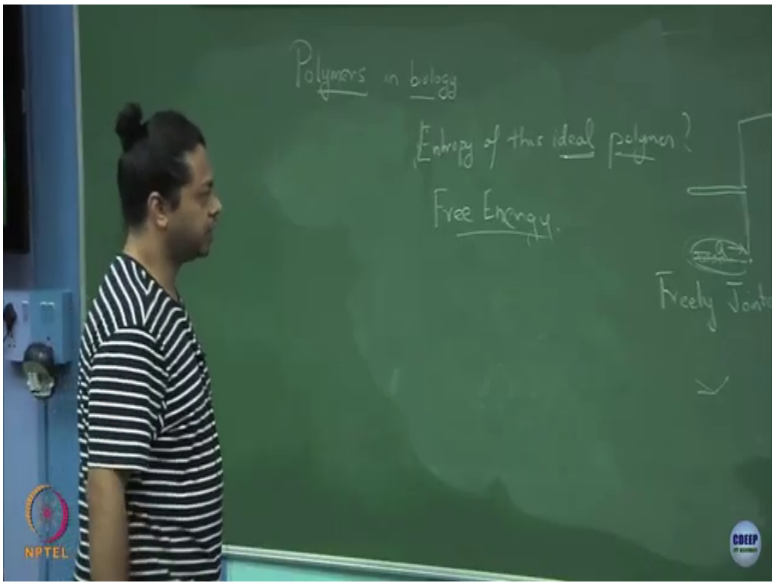
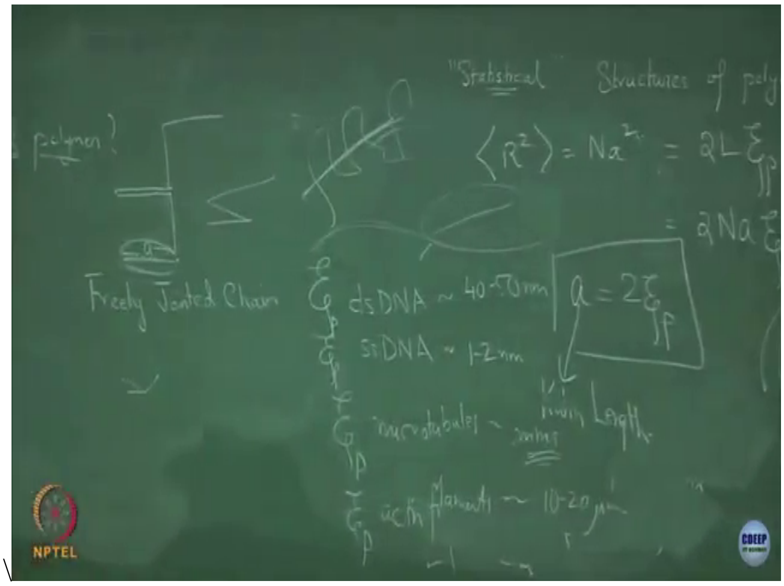
Physics of Biological Systems
Prof. Mithun Mitra
Department of Physics
Indian Institute of Technology, Bombay

Lecture – 31
Freely Rotating Chain Model

(Refer Slide Time: 00:17)

