

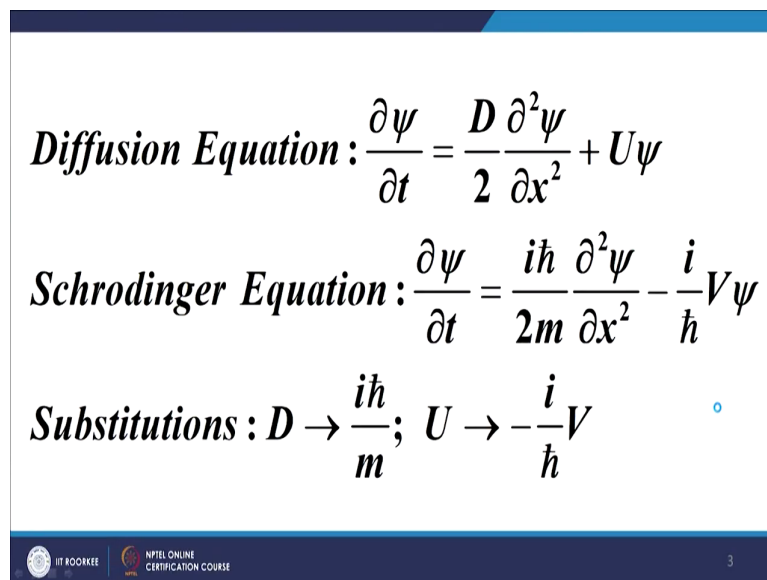
**Path Integral Methods in Physics & Finance**  
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**Lecture - 13**  
**Schrodinger Equation Path Integral, Langevin Equation**

Welcome back. In the last lecture we had a first encounter with the Path Integral. So, what I propose to do today is, to start with a brief recap of the steps that we followed, to develop this concept of path integral. And thereafter as an exercise we will extend this path integral for the diffusion equation to devise the path integral in the form, that Richard Feynman did for as the solution of the Schrodinger equation.

Then we will continue with our study of the Langevin equation, we will try to establish the equivalence between the Langevin equation and the Fokker Planck equation and develop the solution of the Langevin equation.

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The slide contains three mathematical equations and a substitution. The first equation is the Diffusion Equation:  $\frac{\partial \psi}{\partial t} = \frac{D}{2} \frac{\partial^2 \psi}{\partial x^2} + U\psi$ . The second equation is the Schrodinger Equation:  $\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi$ . The third part shows substitutions:  $D \rightarrow \frac{i\hbar}{m}$ ;  $U \rightarrow -\frac{i}{\hbar} V$ . The slide also features logos for IIT Roorkee and NPTEL Online Certification Course at the bottom.

**Diffusion Equation:** 
$$\frac{\partial \psi}{\partial t} = \frac{D}{2} \frac{\partial^2 \psi}{\partial x^2} + U\psi$$

**Schrodinger Equation:** 
$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi$$

**Substitutions:** 
$$D \rightarrow \frac{i\hbar}{m}; U \rightarrow -\frac{i}{\hbar} V$$

So, that is the agenda for today. Let us start, the diffusion equation is given by the first equation on the slide del phi by del psi by del t is equal to D by 2; del square psi upon del x square plus U of psi. In contrast the Schrodinger equation can be written in the form of del psi by del t is equal to ih i is under root 1 minus 1 I am sorry ih upon 2 m del square psi and upon del x square minus i upon h V into psi.

It is written in a slightly different form, but by the rearrangement of various numbers; we can put it in the form that I have presented on the slide.

A comparison of the 2 equations - the diffusion equation and the Schrodinger equation represents the following relationships: D relates to ih upon m; h bar upon m, recall that h is the Planck's constant, U is replaced by minus ih V where V is the potential.



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**Propagator :**

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

**Kernel :**

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

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Now, also to recall we ended up, finding the expression for the propagator in the form that is given in the red box. And we had the expression for the kernel which is the second equation on this slide for the diffusion equation. I emphasize these expressions were obtained for the diffusion equation.

