

Statistical Mechanics
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Lecture – 04
Gaussian Distribution

Good afternoon to all of you. We will continue yesterday's discussion with a continuous random variables. So, if we just recall what we discussed in the last lecture. Some important points that would perhaps help us enable us to carry on further in this lecture. So, we discussed that there is a very powerful method of computing both moments in cumulants using their generating functions.

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$x : f(x)$
Characteristic function $= \tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$
 $\langle x^m \rangle = \left. \frac{\partial^m}{\partial (-ik)^m} \tilde{f}(k) \right|_{k=0} = \int_{-\infty}^{\infty} f(x) x^m dx$
Cumulant generating function $= \ln \tilde{f}(k) = \sum_{j=1}^{\infty} \frac{(-ik)^j \langle x^j \rangle_c}{j!}$
 $\langle x^m \rangle_c = \left. \frac{\partial^m}{\partial (-ik)^m} \ln \tilde{f}(k) \right|_{k=0}$

So, in the last class we saw that for every random variable x which is distributed with pdf p of x , there exists a characteristic function that serves as a generator of moments. Now, the characteristic function is nothing, but the Fourier transform of the pdf and this was defined as p of k ok. And this provided as with a very powerful tool that we could compute any m th moment of the random variable, which is the m th moment here refers to average of the m th power of the random variable as nothing, but the m th derivative of the characteristic function, evaluated at k equal to 0.

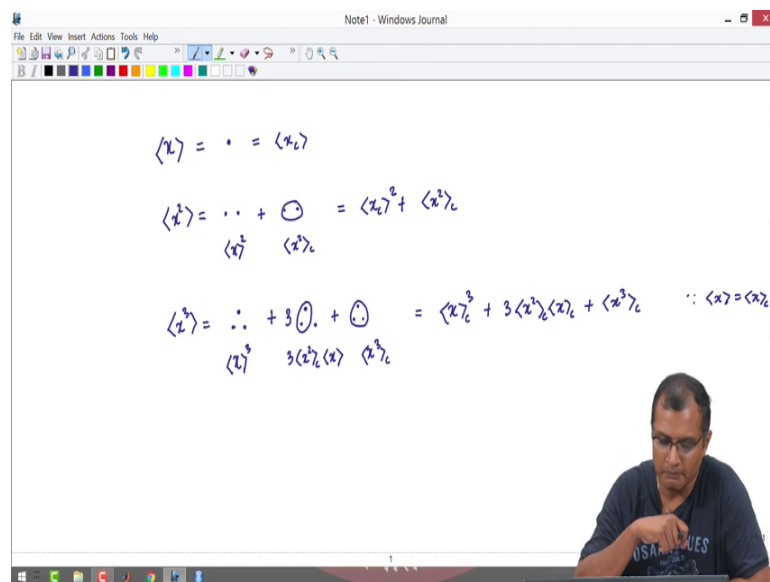
Of course, you could have computed this moment directly by brute force using the integral, but I offered this prescription of cumulated characteristic function, just to

improve your prospects to evaluate the m th moment. And then we also computed the cumulant generating function which is nothing, but the logarithm of the characteristic function and this is given as logarithm of the characteristic function.

And we know that this is given as if you expand p of k , $\ln p$ of k the expansion starts from j equals to 1 to infinity minus $i k$ to the power j j th cumulant over j factorial. And if you look at this expansion, it is straight forward to see that any m th cumulant can be extracted by simply taking m th order derivative of the cumulant generating function.

So, if you take the m th order derivative of the cumulant generating function at k equal to 0, this will give you the m th cumulant which is nothing, but extracting the coefficients of the of the m th cumulant from the series expansion. So, you now have 2 powerful expressions; one is this expression of computation of moments using the moment generating function and second is the powerful method of computing cumulants using cumulant generating function. When we did compute a few cumulants in the last class so, I just to sort of refresh your memories.

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So, the cumulants and the moments are related by this beautiful graphical relationship, you can also compute them analytically using the relations we have just derived. You can also write down the first cumulant as just a single dot as I said, m th order moment can be written as number of ways you can arrange m dots in ways in which we can show connect dots as cumulants and dots which are not connected as moments.

