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## Lecture - 12 Diffusion Equation Path Integral (2), Autocorrelators

Right, welcome back.

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$$\operatorname{Re} call: \Delta = \lim_{n \to \infty} \left\langle \exp\left(\frac{t}{n} \sum_{k=1}^{n} U\left(x + \sqrt{\frac{t}{n}} \sum_{j=k}^{n} y_{j+1}\right)\right) \right\rangle \\ \times \exp\left(\sqrt{\frac{t}{n}} \sum_{k=1}^{n} y_k \frac{\partial}{\partial x}\right) \right\rangle$$
  
with  $y_{n+1} = 0$ . In the lim it  $n \to \infty$ ,  $\langle y_j \rangle = 0$ ,  $\langle y_j^2 \rangle = D$ .  
Thus, by the CLT,  $\sum_{k=1}^{n} y_k \frac{-\operatorname{distribution}(n \to \infty)}{N(0, nD)}$ 

Now, by making use of the property of the translation generator the first derivative in the exponential, we were able to simplify the expression of the propagator and bring all the derivative terms to the right and all the non-derivative terms to the left. This was a very important simplification that we could achieve because of this particular property.

And then we had this important relations that in the limit that n tends to infinity which we ultimately have to do I have to take in the limit n tends to infinity each of these y j's is normally distributed with a mean of 0; and a variance of D, variance of D each of the each of these y j's. And by using the central limit theorem we find that the summation of these y j's up to n are normally distributed with a mean of 0, and a variance of n D, so that is where we concluded the last lecture last class. Let us continue from there.

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Defining a Brownian motion by 
$$W_k = -\sqrt{\frac{t}{n}}\sum_{j=1}^k y_j$$
 with  
 $\langle W_k \rangle = 0; \langle W_k^2 \rangle = \frac{t}{n}kD = \frac{kt}{n}D; dW = W_k - W_{k-1} = -\sqrt{\frac{t}{n}}y_k;$   
 $\langle dW \rangle = 0; \langle (dW)^2 \rangle = \left(\left(-\sqrt{\frac{t}{n}}y_k\right)^2\right) = \frac{t}{n}D = Ddt$ 

Now, we define a Brownian motion? How do we define it? As you recall Brownian motion is the sum of random variables, and each of those random variables are normally as I am sorry the random variables are such that the Brownian motion becomes a sum of those random variables. And at any particular point in time, the random the aggregate of all those random, the sequence of those random variables is normally distributed due to the central limit theorem as a mean of 0, and a variance equal to the length of evolution.

So, we define a Brownian motion by W k is equal to minus root t by n remember that we talked about the step size of under root t t by n that is precisely what is happening here. So, W k is equal to minus under root t by n summation of y j with j equal to 1 to k. Please note these subscripts the indices we have W k is a summation of random variables y 1, y 2, y 3 from 1 to k.

Let us look at the properties of this Brownian motion to ensure that it is a Brownian motion. We have the expectation value of W k is clearly 0, because the expectation value of each y j is 0. The expectation value of W k square now that is interesting, recall that the expectation value of each y j is equal to D.

Therefore, when you are multiplying by under root the you are scaling the variable by under root t by n, the variance gets scaled by t by n, so the variance will be equal to t by n, and since there are n y j's here. So, we have t by n k into D to reiterate to repeat each y j has a variance of D. There are k of them, so the total variance becomes and each of them are independent of the other. So, the total variance becomes k D. And we are scaling each y by under root t by n, so the variance gets scaled by t by n. So, we have t by n into k into D.

And d W the increment W k minus W k minus 1 is nothing but under root t by n y k. And clearly the expectation of d W is 0, because the expectation of y k is 0; and the expectation of d W square is equal to t by n into this expression this particular expression expectation of y k square. Remember the expectation of y k square was D, therefore, it becomes t by n into D, and that is nothing but the D into the step size that is D dt.