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**SOLUTION OF DIFFUSION EQUATION**

*Consider the 1 – D diffusion equation*

$$\frac{\partial \psi}{\partial t} = U\psi + \frac{D}{2} \frac{\partial^2 \psi}{\partial x^2}$$

*Its solution can be written as :*

$$\psi(x,t) = \left\{ \exp \left[ t \left( U + \frac{D}{2} \frac{\partial^2}{\partial x^2} \right) \right] \right\} \psi(x,0) = \Delta \psi(x,0)$$

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How did we go about it? Well, a quick recap we started with the diffusion equation we are obtained the solution of the diffusion equation in the form that is given in the green box. That was the first step; we started with this equation then we proceeded to simplify the expression that is contained in the green box at the bottom of the slide.

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**APPLY TROTTER'S FORMULA**

$$F/A : \psi(x, t) = \exp \left[ t \left( U + \frac{D}{2} \frac{\partial^2}{\partial x^2} \right) \right] \psi(0) = \Delta \psi(x, 0)$$

Set :  $A = U ; B = \frac{D}{2} \frac{\partial^2}{\partial x^2}$ . By Trotter's formula, we have

$$\exp [t(A + B)] = \lim [ \exp(tA/n) \exp(tB/n) ]^n \text{ so that}$$

$$\Delta = \exp \left[ t \left( U + \frac{D}{2} \frac{\partial^2}{\partial x^2} \right) \right] = \lim_{n \rightarrow \infty} \left[ \exp \left( \frac{t}{n} U \right) \exp \left( \frac{t}{n} \frac{D}{2} \frac{\partial^2}{\partial x^2} \right) \right]^n$$



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How did we do it? Well, the first step we did was to use the Trotter's formula, to write it as a product of exponentials to the power n with the limit n tending to infinity we wrote this expression exponential t bracket U plus D by 2 del square upon del x square as a limiting; limit n tending to infinity exponential t upon n U. Exponential t upon n D by 2 d square upon d x square and the whole thing raised to the power n.

Then we took up 1 above the second expression, that is exponential t upon n D by 2 del square upon del x square and we manipulated it a bit.



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To simply:  $\exp\left[\frac{t D \partial^2}{n 2 \partial x^2}\right]$

Gaussian integral:  $\sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dy \exp(-ay^2 + by) = \exp\left(\frac{b^2}{4a}\right)$

Set  $a = \frac{1}{2D}$ ,  $b = \sqrt{\frac{t}{n}} \frac{\partial}{\partial x}$ , we get

$\frac{1}{\sqrt{2\pi D}} \int dy \exp\left[-\frac{1}{2D} y^2 + \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x}\right] = \exp\left[\frac{t D \partial^2}{n 2 \partial x^2}\right]$

How did we manipulate it? Well, it that is very interesting we invoke the Gaussian integral. The Gaussian integral in the form of integral minus infinity to infinity exponential minus a y square plus b y which cannot be integrated by computing d square, and we end up with the expression on the right hand side. This expression that I put now in the within the box.

This expression if I make this substitution in this expression on the right hand expression of a equal to 1 upon 2 D, b equal to under root t upon n del by del x. Then, this right hand expression this right hand corner expression becomes precise with expression that we started with.

So, equivalently we can say that the left hand expression must also represent the same thing with the substitutions a equal to 1 upon 2 D, b equal to under root t upon n D by del x. So, we

make the substitutions, and we end up with the expression that is given at the equation that is given at the bottom of your slide.

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**CONVERT TO GAUSSIAN EXPECTATION**

$$F/A: \frac{1}{\sqrt{2\pi D}} \int dy \exp \left[ -\frac{1}{2D} y^2 + \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right] = \exp \left[ \frac{t D}{n} \frac{\partial^2}{2 \partial x^2} \right]$$

Now, the expression  $\frac{1}{\sqrt{2\pi D}} \int dy \exp \left[ -\frac{1}{2D} y^2 + \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right]$

can be written as the expectation value of  $\omega = \exp \left( \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right)$

under the Gaussian distribution:  $p(\omega) d\omega = \frac{1}{\sqrt{2\pi D}} \exp \left( -\frac{y^2}{2D} \right) dy$


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Now, if you look at the expression that that is brought forward in fact, that is the first equation now on this particular slide. It is very interesting if you carefully analyze this expression it can be written as an expectation value. We have 1 we have a probability distribution 1 upon under root 2 pi D exponential integral of d y exponential minus 1 upon 2 D y square which is clearly a Gaussian distribution.