So, if you want to show graphically what is the first moment, you show it with a single dot and single dot is cannot be connected. So, this is nothing, but the first cumulant. Now if you want to show what is the second moment you use 2 dots, but now you can use 2 dots and keep them disconnected, you can also connect 2 dots with 2 dots the connection is possible. So, when you do not connect them this is nothing, but the first moment and there are 2 of them. So, its first moment square and the 2 dots that you have connected by a logic is the second cumulant and since we call the first moment as the first cumulant this is nothing, but first cumulant square plus second cumulant.

Then you can use it to compute the third moment. Third moment can be constructed by taking 3 dots; now 3 dots can be kept disconnected. There is one more way to sort of connect 2 dots and leave the third one, but you know there are 3 ways to do it. So, you have to attach a pre factor 3 plus you can connect all of them that is it there are no more ways to order 3 dots. So, the first is basically 3 disconnected dots. So, they are nothing, but the first moment to the part 3; plus 3 times the second cumulant into the first moment and 3 connected dots is the third cumulant.

Because we have the logic of keeping connected dots as cumulants and this can be written as because our moment is also first moment is also a first cumulant. In the in the third moment definition or the second moment in the second moment definition right so, 2 open dots are second moment to the power.

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Perfect then that is true; that is true that. So, thank you. So, this is right. So, this way you can continue and compute the fourth moment and so and so forth so.

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Very important distributions in Stat Mech.

(a) Gaussian distribution: $f(x) = N e^{-ax^2}$

N to be determined by normalization

$$\int_{-\infty}^{+\infty} f(x) dx = 1 = \int_{-\infty}^{+\infty} N e^{-ax^2} dx = N \int_{-\infty}^{+\infty} e^{-ax^2} dx = N \sqrt{\frac{\pi}{a}}$$
$$\Rightarrow N = \sqrt{\frac{a}{\pi}}$$

So, much for the recap we will now progress to some very important distributions in statistical mechanics and what immediately figures in my head is the Gaussian distribution. That you find almost everywhere in equilibrium systems. Infact towards the end of this course we will show that the Gaussian distribution is also a the only distribution which has the maximum entropy and hence natural distribution for all systems at equilibrium. But today we will just look at some statistical properties of this distribution without actually proving the maximum entropy principle. So, my first distribution that I am going to discuss is the Gaussian distribution ok. So, this distribution is defined as.

Suppose x is a random variable distributed as a Gaussian you know as a Gaussian distribution, then it is defined as e to the power minus $a x$ square ok. Now x is a random variable a is some constant, which will be shown immediately or in few steps that is related to variance of this random variable. But as of as is I see that this distribution p of x is not normalized ok. Not only that it is easily it is easily seen that the distribution is not normalized, because the dimension of distribution is missing e raised to minus $a x$ square is dimensionless.

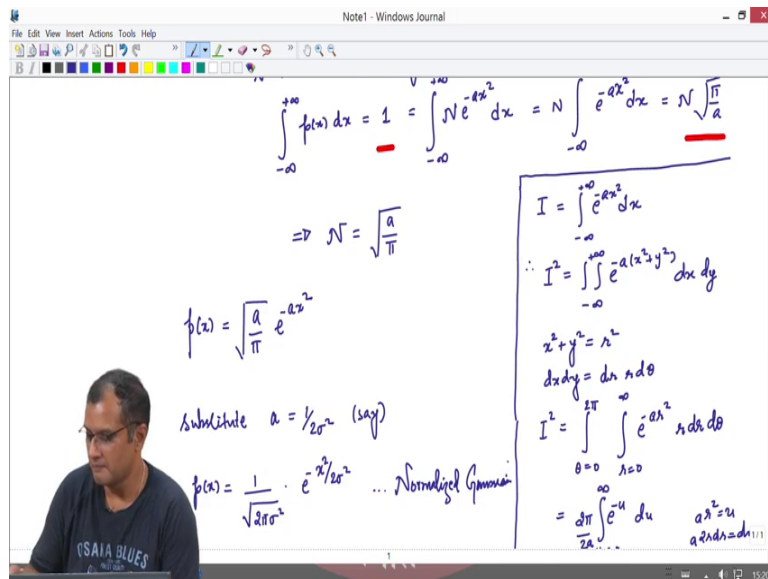
And I have told that p of x is a probability density function. So, it must have dimensions of 1 upon x . So, let us say I attach a pre factor N here which has the dimensions of 1 upon x , this N needs to be determined ok. N to be determined and to be determined by

normalization its a very important condition on any pdf that it should be normalized. So, our normalization condition is the integral of $p(x) dx$ should be equal to unity ok.