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$$F \mid A : \Delta = \lim_{n \to \infty} \prod_{j=1}^{n} \left\langle \exp\left(\frac{t}{n}U\right) \exp\left(\sqrt{\frac{t}{n}}y_{j}\frac{\partial}{\partial x}\right) \right\rangle$$
$$= \lim_{n \to \infty} \left\langle \exp\left(\frac{t}{n}\sum_{k=1}^{n}U\left(x + \sqrt{\frac{t}{n}}\sum_{j=k}^{n}y_{j+1}\right)\right) \exp\left(\sqrt{\frac{t}{n}}\sum_{k=1}^{n}y_{k}\frac{\partial}{\partial x^{\circ}}\right) \right\rangle$$
$$\Delta = \lim_{n \to \infty} \left\langle \exp\left(\frac{t}{n}\sum_{k=1}^{n}U\left(x + W_{k} - W_{n}\right)\right) \exp\left(-W_{n}\frac{\partial}{\partial x}\right) \right\rangle$$
$$This is the operator form of the propagator.$$

So, let us now what do we have? We started with this first expression for delta, we simplified it by translation generator property, and we got all the derivatives to the right, we got all the other terms to the left, and then we introduced the concept of Brownian motion.

By introducing the concept of Brownian motion to represent the sum of divisors, we simplify the summation the terms; within the summation and we write them as a Brownian motions it is quite straightforward. We write summation of y k as W k, and we write summation of y j plus 1 from j equal to k to n as a difference of two Brownian motions from j equal to 1 to n and then from j equal to 1 to k.

So, j equal to 1 to n minus j equal to 1 to k. In other words, it is equal to y n minus y k, but there is a minus sign here in defining the Brownian motion and therefore it becomes y k minus

y n. So, this is the operator form of the propagator. The y operator form because it contains the derivative operator to the extreme right.

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To obtain the expression for the kernel i.e. of 
$$K(x,t;y)$$
  
that satisfies  $\psi(x,t) = \int d\theta K(x,t;\theta)\psi(\theta,0)$  we have  
 $\psi(x,t) = (\Delta\psi)(x,0)$   
 $= \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n}\sum_{k=1}^{n}U(x+W_k-W_n)\right] \exp\left(-W_n\frac{\partial}{\partial x}\right)\psi(x,0)\right\rangle$   
 $= \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n}\sum_{k=1}^{n}U(x+W_k-W_n)\right]\psi(x-W_n,0)\right\rangle$  (Set  $\theta = x - W_n$ )  
 $= \int d\theta \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n}\sum_{k=1}^{n}U(\theta+W_k)\right]\delta(x-W_n-\theta)\right\rangle\psi(\theta,0);$ 

Now, we move on to find the expression for the kernel. The kernel has to satisfy this equation which is given at the top in the green box phi of psi of x t is equal to integral d theta kernel x, t subject to theta psi theta comma 0.

In other words, it transform the state theta 0 to the state psi theta 0 to the state psi x t. It transform the state psi theta 0 to the state psi x t. Recall that the propagator transform the state psi theta 0 to this state psi theta t. Here we have the kernel doing a slightly different job. It is transforming the state psi theta 0 to the state psi theta sorry x t.

Now, as I mentioned the propagator and did the job of transforming the state  $x \ 0$  to the state xt, or the state at  $x \ 0$  to the state at x t, this is transforming the state at theta 0 to the state at xt. How to work it out? Let us start with the continue with the expression for the propagator. And let us operate that on psi  $x \ 0$ , we get this expression with the d by d x operating on psi  $x \ 0$ . We make a simplification.

We now again we use this translation property of exponential del by del x exponential the second term exponential minus W n del by del x operating on psi x 0 does a translation in spatial coordinates and it gives you psi x minus W n comma 0.

The this because it is a derivative with respect to the spatial coordinate, it does a translation with respect to the spatial coordinates, and it shifts psi from x 0 to psi at x minus W n comma 0; 0 is the time coordinate. So, it does not affect the time coordinate, it does not because there is no time coordinate involved in the derivative. So, it only the spatial coordinate is there.

And the spatial derivative operates on the spatial coordinates, and it gives you psi of x minus W n comma 0. So, this expression gives me the expression in this blue box due to the translation generation property of the exponential of the derivative.