And we have the other term which is exponential under root t upon n y del by del x. So, we can this whole expression can be seen as the expectation of the variable; which is represented by omega, omega equal to under root t upon n y del by del x with the probability distribution

being this particular Gaussian distribution which is given right in the red box right at the bottom of this slide.

This is the probability density function the pdf and the random variable is given by exponential under root t upon n y del by del x. If you putting it the other way around; suppose, I were to work out the expectation of omega given by exponential under root this expression with respect to the probability distribution or pdf given by the expression in the red box, I would precisely end up with the first the left hand side of the first equation given on this slide.

Which we have already established is equal to the right hand side, and which we started with. So, that is the sequence of events that have taken place so far. And we now ended up with the right hand side of the first equation being equal to an expected expectation value which is given in the green box right at the bottom of this slide.

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$$\frac{1}{\sqrt{2\pi D}} \int dy \exp \left[ -\frac{1}{2D} y^2 + \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right] \text{ is expectation value of}$$

$$\omega = \exp \left( \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right) \text{ under the Gaussian distribution :}$$

$$p(\omega) d\omega = \frac{1}{\sqrt{2\pi D}} \exp \left( -\frac{y^2}{2D} \right) dy. \text{ Hence } \exp \left[ \frac{t D}{n} \frac{\partial^2}{2 \partial x^2} \right]$$

$$= \frac{1}{\sqrt{2\pi D}} \int dy \exp \left[ -\frac{1}{2D} y^2 + \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right] = \left\langle \exp \left( \sqrt{\frac{t}{n}} y \frac{\partial}{\partial x} \right) \right\rangle$$





As represented by this ah arrow exponential this becomes equal to this through the intermediate steps that, I have just enumerated.

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**INTRODUCE SEQUENCE OF GAUSSIAN EXPECTATION**

Now consider  $\left[ \exp\left(\frac{t D}{n} \frac{\partial^2}{2 \partial x^2}\right) \right]^n$ . For each one of these  $n$  factors, we introduce an independent Gaussian random variable  $y_j$  with the corresponding probability density

$$p(\omega_j) d\omega_j = \frac{1}{\sqrt{2\pi D}} \exp\left(-\frac{y_j^2}{2D}\right) dy_j; j = 1, 2, \dots, n$$



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Now, but if you look at the where we started with when we use Trotter's formula we had this exponential. But we had it to the power  $n$ ; exponential  $t$  upon  $n D$  by  $2$  del square upon del  $x$  square to the power  $n$ , that is what we had. We have so far simplified only the inner part without the power that is we have simplified exponential  $t$  upon  $n D$  by  $2$  and  $d$  square upon  $d x$  square and we are expected expressed as a expectation value.

But, when we have where that means, in other words we need to take the  $n$ th power expectation or expectation of  $n$  such variables. And that is precisely what we do we introduce

$n$  such  $y$  variables  $y_1, y_2, y_3$  having similar Gaussian distributions which is given in the red box at the bottom of your slide. And these are the  $j$  it is ranging from 1 to  $n$ .

So, we introduce  $n$  such variables corresponding to  $n$  factors which are represented by the  $n$ th power of this particular expression. This particular expression within the brackets the exponential expression is itself equal to 1 term.

And this because of the power  $n$  there are  $n$  terms and to account for those  $n$  terms we have introduced  $n$  Gaussian random variables; each of which follows this particular distribution. Each of which follows this particular distribution the distribution that is given in the red box in your at the bottom of your slide the dark red box.

And, recall please note this all these variables  $y_1, y_2, y_3$  are independent. And of course, they are Gaussian, but they are independent. That is very important property otherwise analysis would be very much impeded the variables are independent of each other right.