So, the left hand side is nothing, but integral $N e^{-ax^2} dx$. So, I can take N outside and this become simply integration of $e^{-ax^2} dx$. Now if you know the result of this integral this Gaussian integral, you can simply substitute that result which is square root of π/a and that gives you your N .

So, you can compare you can compare this one here and N into square root π/a and write down the value for N . So, comparing our result for N is nothing, but $\sqrt{\pi/a}$ ok. Now if you do not recall your Gaussian integral and you are wondering how did I write square root π/a for $\int_{-\infty}^{\infty} e^{-ax^2} dx$.

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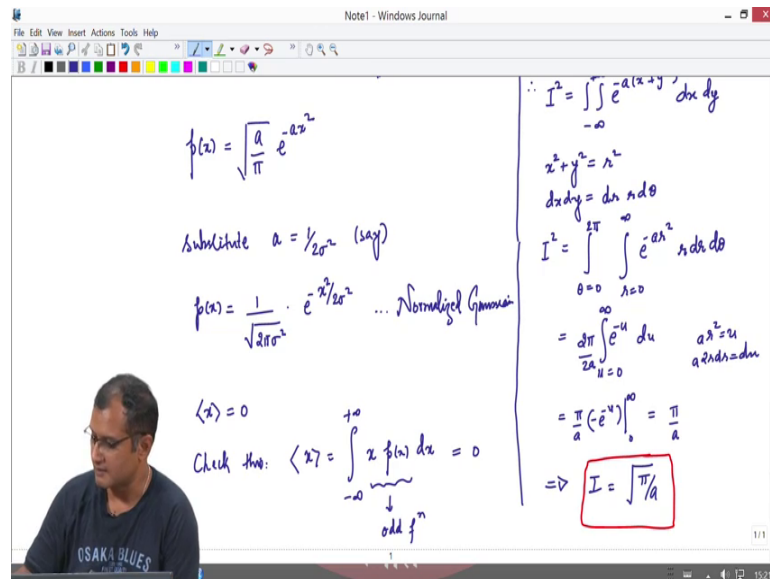


This is a very simple calculation that you can do this is just for those who have not who do not remember this result of Gaussian integral. So, if I write down this Gaussian integral $I = \int_{-\infty}^{\infty} e^{-ax^2} dx$, this means my I^2 has to be double integral $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-a(x^2+y^2)} dx dy$ ok. So, now, because I can change the integration variable from x to y , that is that amounts to square in the integral and if I simply make the substitution into polar coordinates and the area element $dx dy$ which is the area element in the polar coordinates as $r dr d\theta$.

Then my integral I square simply becomes integral theta going from 0 to 2 pi, integral r going from 0 to infinity e raised to minus a r square r d r d theta ok. Integral on theta simply gives me a factor of 2 pi and if I substitute r square as u, then I can simply write down twice r d r as d u and the inner integral will become integral on u going from 0 to infinity, e to the power minus a u d u by 2. In fact, I am going to substitute a r square as u.

So, I will get a into 2 r d r d u. So, I will get a 2 here and I will get an e raised to minus u and so, this would be just phi by a, integral e raised to minus u is minus e raised to minus u and you supply the limits 0 to infinity this is simply pi by a ok.

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And this is I square which means I is square root of pi by a there you go. So, this is the Gaussian integral formula in case you have forgotten or do not remember it ok. So, I have just substituted this here, now let us put this normalization constant back into the definition of our pdf. So, our pdf becomes Gaussian; Gaussian pdf becomes now with the formula for N as a pi square root e raised to minus a x square. I am just going to just to make it more consistent with the literature, I am just going to make a substitution here.

