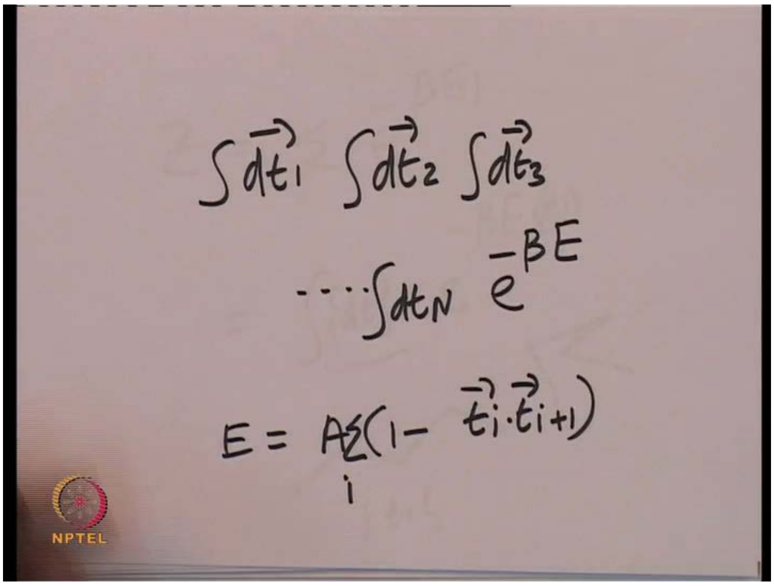

$$\int d\vec{t}_1 \int d\vec{t}_2 \int d\vec{t}_3 \cdots\cdots \int dt_N \, e^{-\beta E}$$

$$E = A\sum_i (1 - \vec{t}_i \cdot \vec{t}_{i+1})$$

So, the way to write it is, the first tangent vector d t 1 can take any values integral over all possible angles and the second one also can take all possible conformations, the third tangent vector can also take all possible conformations dot dot dot and similarly, there could be N tangent vectors. So, each of this tangent vector can take all possible conformations and e power minus beta total energy and total energy we know is A times 1 over t i dot t i plus 1 and sum over i. So, A into sum over i 1 minus t i dot t i plus 1 will be the energy and this will give you this answer. So, now let us think about this d t 1 A bit. So, i just said in a, we just discussed that, we can have all possible angles. So, now in 3 D, we can have, there are two angles phi and theta. So, we can sum over phi and theta.

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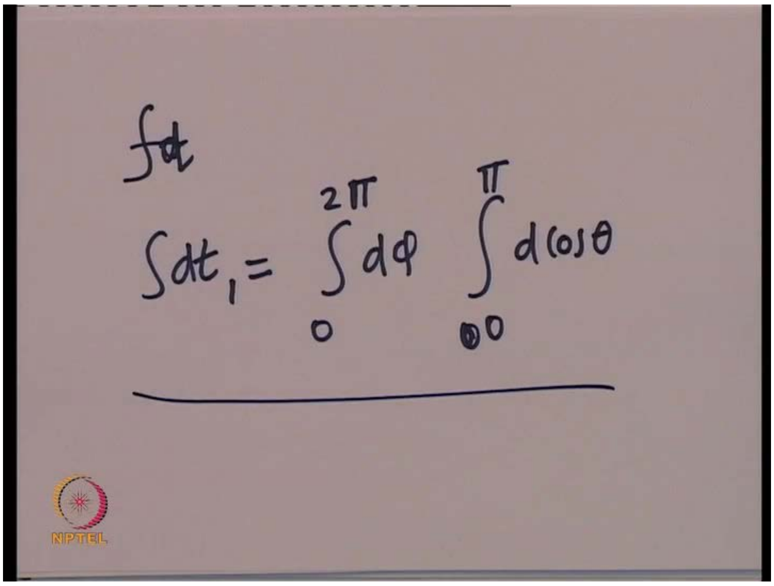

$$\int dt$$

$$\int dt_1 = \int_0^{2\pi} d\phi \int_0^{\pi} d\cos\theta$$

So, it turns out that, the way of representing A 3 D volume element given that the length is a constant is so, integral d t 1 integral d t 1 will be integral d phi 0 to 2 pi integral 0 0 to pi d Cos theta, this will turn out to be the volume element, but we will discuss about that in detail in another lecture, but what I just want to say here is that, we have to sum to over all possible volume elements and you sum over d t 1, d t 2 like this, you will get the conformation of all this and if you know the conformation then we can calculate the partition function for this particular D N A and known the partition function, you can answer the question, what is the probability of having D N A in a particular conformations.

So, if you want to have the close conformation we can ask the question, what is the probability of finding D N A in the close conformation. Now, we we know now, how to calculate partition function and we know how to calculate, what are in principle how to calculate the partition function of D N A for a D N A under worm like chain model. We will do this explicitly in the coming lecture, we will explicitly do and calculate the partition function for D N A and we will calculate some quantities such that of interest to us.

But for the moment, we we will stop with today's lecture here, and then continue calculating in this in in the next lecture. So, today's lecture to summarize, we learnt how to calculate partition function, we learnt how to calculate free energy, and we also learnt, how to calculate the probability of finding of the system in a given state i. So, with this, I will stop today’s lecture, we will continue tomorrow. Bye.

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