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$$\exp\left[\frac{t D \partial^2}{n 2 \partial x^2}\right] = \left\langle \exp\left(\sqrt{\frac{t}{n}} y \frac{\partial}{\partial x}\right) \right\rangle \text{ so that}$$

$$\Delta = \exp\left[t\left(\frac{D \partial^2}{2 \partial x^2} + U\right)\right] = \lim_{n \rightarrow \infty} \left[ \exp\left(\frac{t}{n} U\right) \exp\left(\frac{t D \partial^2}{n 2 \partial x^2}\right) \right]^n$$

$$= \lim_{n \rightarrow \infty} \prod_{j=1}^n \left\langle \exp\left(\frac{t}{n} U\right) \exp\left(\sqrt{\frac{t}{n}} y_j \frac{\partial}{\partial x}\right) \right\rangle$$

So, that is what we precisely do when we put these values when we use this sequence of  $n$  independent Gaussian random variables and express each term as an expectation of one of these random variables. In these Gaussian random variables we end up with a product of this this expression, which is given in the green slide at the bottom of your, green box at the bottom of your screen.

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- The expectation bracket stands for all  $n$  expectation values or Gaussian integrals;
- In each term of the product the lower index  $y_j$ 's are written to the right by convention;
- The product is an ordered product where a factor with  $\frac{\partial}{\partial x}$  is followed by a factor of  $U(x)$  then followed by a factor of  $\frac{\partial}{\partial x}$  and so on.



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**INTERCHANGE TERMS BY TRANSLATION OPERATOR**

$$\Delta = \lim_{n \rightarrow \infty} \prod_{j=1}^n \left\langle \exp\left(\frac{t}{n} U\right) \exp\left(\sqrt{\frac{t}{n}} y_j \frac{\partial}{\partial x}\right) \right\rangle$$

$$= \lim_{n \rightarrow \infty} \left\langle \exp\left(\frac{t}{n} \sum_{k=1}^n U\left(x + \sqrt{\frac{t}{n}} \sum_{j=k}^n y_{j+1}\right)\right) \exp\left(\sqrt{\frac{t}{n}} \sum_{k=1}^n y_k \frac{\partial}{\partial x}\right) \right\rangle$$

*with*  $y_{n+1} = 0$ .



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Now, this we discussed not much to say about this now we come to a very important property, you see how does our term look like? Let us go back if you look at this term if you look at this term, if you write it out in completely without the abbreviated notation then, what you find is quite; obviously, it has a term in d by d x.

Then it has a term in U, it has a term in d by d x, it has a term in U and so on. In other words the terms in d by d x or del by del x and in you are alternating with each other. We do not have del by del x together and U's together, we do not have that. The terms alternate with each other the del by del x term and the U terms.

But the important part is del by del x in itself acts as a translation operator. And this property of this translation operator enable this to interchange wherever required, the position of the 2 terms and then to write ah and to write all the del by del x terms to the right hand side, and all

the U terms to the left hand side. This is the very important maneuver which is facilitated by the interpretation of  $\delta$  by  $\delta x$  as a translation operator.

It enables us to shift the U terms and the  $\delta$  by  $\delta x$  terms inter se and as a result of which we can now end up with a situation. Where we have all the  $\delta$  by  $\delta x$  terms existing to the right and all the U terms existing to the left and we write it in the form which is given in the blue box at the bottom of your slide right.

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Recall:  $\Delta = \lim_{n \rightarrow \infty} \left\langle \exp \left( \frac{t}{n} \sum_{k=1}^n U \left( x + \sqrt{\frac{t}{n}} \sum_{j=k}^n y_{j+1} \right) \right) \times \exp \left( \sqrt{\frac{t}{n}} \sum_{k=1}^n y_k \frac{\partial}{\partial x} \right) \right\rangle$

with  $y_{n+1} = 0$ . In the limit  $n \rightarrow \infty$   $\langle y_j \rangle = 0, \langle y_j^2 \rangle = D$

Thus, by the CLT,  $\sum_{k=1}^n y_k \xrightarrow{\text{distribution } (n \rightarrow \infty)} N(0, nD)$

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So, what are the properties of  $y$ ? That is a question forward if you look at the relationship in fact, you can directly infer it from the probability density function  $y$  if you if you want to go back we can go back and have a look at it is here the variance is  $D$ , and the mean is  $0$ . So, they are normally distributed all the  $y$ 's are independent of each other, they are Gaussian, they are and distributed with a mean of  $0$  and a variance of  $D$ . So, that is quite straightforward.