Just substitute without loss of generality this a as 1 upon 2 sigma square; a is anyway a variable substitute a as 1 upon 2 sigma square. Then you will see that this pdf becomes the Gaussian pdf of that is naturally commonly found in literature. So, with a as 1 upon 2

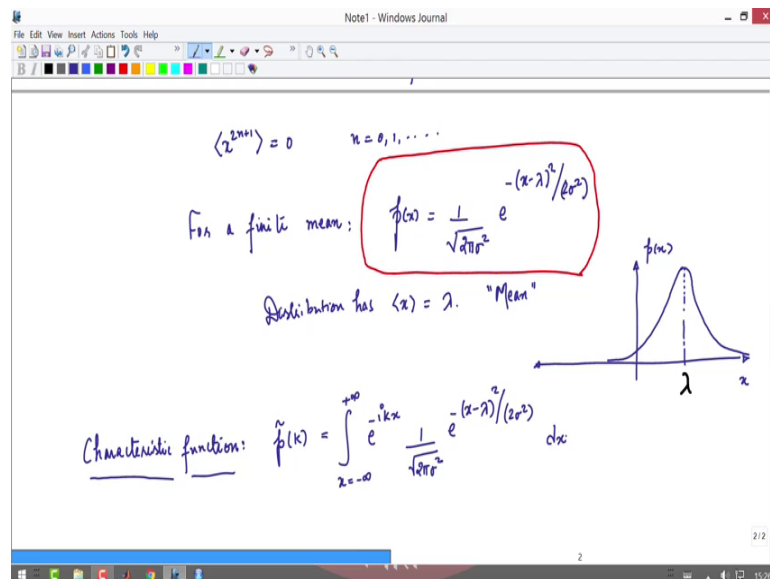
sigma square, this becomes standard Gaussian that you find in literature and this is the normalized Gaussian distribution ok.

Couple of things that I would like to mention here before proceeding is that, this is the distribution with 0 mean you can check this by simply computing the mean by brute force. So, the mean is nothing, but integral minus infinity plus infinity x into p of x d x.

And I can see p f p of x is Gaussian distribution, which is a even function; now if even function is multiply to an odd function which is x, it becomes a odd function itself. So, x times p x becomes an odd function and hence the integral of this odd function in the symmetric interval minus infinity plus infinity is 0. So, it is not surprising to me that the average value of x is 0.

Infact all even moments of x will be 0 because p of x is even by itself all odds I am sorry all odd moment of x will become 0, because p of x is even ok.

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So, you can write down as x to the power some 2 n plus 1 will be 0 for any n, but we can write down a Gaussian distribution with finite mean ok. So, for a finite mean you can rewrite the Gaussian distribution as p of x equals to everything remains the same, it is just that you accommodate for a finite mean as x minus lambda to the power 2 upon twice sigma square. Now this is a distribution has a finite mean which is lambda ok. So, this is

the mean. Now you can check that this is the mean by the tools that are discussed already or have some patience we will discover that this is a mean in a short while.

So, you can sketch this distribution p of x as a function of x would be a Gaussian distribution, which means it will extend up to infinity on both sides around the mean. So, this would be the location of the mean λ ok. So, if λ is 0 this would be a Gaussian center at the origin ok. Otherwise, this would be a Gaussian that is shifted from this origin ok. So, let us now look at some of the important properties of this distribution

So, if p of x is given as this ok. So, let us look at our p of x , this is our general Gaussian distribution with a finite mean that is λ and if you want to find out the characteristic function of this Gaussian distribution, then you can simply compute that by taking a logarithm by taking a Fourier transform of this Gaussian distribution.

Why are we doing this? We are doing this because we want to understand or we want to derive a neat formula for the moments and cumulants of this Gaussian distribution and in doing so, we were we shall also be greeted with a very important result in the context of Gaussian distribution, that is this is the only distribution in nature that has only the first 2 surviving cumulants. It is completely specified by its first 2 cumulants and we shall discover that in due course.