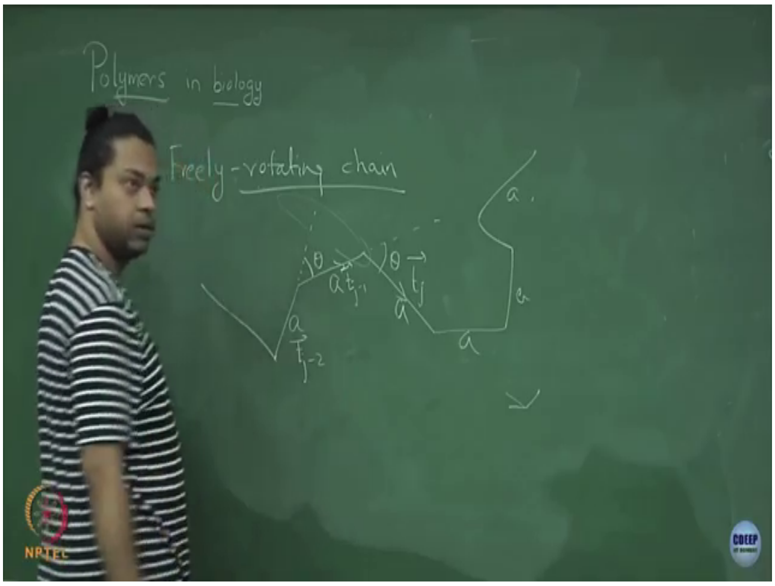


(Refer Slide Time: 00:24)



Let me do one more sort of a polymer model; just to show you that this is a generic sort of a feature, this R square growing as N. So, let me do a model of polymer which is called a Freely Rotating Chain. What I did was this call this freely jointed chain where each bond could do anything that it wanted. There are different models; there are class of models of growing complexity.

(Refer Slide Time: 00:43)

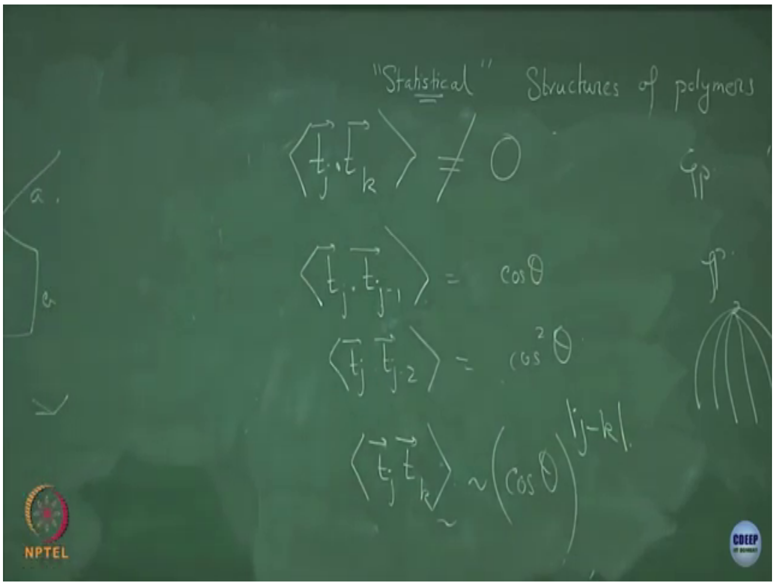


So, the generally the next sort of complex one is called a freely rotating chain ok. So, how do you construct a freely rotating polymer chain? So, what you do is that you take a length, let say all lengths are of length a ok. And then you place the next length along an angle theta with respect to the previous one.

So, you place it at an angle theta which is fixed let say do an approximation. And then the next one again you place it at an angle theta like this. It could be anywhere in this theta cone that is not fixed, but you just the relative angle is theta and then you keep going, keep adding monomers like this.

So, there is now a constraint in compared to the freely jointed chain where there was no such angular constraint, it could be anything. Here I was constrained that this angle must be theta, but it still the lengths are all the same; let us say, the lengths are all still a. And so, therefore, what I if I write down the tangent correlations unlike in the freely jointed chain; this would no longer be 0. There would be some correlations right because, my bonds are restricted to lie on that cone of angle theta.

(Refer Slide Time: 02:14)



"Statistical" Structures of polymers

$$\langle \vec{t}_j \cdot \vec{t}_k \rangle \neq 0$$

$$\langle \vec{t}_j \cdot \vec{t}_{j-1} \rangle = \cos\theta$$

$$\langle \vec{t}_j \vec{t}_{j-2} \rangle = \cos^2\theta$$

$$\langle \vec{t}_j \vec{t}_k \rangle \sim (\cos\theta)^{|j-k|}$$

So, what I want to do is that what I want to do is that I want to calculate these tangent-tangent correlations or at least I am going to argue for these tangent-tangent correlations, how they will look like. In the freely jointed case, this was 0. In the freely rotating chain, this will no longer be 0. We will have some tangent tangent correlations. And what will that look like? Let say I wanted to calculate the average of this quantity; t j dot t j minus 1.