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**INTRODUCE BM**

*Defining a Brownian motion by*  $W_k = -\sqrt{\frac{t}{n}} \sum_{j=1}^k y_j$  *with*

$$\langle W_k \rangle = 0; \langle W_k^2 \rangle = \frac{t}{n} kD = \frac{kt}{n} D; dW = W_k - W_{k-1} = -\sqrt{\frac{t}{n}} y_k;$$

$$\langle dW \rangle = 0; \langle (dW)^2 \rangle = \left\langle \left( -\sqrt{\frac{t}{n}} y_k \right)^2 \right\rangle = \frac{t}{n} D = Ddt$$



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Now, to analyze the situation further we introduced the concept of Brownian motion. We introduced the Brownian motion in the form given in the red box  $W_k$  is equal to minus under root  $t$  upon  $n$  summation of these, these Gaussian variables summation of this Gaussian variables represent Brownian motion that is quite; well-known that is we have discussed it, in fact, in an earlier lecture as well.

$W_k$  is we write as a summation of a scaled summation under root  $t$  upon  $n$  is a scaling factor. As a scaled summation of the summation of all the  $y$ 's and recall, each  $y$  is Gaussian distribution normally distributed with a mean of 0, and a variance of  $D$ . These are the various parameter that are apparent you know quite obvious from the definition itself.

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$\psi(x,t) = (\Delta\psi)(x,0)$ ;  $\Delta$  is the propagator

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

$\psi(x,t) = \int dy K(x,t;y) \psi(y,0)$ ;  $K(x,t;y)$  is kernel

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

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So, after all these maneuvers we end up with the 2 expressions we end up with the expression for the propagator; which is given in the red box and we end up with the expression for the kernel which is given in the in the important part of this slide. So, we have these expressions where we ended the discussion last time.



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**REVERSION TO ORIGINAL DISCRETE VARIABLES**



*The expression for the kernel :*

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

*Revert to original Gaussian discrete variables  $y_j$  :*

$$W_k = -\sqrt{\frac{t}{n}} \sum_{j=1}^k y_j \text{ whence : } K(x, t; y)$$

$$= \lim_{n \rightarrow \infty} \left\langle \exp \left[ \frac{t}{n} \sum_{k=1}^n U \left( y - \sqrt{\frac{t}{n}} \sum_{j=1}^k y_j \right) \right] \delta \left( x - \sqrt{\frac{t}{n}} \sum_{j=1}^n y_j - y \right) \right\rangle \quad (1)$$



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Now, we move to as an exercise as an application of this concept, we try to solve this Schrodinger equation in the form of a path integral, which is very commonly known as the Feynman path integral. So, we start with the original version that is the version that we had in the last slide that we derived in the last class that is here.

And from here we go back a bit and what we do is we substitute  $W_k$  and  $W_n$  in terms of the random variables the Gaussian distributed random variables  $y_1, y_2, y_k$  and so on. We go back a bit replace the Brownian motion by the constituent random variables.

And, we get the expression that is given at the bottom of your slide. I will mark it as equation 1.

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**PROPERTIES OF  $y_j$**

$$y_j = z_j \sqrt{D} + D \sqrt{\frac{t}{n}} \frac{\partial}{\partial x}$$
$$z_j \xrightarrow{\text{distribution}} N(0,1).$$

Hence, in the limit  $n \rightarrow \infty$ ,  $\langle y_j \rangle = 0$ ,  $\langle y_j^2 \rangle = D$ .

Thus, by the CLT,  $\sum_{k=1}^n y_k \xrightarrow{\text{distribution } (n \rightarrow \infty)} N(0, nD)$

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As far as properties of  $y$ 's are concerned just to recollect they are normally distributed, they are independent, they have a mean of 0 and a variance of D each of them.

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**INCORPORATING THE PROBABILITY DISTRIBUTIONS**

$$K(x, t; y) = \lim_{n \rightarrow \infty} \left\langle \exp \left[ \frac{t}{n} \sum_{k=1}^n U \left( y - \sqrt{\frac{t}{n}} \sum_{j=1}^k y_j \right) \right] \delta \left( x - \sqrt{\frac{t}{n}} \sum_{j=1}^n y_j - y \right) \right\rangle$$

*Incorporating the probability distributions in the expectation. We replace the averages over  $y_1, y_2, \dots, y_n$  by their explicit form as integrals. In this case an integral over  $y_1, y_2, \dots, y_n$*

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Now, what we do is, these angular brackets as you know very well represent expectations. They represent the expectation of whatever is contained within them and, with respect to the probability distribution that we just talked about.