So, let us do the standard mathematics here. So, the characteristic function which is the generator of moments is basically the Fourier transform of the pdf and the pdf here is the Gaussian distribution. So, let me just write it in one step, this is the Fourier transform of the Gaussian distribution. So, I will write down the Gaussian distribution here ok.

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And you can pull out the constant pre factor and rearrange the terms inside. So, I would like to make say I would like to take advantage of the basically I would like to take advantage of this Gaussian intergral, that e raised to minus a x square when integrated from minus infinity to plus infinity, a square root of phi by a or result that we just derived a few minutes ago. I would like to take advantage of this. Now I can only do that if I can write down the complex exponential and second exponential together with a power that is looking like some x square ok. So, let us do that.

So, I am going to combine these 2 exponentials and write down a single exponential with a power x minus lambda and that would give me x minus lambda the whole square plus sigma square i k to the power 2 by 2 sigma square ok. And I am just going to rub rub it from here because that is just indicated and get back to my. This is not yet complete because it has given me some extra exponentials that I must eliminate. So, as you can see x minus lambda the whole square will give me this second exponential and twice of sigma square will cancel with twice sigma square in the denominator and I will get i k into x minus lambda of which minus i k is already there. So, I need e to the power minus i k ok minus i k lambda into extra k square minus k square sigma square by 2 into d x ok.

So, if you combine the 3 exponential you get the numerator, the expression is written one step above. As usual I can pull out e raised to minus i k lambda because this is an integral on x. So, e raised to minus i k lambda comes out divide by 2 pi sigma square and so,

does e raised to minus k square sigma square by 2 and what I have inside is basically an integral x going from minus infinity to plus infinity e to the power minus of x minus lambda plus sigma square i k square by 2 sigma square dx ok.

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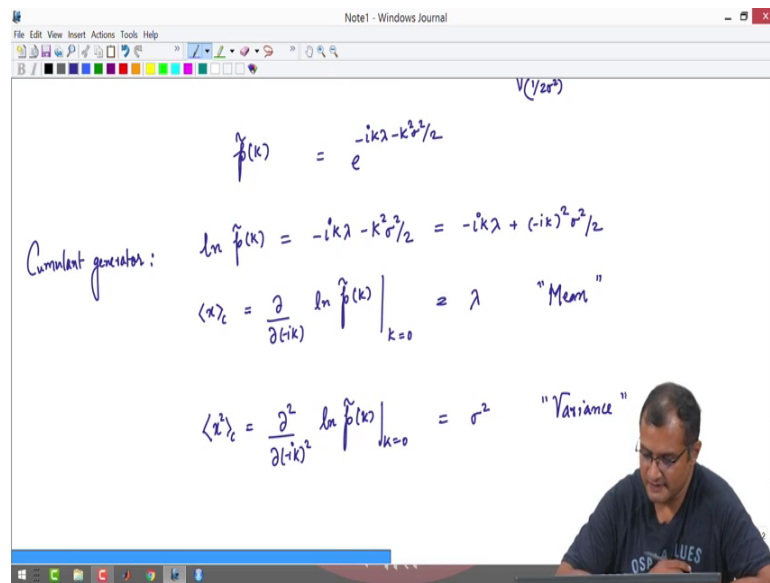
$$= \frac{e^{-ik\lambda - k^2\sigma^2/2}}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} e^{-u^2/2\sigma^2} du$$

$$= \frac{e^{-ik\lambda - k^2\sigma^2/2}}{\sqrt{2\pi\sigma^2}} \cdot \sqrt{\frac{\pi}{(1/2\sigma^2)}}$$

And here I will make a simple substitution that x minus lambda plus sigma square i k if I substitute as some u then this intergral simply becomes e raised to minus ik lambda minus k square sigma square by 2 upon square root of 2 pi sigma square into integral u going from minus infinity to plus infinity, e raised to minus u upon 2 sigma square d x d u.

Gaussian integral tells me that this integral is nothing, but square root of pi by 1 upon 2 sigma square which will cancel off with the denominator and I will simply get and I will simply get e raised to minus i k lambda minus k square sigma square by 2 everything will cancel ok. So, fine.