So, let say this is my t j this vector, this vector is t j minus 1, this vector is t j minus 2 and so on Right. And I want to calculate any general correlation t j dot t k, t j dot t k, but let me just start with t j dot t j minus 1. What is what will that be? Given that these angles are theta are restricted to be theta cos theta right with an l square. Oh, no these are tangents. So, no l squared also. If this were r j dot r j minus 1, I would have an l square. So, this would just be cos theta right. What would be t j dot t j minus 2 hm?

Student: Cos (Refer Time: 03:46).

Cos square theta. Similarly, in general if you write t j dot t k the tangent tangent correlations; this will go as cos of theta to the power of let me write mod mod j minus k.

So, basically when you do this averaging, the only component that you will carry through is this cos theta component and so on. From here again if you carry the component onto this one, you will carry the cos theta component of that t j minus 2 onto j minus 3. So, every time you do this, every time you go back a monomer; you will pick up a cos theta. So, if you are doing the tangent tangent correlation between two monomers separated by this j minus k, you will pick up that many cos thetas ok. So, that is how your tangent-tangent correlation decays.

Student: How is that (Refer Time: 04:45).

Yes.

Student: It will be in an (Refer Time: 04:55).

It will be.

Huh.

Student: Schematic like (Refer Time: 04:58).

Yes

Student: (Refer Time: 05:01).

A schematic like this.

Student: Actually this systematically (Refer Time: 05:05).

Yes, but your remember your averaging over all come all of these this averaging is an average over all possible t j's that you have right. So, the only component let say if I think of this t j minus 1 onto this j minus 2, the only component that will survive is the projection of this t j minus 1 in the direction of this t j minus 2 right which is a cos theta right.

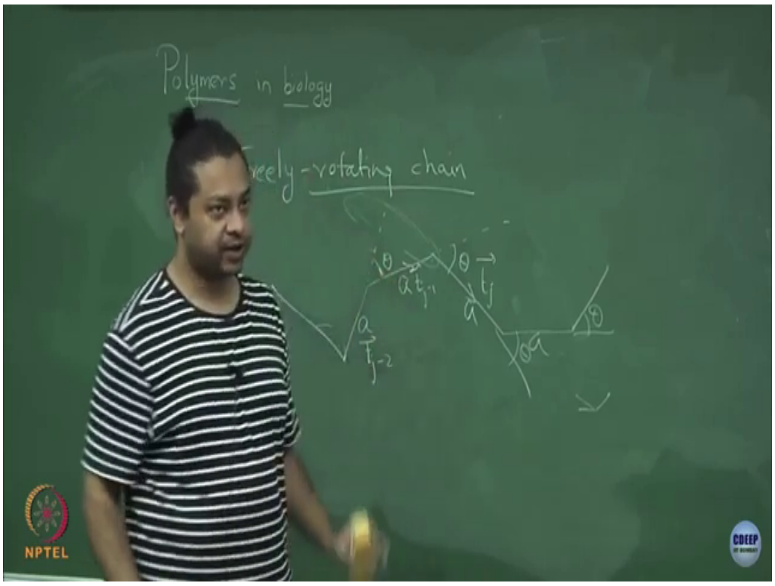
Student: (Refer Time: 05:33).

Over here.