Now, what I do is, I said theta equal to x minus W n. To simplify further recall I have to bring this in the form theta comma 0 psi theta comma 0. So, what I do is, I substitute theta equal to x minus W n.

When I substitute psi, when I substitute x minus W n minus theta to introduce this constraint into this expression, I use a direct delta function, I introduce this direct delta function within the integration and I write the integration together with delta x minus W n minus theta that is precisely x minus W n minus theta is precisely representing this particular change in coordinates. We are shifting x minus W n or we are changing x minus W n as theta substituting x minus W n as theta. And in order to implement that substitution, I introduce a delta function x minus W n minus theta. So, that this integral operates now only over the expressions where this theta equal to x minus W n holds. The rest is simplified x minus W n is written as theta. So, it becomes U theta plus W n. And now psi which was written as psi x minus W n comma 0 now becomes psi theta comma 0. And we have the expression for the kernel.

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$$F/A:$$

$$\psi(x,t) = \int d\theta \lim_{n \to \infty} \left( \exp\left[\frac{t}{n} \sum_{k=1}^{n} U(\theta + W_{k})\right] \delta(x - W_{n} - \theta) \right) \psi(\theta, 0)$$

$$Also, by definition \psi(x,t) = \int d \mathbb{K}(x,t;\theta) \psi(\theta,0). Hence$$

$$\mathbb{K}(x,t;\theta) = \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n} \sum_{k=1}^{n} U(\theta + W_{k})\right] \delta(x - W_{n}^{\circ} - \theta) \right\rangle$$

And the kernel is now in can be written or is in the form of this expression the last red box that we have K of x, t theta is equal to limit n tending to infinity this whole expression together with this and delta function, together with this delta function including this delta function. And that is clearly seen by comparing these two equations and comparing the expression for the K in this expression and this integrand. (Refer Slide Time: 11:10)

$$\psi(x,t) = (\Delta\psi)(x,0) : \Delta \text{ is the propagator}$$

$$\Delta = \lim_{n \to \infty} \left\langle \exp\left(\frac{t}{n} \sum_{k=1}^{n} U(x+W_k - W_n)\right) \exp\left(-W_n \frac{\partial}{\partial x}\right) \right\rangle$$

$$\psi(x,t) = \int dy K(x,t;y) \psi(y,0) : K(x,t;y) \text{ is ker nel}$$

$$K(x,t;y) = \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n} \sum_{k=1}^{n} U(y+W_k)\right] \delta(x-W_n - y) \right\rangle$$

Now, one more step of simplification can be achieved. This is the relative expressions for the propagator and the kernel. The upper expression within the red box is that for the propagator that we had earlier; and the lower expression is for the kernel. And important thing is that in the propagator we have this first derivative the translation generator and in the second the kernel that translation generator is replaced by the delta function.

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$$F/A: K(x,t;y) = \lim_{n \to \infty} \left\langle \exp\left[\frac{t}{n} \sum_{k=1}^{n} U(y+W_k)\right] \delta(x-W_n-y) \right\rangle$$
  
In the continuum limit of BM, we can assume W(s) as a BM  
path initiating at y i.e W(0) = y at s = 0;  
W(t) = (y+W\_n) at s = t = n.  $\frac{t}{n}$  and  
W(s) = (y+W\_k) for arbitrary s = k.  $\frac{t}{n}$ .  
Then,  $K(x,t;y) = \left\langle \exp\left[\int_0^t U(W(s))ds\right] \delta(x-W(t)) \right\rangle$ 

Now, we do a little bit more of simplification. What we do is, we define a Brownian motion again, we define a Brownian motion by the expression that if the Brownian path starts at y at t equal to 0, therefore, W of 0 is equal to y. We define a Brownian motion that way W is 0 is equal to y it starts at the path Brownian path starts at y. So, we have W 0 equal to y at s equal to 0; s is now the new time coordinate representing the time coordinates.

So, at s equal to 0, we have W 0 equal to y and at s equal to t that is the conclusion of the path, the terminal point of the path. We have W of t small t that is W of small t is equal to y plus W n, y plus W n that is at s equal to t that represents. And at any intermediate path we can represent for any intermediate value of s, what do we have we have W s is equal to y plus W k. Where.