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The whiteboard shows the following derivations:

$$\hat{f}(k) = e^{-ik\lambda - k^2\sigma^2/2}$$

Cumulant generator: $\ln \hat{f}(k) = -ik\lambda - k^2\sigma^2/2 = -ik\lambda + (-ik)^2\sigma^2/2$

$$\langle x \rangle_c = \left. \frac{\partial}{\partial (ik)} \ln \hat{f}(k) \right|_{k=0} = \lambda \quad \text{"Mean"}$$
$$\langle x^2 \rangle_c = \left. \frac{\partial^2}{\partial (ik)^2} \ln \hat{f}(k) \right|_{k=0} = \sigma^2 \quad \text{"Variance"}$$

So, then this is the characteristic function corresponding to the Gaussian distribution. Now we can see very easily that, as I said in the beginning that the Gaussian distribution is the only distribution that has it is completely specified by express to culminates and here we see what.

So, you can take the logarithm of this that is nothing, but the cumulant generator and this comes out to be just minus $i k \lambda$ minus $k^2 \sigma^2$ by 2 if I take the logarithm both sides. And just re writing it as minus $i k \lambda$ plus minus $i k$ whole square, σ^2 by 2 ok. So, now, you know that the first cumulant is nothing, but the first derivative of the cumulant generator evaluated at k equal to 0 which comes out to be just λ . So, this is the mean and that we already know that the first cumulant is the mean ok. λ was declared as the mean and so, it is not surprising to me that the first cumulant is λ .

Let us see what is the second cumulant? The second cumulant is the second derivative of the cumulant generator at a origin which is nothing, but σ^2 we call this as variance.

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$$\langle x^2 \rangle_c = \frac{\partial^2}{\partial (ik)^2} \ln \hat{p}(k) \Big|_{k=0} = \sigma^2 \quad \text{"Variance"}$$

$$\langle x^3 \rangle_c = 0$$

$$\langle x^4 \rangle_c = 0$$

$$\vdots$$

$$\langle x^m \rangle_c = 0$$

Gaussian PDF is completely specified by first two cumulants - $\langle x \rangle = \lambda$ & $\langle x^2 \rangle_c = \sigma^2$

And you can see any other derivative all other you know x 3 third cumulant, fourth cumulant all other cumulants are 0 because you do not have terms which are above quadratic in k in the cumulant generating function ok. So, this is the beautiful property possessed only by Gaussian distribution, its completely specified (Refer Time: 29:23) the Gaussian pdf can you know this is denoted here as by first 2 cumulants, which are basically the mean and the variance; lambda and sigma square will completely specified the Gaussian pdf ok. So, you can also write down their your their higher order moments.

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Some moments of $p(x)$: Gaussian:

$$\langle x \rangle = \dots = \langle x \rangle_c = \lambda$$

$$\langle x^2 \rangle = \dots + \odot = \lambda^2 + \sigma^2$$

$$\langle x^3 \rangle = \dots + 3\odot + \ominus = \lambda^3 + 3\sigma^2\lambda + 0 = \lambda^3 + 3\sigma^2\lambda$$

$$\langle x^4 \rangle = \dots + 4\ominus + 6\odot\odot + 3\ominus\ominus + \oplus = \lambda^4 + 4\sigma^2\lambda^2 + 6\sigma^2\lambda^2 + 3\sigma^4 + 0 = \lambda^4 + 6\sigma^2\lambda^2 + 3\sigma^4$$

So, you can write down for example, moments of the Gaussian pdf our Gaussian pdf. So, you can take the first moment which we know already its a single dot. So, I will use the diagram method which is nothing, but the our first cumulant that is our lambda is second moment is constructed by 2 points. The 2 points can be either disconnected or connected; connected disconnected points are nothing, but your moments. So, they are lambda square plus connected dots are cumulant, this is a second cumulant which is sigma square. And third moment would be you take 3 dots; 3 dots can be disconnected or you can connect 2 of them and leave the third guy.

And there are 3 ways of doing it and you have connections on all of them this is that now further. So, 3 open dots as we know are moments. So, that is lambda cube plus 3 times this would be second cumulant sigma square into lambda plus you have third cumulant, which is 0. We have just shown that the cumulants above order 2 are all 0 and similarly you can compute the fourth as 4 dots all of them open plus connect 3 of them not there are four ways of doing it plus connects 2 of them and leave the other 2 open there are 4 c 2 ways of doing it which is 6 plus connect 2 of them and the other 2 of them there exactly half of 6 which is 3 ways of doing it and connect all of them no more ok.