Student: Yeah

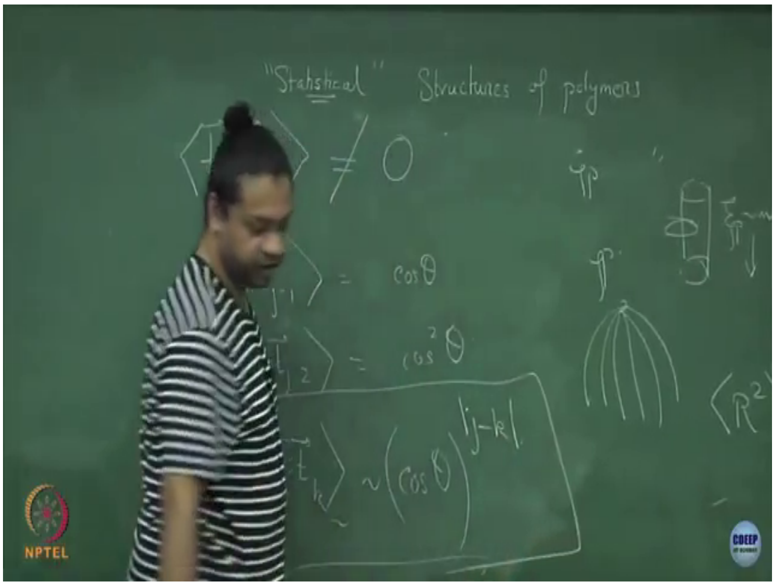
Oh that, that I have drawn very badly, but I do not know.

(Refer Slide Time: 05:46)



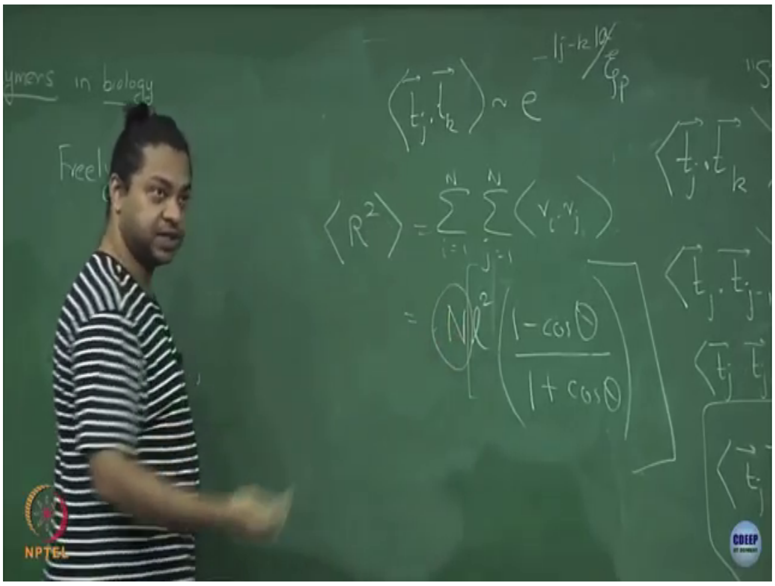
So, this is theta and then again this is theta, it continues. So, between all bonds so that is the model of this freely rotating chain; between all bonds I have an angle which is theta. That is my only restriction ok.

(Refer Slide Time: 06:05)



So, then the tangent tangent correlation looks like this; in this sort of a freely rotating chain. On the other hand in order to define my persistence length what I claim is that my tangent tangent correlations.

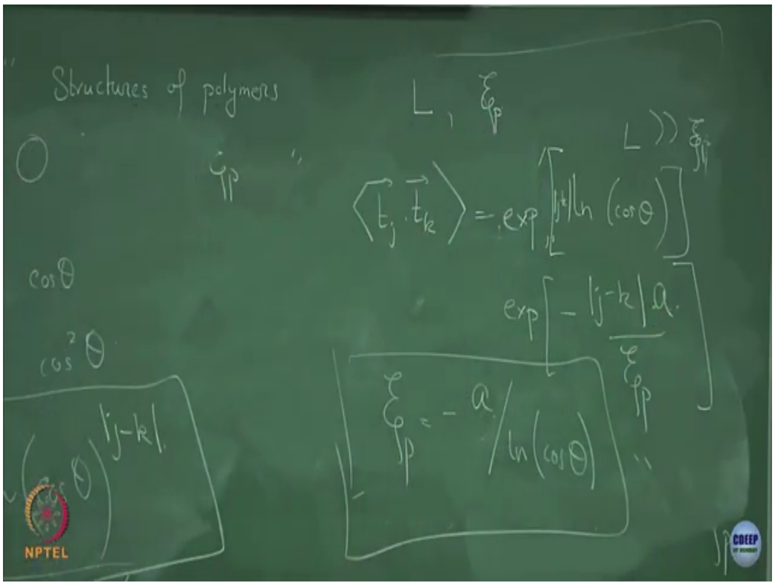
(Refer Slide Time: 06:15)