How do we define k or what is the relation between k and s? s is equal to k under root t upon n. k is, recall k is the number of steps right time steps and each step is of length t by n. So, the it in terms of continuous time it works out to k into t upon n which is the arbitrary or the general value of s lying between 0 and small t.

Making these substitutions, I can write this summation as an integral. Now, assuming that this W that we have defined now is continuous Brownian motion, I can make this substitution replace this summation by the integral u t u of W s, integrated within the limit 0 to t, so this gives, and the rest is this quite simple.

The delta function now operates because it is W n minus y x minus W n minus y, it becomes x minus W t. Recall what is W t? W t is equal to y plus W n. So, substituting y plus W n is equal to W t, we get this expression the delta function, and the rest is mere substitution. So, we are now able to write we are now able to write the expression for the kernel in terms of a continuous Brownian motion an integral of a function of a Brownian motion rather than summation of a discrete sum of random variables.

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Then, 
$$K(x,t;y) = \left\langle \exp\left[\int_{0}^{t} U(W(s))ds\right]\delta(x-W(t))\right\rangle$$
  

$$= E_{t}\left\{\exp\left[\int_{0}^{t} U(W(s))ds\right]\delta(x-W(t))\right\}$$

$$= E_{xt}\left(\exp\left(\int_{0}^{t} U(W(s))ds\right)\right) \text{ where } E_{xt}(\zeta) = E_{t}\left(\zeta\delta(x-W(t))\right)^{2}$$

So, now the important thing, what have we got, we have got the kernel as the expectation value of a certain quantity. We expectation value of the exponential of an integral, now when we have the expectation value, obviously, it will be integrated, it will involve a probability density function because, or a probability mass function either way. And then it has to be summed over or integrated over as the case may be with respect to this expression of random variables.

So, the basic point that I want to emphasize is that here we are having to talking about the continuous case, we have having a probability density function, and then we are having this random variable here. We are integrating the expression in order to arrive at the expected value.

And we have to do this integration over the various possible realizations, various possible realizations of this random variable. And because this random variable is continuous, there is a integration here. What do we find it is an integration over all possible paths, and therefore it is called a path integral right. So, we have arrived at this expression. Recall this is the origin of this path integral can be traced back to the diffusion equation. Therefore, this represents an explicit solution of the diffusion equation.

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Now, some definitions before we proceed further, the concept of autocorrelation functions. As I mentioned several times, a stochastic process involves a sequence of random variables. Random variable at t equal 1, random variable representing the process at t equal to 2, random variable representing the process at t equal to 3 and so on a sequence of random variable which is usually indexed with respect to time. Now, the correlation between these random variables at different points in time is conveys very important information about the dynamics of the process about the memory of the process. And therefore, it is a very important parameter as far as various stochastic processes are concerned. It is defined as the correlation function.

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We have 
$$E[X(t_1)X(t_2)] = \sum_{j=k} x_j x_k P_2(k,t_2;j,t_1)$$
  
 $= \sum_{j=k} \sum_{k} x_j x_k P_2(k,t_2|j,t_1) P_1(j,t_1)$   
For a stationary random process, on writing  $t_2 - t_1 = t$   
 $C_X(t) = E[X(0)X(t)] = \sum_{j=k} \sum_{k} x_j x_k P(k,t|j) P(j)$   
This is the autocorrelation function  $C_X(t)$  of the stationary, discrete random process X(t), in the case when the mean value is zero at all times.

Precisely, we have the expectation the correlation function is defined as the expectation of X at t 1, and X at t 2. The expectation of this value, you see you will have various realizations of t 1 x at t 1. And you will have various realizations of x at t 2. Work out the correlation between them, and that is precisely what gives you an indication of how the process is moving forward in time.

And this is as you can see on the right hand side, this represents the summation in the case of discrete processes, it represents the summation over j and k of all possible realizations of the

of the stochastic process at t equal to 1, at t equal to 2 together with the joint probability together with the two time joint probability of the process being in state j at time t 1, and the process being in state k at time t 2 that is what is called the correlation function.