So, the first guy which is the all four of them disconnected is nothing, but lambda to the power 4 first moment to the power 4 plus 4 times third cumulant which is 0 into lambda plus 6 times second cumulant sigma square into lambda square plus 3 times sigma 4 sigma square into sigma square plus all 4 of them connected which is fourth cumulant and that is 0.

So, these 2 terms are 0 and ok. So, basically you can simply this you can simply write as lambda cube plus 3 sigma square lambda and here you can simply write down lambda 4 plus 6 lambda square sigma square plus 3 times sigma to the power 4. So, these are the four moments of the Gaussian random variable. So, this is how you can completely specify the moments and the cumulants of a Gaussian pdf and what we have learnt today is a very important property or unique property of the Gaussian distribution that it can be completely constructed knowing just the. So, the meaning that a distribution can be constructed completely by just the 2 cumulants actually means that if you are given the 2 cumulants.

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Handwritten notes on a whiteboard:

$$\langle x \rangle = \dots + 4 \dots + 6 \dots + 8 \dots + \dots - \lambda + 7(0)\lambda$$

$$+ 6\sigma^2\lambda^2 + 3\sigma^4 + 0 = \lambda^4 + 6\sigma^2\lambda^2 + 3\sigma^4$$

Suppose you are given:

$$\langle x \rangle_c = \lambda$$

$$\langle x^2 \rangle_c = \sigma^2$$

$$\ln \hat{f}(k) = \sum_{j=1}^N \frac{(-ik)^j \langle x^j \rangle_c}{j!} = (-ik)\lambda + \frac{(ik)^2 \sigma^2}{2!} = -ik\lambda - \frac{k^2 \sigma^2}{2}$$

Let us say you given the first cumulant it is the mean and the second cumulant as the variance, you can construct the Gaussian pdf as follows. So, this is the reverse question, knowing the mean and cumulant how you construct. Well you know that the cumulant generating function is basically the sum of is an expansion in powers of minus i k. Now in this expansion there only the 2 terms the first 2 terms all the terms are 0. So, the first term is minus i k into lambda because that is the first cumulant and the second term in the expansion is minus i k to the power 2 upon factorial 2 into sigma square ok, which is basically minus i k lambda minus k square sigma square by 2 ok.

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Handwritten notes on a whiteboard:

$$\hat{f}(k) = e^{-ik\lambda - k^2\sigma^2/2}$$

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} \underbrace{e^{-ik\lambda - k^2\sigma^2/2}}_{\hat{f}(k)} dk$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\lambda)^2/2\sigma^2}$$

\equiv Reversed Gaussian PDF \equiv

So, now if you compare these two terms, you simply raise both sides to exponential you get p of k as e raised to minus $i k \lambda$ minus $k^2 \sigma^2$ by 2. Now once you have p of k you can compute p of x via an inverse Fourier transform and get your pdf.

So, this is my p of k this exponential is nothing, but my p of k which whose inverse Fourier transform I am taking right now and you know that the Fourier transform of a pdf of a Gaussian distribution is also a Gaussian distribution. So, what you will get at the end of this exercise is your, is Gaussian distribution $\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x-\lambda}{\sigma}} e^{-\frac{x-\lambda}{\sigma}}$. So, this is how you recover your your Gaussian pdf. So, that is how you recovered your Gaussian pdf.

In general you can construct any pdf like this suppose you know all the cumulants if you know all the cumulants then you can simply construct the cumulant generating function. Suppose you have five cumulants and you say that there are only five cumulants in this distribution. Please write down there is an expansion, compute your cumulant generating function and take its inverse Fourier transform that would give your pdf.

So, we end the lecture here and when we meet in the next class we will discuss another important distribution which is the Poisson distribution and we have one more important discussion to cover that is on binomial distribution. So, these are the 3 major distribution that I will cover in the class and discuss the features of each one of them ok.