t j dot t k should decay as e to the power of minus j minus k by xi p right. Actually, I should write if these are indices then I should write t j minus k into a in order to get a length as the persistence length dimension ok.

So, then given these two expressions, what is the persistence length of this freely rotating chain? So, I will I can just rewrite this thing right, I can just rewrite this cos theta to the power of j minus k as some So, t j dotted with t k.

(Refer Slide Time: 07:12)



A some exponential of exponential of log of cos theta to the power of j minus k, which means j minus k log of cos theta right which means, if I now want to write this as exponential of minus j minus k l by xi p, then my xi p comes out to be persistence length is like minus l by log of cos theta. I have just rewritten it in this form and read off what would be is what xi p would need to be in order to write it like this.

So, the persistence length I am writing l maybe I am writing different things, I was writing a over there. So, let me keep writing a. So, you had a polymer whose chemical units had a length l, but they had this restriction that it would their bond angles had to be theta ok. So, if you go to this limit of a very long polymer, you can effectively replace it by this coarse grain beads; which where the beads would be given by this size scale the size scale of the persistence length which would depend on a which is your chemical information, the bond length, but also on this restriction that the bond angles have to be theta which comes into this log of cos theta a by log of cos theta.

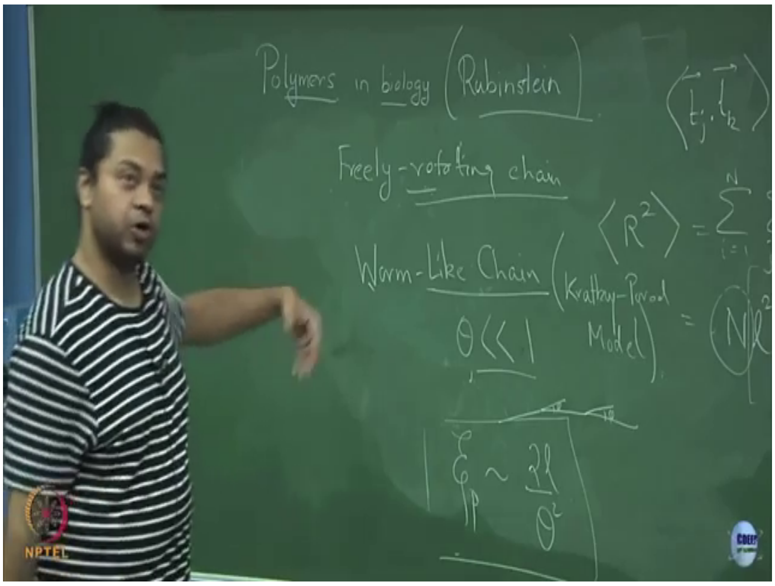
Once you build up once you build these coarse grain monomers of this length scale, then you can replace this by a freely jointed model and in fact, you can calculate this. So, I will leave this for you to do. You can calculate what is R square for a for a freely rotating chain like this.

You can calculate; what is R square for a freely rotating chain like this. So, you can just do this sum over i equal to 1 to N, sum over j equal to 1 to, r i dot r j average and you can show that this comes out as; let me just write it N l square 1 minus cos theta by 1 plus cos theta.