Now, this probability point issue can be simplified further. And we by using Baye's theorem, we can express it at a two time conditional probability. And a onetime probability for a stationary process; it gets simplified further because time translation does not change the properties of the system.

Therefore, we can write t x E of X t, X t 1, X t 2 as equal to E of X 0 X t, and the rest of the properties also get simplified the conditional probability also gets simplified. It becomes and then this probability the one time probability also gets simplified, you can use the probability at t equal to 0 for that matter. And from t equal to 0, you can have the conditional probability that this system moves to the state k at time t, and work out the conditional work out the correlation function auto correlation function.

And that in that way with respect to t equal to 0 you can work out the auto correlation function. At any other point in time, it would be representative of other auto correlation functions also provided the system is a stationary random process, a stationary stochastic process that is time translation does not influence the system. (Refer Slide Time: 20:17)

When the mean value of a stationary random process is  
non-zero, the autocorrelation function is defined in terms  
of the deviation from the mean value, namely 
$$\delta X = X - E(X)$$
. In this case:  
$$C_{X}(t) = E\left[\delta X(0)\delta X(t)\right] = \sum_{j}\sum_{k}x_{j}x_{k}P(k,t|j)P(j) - \left[E(X)\right]^{2}$$
$$E\left(X\right) = \sum_{j}x_{j}P(j)$$

Now, this is the case where the definition that I have given above is the situation when the mean value of the random process is non is zero. If the mean value of the process is 0, then the above formula operate. If the mean value of the processes is not 0, then we measure correlations in respect of deviation from the mean.

We define deviation from the mean as delta of X is equal to X minus the mean of X, then delta X is equal to X minus mean of X that is the standard formula for deviations. And we work out the correlation as the expected value of delta X 0 delta X t. The correlation between these two and the formula change slightly this additional term in the green box comes into play.

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For Markov processes, the autocorrelation becomes all the more important. Recall what are Markov processes? Markov processes are those processes where the process has limited memory the memory is confined to the immediately preceding state. So, in the case of Markov processes, the autocorrelation function has special significance because the auto correlation function depends on the conditional probability, and the conditional probabilities determine all the joint probabilities in the case of Markov processes.

And the joint probabilities are what we want ultimately, because our path probability is a sequence of joint probabilities. So, knowing the joint probabilities, we can calculate path probabilities, and joint probabilities are determined by conditional probabilities in the case of Markov processes.

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For continuous stochastic processes, these are the formula a slightly different from what we have for the discrete expression, only basic difference is that we replace the summation by integration, and the probability functions by probability density functions, the rest is more or less absolutely parallel right.

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Now, I have talked about the diffusion equation in a lot of detail. You would recall I when I started with deriving the diffusion equation. What do you do what we did was we talked about the random motion of a particle in a fluid, we had certain predefined probabilities of these particle moving to the left moving to the right in an infinite decimal time; and on that basis we arrived at the diffusion equation.

We did not, we did not explicitly encounter the Newtonian force equation we did not present the dynamics of the particle in the form of a Newtonian force equation and then try to solve it. We had a slightly obscure approach to the study of the dynamics. We studied the dynamics purely in the context of probabilities. We did not talk about the dynamics per say as a Newtonian framework as a dynamical framework where the laws of motion manifest themselves explicitly. Recall now the Langevin equation does just that. It gives you or it presents the dynamics of the system which is subjected to some kind of a stochastic force field, and as explicitly presenting it in the Newtonian framework, and that is what I want to take up now.

We are talking about the dynamics of the Brownian particle. Recall that a Brownian particle is a microscopic particle which is immersed in a fluid, and which executes random motion due to the collisions that it encounters with the various molecules of the fluid.

Let us assume for simplicity the mass is assumed to be unity in any case we can rescale other quantities if we so desire and make the mass unity. So, that is not an issue really and that does not affect the generalization of the exposition. Now, we can write the assuming that the mass to be unity, the force equation, recall that we are working in non relativistic dynamics in Newtonian dynamics.