So, whatever is the chemical information gets encoded in this part. For a freely jointed chain this part, there was nothing here it was just N times l square. For the freely rotating chain, it is N l square into this object, but this fact that this size grows so, the square of the size grows as N, this is universal, At least for a class of polymers, this is universal. It will no longer for example, be true if your monomers were self avoiding. So, you could not cross, then you would it you would no longer grow as N.

But for, otherwise if you allow self intersecting polymers, but regardless of the details of the chemistry whether you have a cos theta or not and so on. You will this fact is an universal sort of scaling R square will grow as N. In fact, so this is call the freely rotating chain right.

(Refer Slide Time: 10:49)



This is call the freely rotating chain. So, this you should try to derive and see the small theta limit of this is what is called as the worm like chain. So, the worm like chain, worm like chain is the limit of the freely rotating chain when this theta is much smaller than 1.

If the angles between neighboring bonds is very small, which means this polymer is very stiff; the next one can only go a little bit. This is theta and the next one can only go a little bit more and so on. Then this is called as the worm like chain or another name for it is the Kratky Porod is the Kratky Porod model.

There is this theta much much less than 1 limit and in this limit you can write down the xi p because, xi p is remember minus l by log of cos theta. If you take a small theta approximation; that is turns out around 2 l by theta square which for small theta is pretty large. So, if because this chain is very stiff, I expect my correlations to persist for a longer length and that will come out in the xi p, that the xi p for small theta is going to be pretty large because this is call the worm like chain model and polymers.

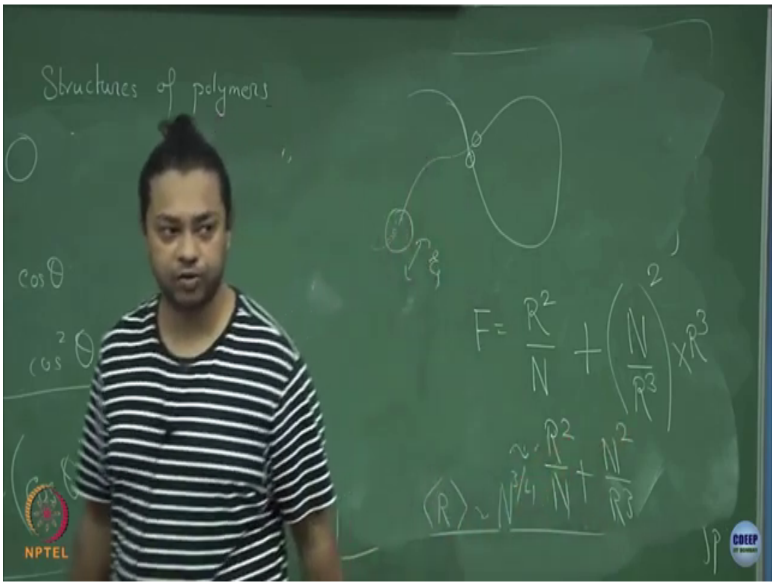
Lastly let me just put in some numbers. So, you can keep building sort of complexity this is not on a for a good book actually, if you are interested is this book on Polymers by Rubenstein, Polymers by Rubenstein which has a discussion of more models like this, this whole class of models, how to put in more and more complexity into this chemical into this molecular level details and still work out this average properties.

Let me just do one more thing. So, one thing we have calculated is this end to end distance and that we see goes as this l times xi p all right.

Student: (Refer Time: 13:07).

Yes and no. Yes and no, because you would imagine so, right.

(Refer Slide Time: 13:16)



That if I take a polymer chain like this, how does it go like cross itself? And that would be true if your units that you are using to describe the polymer or your real chemical subunits, but remember it is not. It is a coarse grain it is a coarse grain model when each unit is of this length of xi p.

So, there is empty space within these units as well, if you think about it right. There is some there is some bonds and here and so on. But, it is not it is not a single bond ok. So, in principle actually a polymer can in fact self intersect. So, for example, if you have if you put a polymer in a good solvent versus a bad solvent. In a bad solvent; the polymer does not like to interact with the solvent. So, it tries to sort of stay close to itself and then the relevant description is that of a self intersecting polymer.

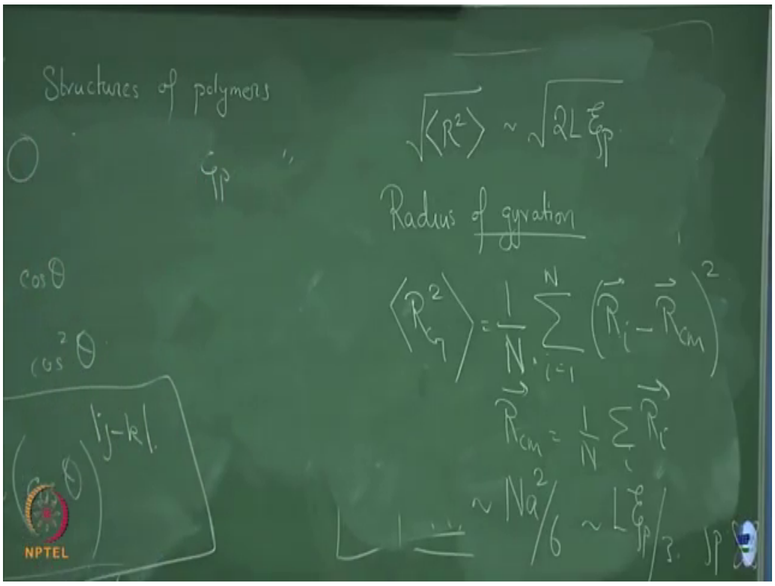
On the other hand, in a bad solvent where it wants to interact with the solvent molecules preferentially compared to its own monomers, the relevant description would be provided by a self avoiding polymer ok. And in fact, you can maybe I will do this later a little carefully. So, remember, I wrote down this I wrote down that the free energy goes as R square by N for this Gaussian polymer right. You can sort of hand wavingly say, how this would be modified if I introduce self avoidance in here.

So, if I had polymers which could not self intersect right; which means that there would be an energy cost if they came together. What would that energy cost be proportional to? It would in some sense be proportional to the density of these polymers right. If there were more dense, then it would be more likely to meet. So, you can write something like rho square over here right and rho is what is the density which is like the number divided by the volume right whole square N square by. So, this would be the energy density into the volume itself that would be r's cube.

So, you can show that approximately the free energy would be given by this R square by N term plus N square by R cube sort of a term. And then if you minimize this free energy that would tell you, how this R would go as a function of m. It would no longer go as square root of N, but in fact, you can show for a self avoiding polymer at least in this sort of a model it would go as n to the power of three fourth.

So s that sort of a model is a different universality class compared to this self intersecting ones and anything. I will, if I have time I will do self avoiding polymers better. What was I saying? It is saying about this end to end distance.

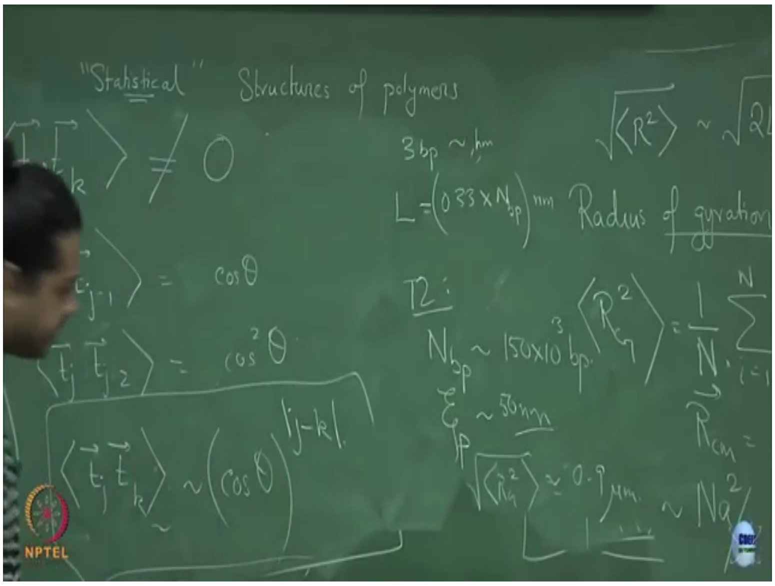
(Refer Slide Time: 16:30)