In Newtonian dynamics, we can write the equation of motion as the acceleration that is the rate of change of velocity is equal to minus gamma V is the velocity plus L t. The in the terms I will explain in a minute, but this is what is the Newton's equation of motion for the Brownian particle which is encountering collisions from various sides randomly by other particles of the fluid.

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Now, what is the property of the force that we are talking about in the current context? Number 1, there be one in this particular equation in fact we have introduced a damping term as well, the first term this first term minus gamma V is a damping term and it operates linearly in velocity.

And in the absence of any force it will cause the dissipation of energy, and result in the absence of any L t that is any external force the particle will gradually come to rest due to the damping term. So, we have one damping term which is a gamma is a constant quantity, and it is linear in the velocity. And then we have a stochastic term which is L t.

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Let us look at the properties of L t. The L t is a, L t is a random force; random in the sense that it is an impulse which takes place at random intervals of time. The force is the manifestation or of collisions between the various fluid molecules and the Brownian particle. So, let us explore the physical characteristics of this particular force before I talk about the statistical properties. (Refer Slide Time: 27:11)



Now, the first thing is that each the collision the time of collision is a very small. As a result of which the collisions may be assumed to be instantaneous. And then the collisions from one particle due to one particle the impact of the collision due to one particle and the impact of the collision due to another particle are mutually independent. They do not influence each other. And thirdly the force with which they collide with each other that force is not constant that is also varying rapid varies rapidly.

Now, the keeping in view these three properties, keeping in view the first property, collisions are spontaneous, collisions are uncorrelated with a between each other. And the collision force varies rapidly. We are able to model it in as a or together with a delta function, and that gives us the following two properties of the random force or the external force.

Number 1 is on the average L t will be equal to 0, and number 2 the correlation or the autocorrelation of L t at different points in time is delta is a delta function or is a modified delta function with gamma capital gamma here representing the strength of the force. And L t, L t dash is the autocorrelation expected value of L t L t dash is the autocorrelation.

So, the autocorrelation of the random force that is exerted on the Brownian particle due to collision between various molecules is in a sense delta correlated with an additional term that represents the magnitude of the that a scaling term. This is nothing but a scaling term which represents the magnitude of the force by which they are impacted right.

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Now, the by talking about this we have taken a certain approximation and a very strong approximation. The approximation is that the time span in which the effect of the force acts on the impulse of the force acts on the Brownian particle due to the collision is very very small. It

is in it is much smaller than other time scales that are relevant to this particular problem. And as a result of which not much approximation is introduced by the in use of delta function to model this collision in colliding force.

Now, we have talked about average force being average of L t being 0 or the average of the external force being 0, we have talked about autocorrelation, so there must be the issue of ensemble error. Now, when we talk about ensemble the assembled ensemble in this particular situation can consist of many many particles, at the same time they which are observed and the properties assessed many particles being observed and their properties determined in the same field.

Or the as same of single particle may be tracked over a sustained period of time in such a way that or to such an extent or to such a length to such a length that the time span is large enough for the impact of one collision, and not to impact the or not to influence the impact of the other collision. This is the fundamental condition that has to be met when we talk about the ensemble on the basis of which the averages or the statistical properties that I have mentioned earlier that is these two properties.

Property 1 and property 2, these two properties that I have mentioned these two properties must be calculated very carefully with respect to ensembles which satisfy either of these two conditions.

Either we have many particles in the same force field and they are assessed at the same point in time, or we have a single particle being tracked at different points in time with the points in time being so far apart that the influence of one collision does not carry over to the other collision. And even in the first case the particles that are studied together at the same time must be distant enough such that they do not get influenced by each other.

So, the Langevin equation is a special case of the general stochastic differential equation. My next program is to take up a detailed solution of the Langevin equation where again we will encounter the path integral.

And then will also establish a similarity between the Langevin equation which represents the pure dynamics of the system which represents which is explicitly showing you the Newtonian dynamics, the laws of motion governing the system, and the Fokker-Planck equation which represents the probabilities of this is of the conditional probabilities of various issues involved in the dynamics of the system. So, that is what I have in the agenda.

Thank you.