So, remember, I calc well, I half calculated this end to end distance and this went as some 2 L times the persistence xi p, this was my end to end distance. You can use this to characterize how big your polymer is, but often what people will use is a different measure which is called a radius of gyration. Radius of gyration and that is defined like this that R G square average is 1 over N, averaged over all monomers i equal to 1 to N R i minus R of the center of mass whole square.

So, for each monomer R i minus, so, this R c m is the average of all of these R's. So, that is defined as R G. So, let me just write R c m is 1 by N sum over i Ri right that is my center (Refer Time: 17:39). So, this is more often you will find people quoting RG values to when they want to say what is the typical size. And again if you expand all of this and you calculate the averages, you can show that this RG's comes out as sum N a square by 6 or in terms of the persistence length L xi p by 3. It is just a matter of writing out this R is and then doing these averages which we know how to do.

So, if you do the maths, you can show that this R G comes out as N a square by 6 or L xi p by 3 ok. I just wanted to write in this because, I just wanted to put in the numbers for a few organisms. (Refer Slide Time: 18:30)



So, remember, 1 base pair of DNA 3 base pairs of DNA is around 1 nanometer 1 nanometer. So, 1 base pair is 0.33 nanometers. So, the contour length of the DNA is 0.33 into the number of base pairs in nanometers right. So, now, if we can just put in different sort of organisms. So, for example, I have this virus bacteria phage T 2 has the number of base pairs in its genome as some 150 kilo bases. So, 150 into 10 to the power of 3 base pairs and as we as I said; the persistence length of DNA is of the order of 50 nanometers. So, you can calculate, how large that genome would be based on this sort of a based on this sort of a polymer theory.

So, this virus has these many base pairs, the persistence length of DNA is 50 nanometers; you can calculate what this R G square is going to be and that comes out to be so, square root of RG square comes out to be roughly around 0.9 microns.

Similarly, if you were to do; E. coli bacteria for example, if we were to do E. coli N, so this is E coli; E. coli has sum 4 into 10 to the power of 6 base pairs and again xi p is the same, it is 50 nanometers and that gives you a size. So, square root of R G square for E. coli comes to around 5 microns. Did you put in the numbers roughly. And people have experimented that how big is the genomes if I look at the E. coli genome and see how large is its size. So, from experiment; if you calculate this RG square. Experimentally, it comes out as around roughly 2-3 microns.

So, a theory like this where you have not taken into account any of the molecular sort of or any of the chemistry, we have just looked at these large scale properties at the scales where this lengths are much larger than the persistence length. The match is not is actually pretty decent in that sense, of course, there are other factors that play there is chemistry there is confinement and so on. But, even so, a calculation like this sort of gives you an idea that given the length of the genome in base pairs roughly how large would you expect that genome to be. For different organisms, you can work this out depending on how many how large in base pairs their genome is ok.

So, this sort of theories are powerful in that sense that it does not really need to you do not need to know a lot of the biology, but these are also limited therefore, in the sort of questions that you can ask. You cannot ask questions at the scales of the persistence length that what happens at you know xi p by 10 or xi p by 100 at those levels, you will have to use different methods. But if you are talking about polymers which are much longer than the persistence lengths genomes a genome wide polymer or some D N A or something like that.

Then statistical theories like this are actually fairly powerful tools to compute average quantities. So, we will see a little more on this particularly in the context of DNA and how it packages inside the nucleus in and how what are the predictions of theories like this versus how they compare with real experimental measurements from these high C or sort of whatever. So, we will talk a little bit about how DNA packages inside the nucleus and how we can use theories like these to under try to understand at least partially the properties of such packaging. All right that, we will do on Friday.