Let us make it explicit. Instead of representing the expectation by these angular brackets; we now introduce explicitly the probability distributions of the random variables you see if you can very well see here that the only random variables are  $y$ .

So, we introduced the respective  $y_1, y_2, y_3$  and so on. So, we introduced the probability density functions of these particular variables and write the expectation in an explicit form in the form by incorporating the Gaussian probability distributions or probability density functions together with whatever we have inside the angular brackets.

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$$y_j = z_j \sqrt{D} + D \sqrt{\frac{t}{n}} \frac{\partial}{\partial x}; \quad z_j \xrightarrow{\text{distribution}} N(0,1).$$

Hence, in the limit  $n \rightarrow \infty$ ,  $\langle y_j \rangle = 0$ ,  $\langle y_j^2 \rangle = D$ .

$$p(\omega_j) d\omega_j = \frac{1}{\sqrt{2\pi D}} \exp\left(-\frac{y_j^2}{2D}\right) dy_j \quad (2)$$


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So, let us see what we get. The this is the distribution of each  $y_j$  is distributed in this form. The let us call it equation 2 equation 2 represent the probability density function of each of these random variable.

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

$$K(x, t; y) = \lim_{n \rightarrow \infty} \int dy_1 \dots dy_n (2\pi D)^{-n/2} \exp \left[ - \left( \frac{1}{2D} \right) \sum_{k=1}^n y_k^2 \right]$$

$$\times \exp \left[ \frac{t}{n} \sum_{k=1}^n U \left( y - \sqrt{\frac{t}{n}} \sum_{j=1}^k y_j \right) \right] \delta \left( x - y + \sqrt{\frac{t}{n}} \sum_{j=1}^n y_j \right)$$

So, let us put them there and we can write the expectation energy which is the upper equation in the form of the lower equation.

We have done nothing else except to substitute or to introduce substitute. In fact, we can call it substitution of the angular brackets by the explicit expression for the expectation incorporating there in the Gaussian probability distributions why? Because all the  $y_j$ 's are Gaussian distributions each has a mean of 0, each has a variance of  $D$ .

And therefore, because there are  $n$  such variables you can see here the factor of  $2\pi D$  is raised to the power  $n$  each of that contribute factor of under root  $2\pi D$  in the denominator. And therefore, because there are  $n$  such variables we have  $2\pi D$  to the power minus  $n$  by 2 and the rest is also and quite straight for this mere substitution nothing else.

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**NOTATIONAL SIMPLIFICATION**

*In an effort to restrict the proliferation of notation we define*

$$\xi_k = y - \sqrt{\frac{t}{n}} \sum_{j=1}^k y_j \quad \text{and} \quad \xi_0 = y$$

*With  $\xi_k, k = 1, \dots, n$  as the integration variables, we have :*

$$K(x, t; y) = \lim_{n \rightarrow \infty} \int d\xi_1 \dots d\xi_n (2\pi Dt/n)^{-n/2} \\ \times \exp \left\{ -\frac{1}{2Dt/n} \sum_{k=1}^n (\xi_k - \xi_{k-1})^2 + \frac{t}{n} \sum_{k=1}^n U(\xi_k) \right\} \delta(x - \xi_n)$$


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Now, we make a bit of notational simplification. So, let us simplify the notation of a bit to reduce the proliferation of notations, what we do is, we make these small substitutions in order that the notation becomes more compact. And clearly when you put these substitutions here you get the expression that is there in this dark red box, at the bottom of this slide.

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### FURTHER STEPS

- The path integral appearance is now clearly pronounced. We do the remaining steps:
- 1. If the integral over  $\xi_n$  is performed the  $\delta$ -function forces  $\xi_n = x$ .
- 2. Next, to correlate with the Schrodinger equation, we set  $D = i\hbar/m$  and  $U = -iV/\hbar$ .
- 3. Calling  $\varepsilon = \frac{t}{n}$ , we get the following expression for K:

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Now, we are literally through some fundamental steps need to be done. We have a delta function here, and delta of  $x$  minus  $\xi_n$  when this integration is done over  $\xi_n$  we get all the  $\xi_n$ 's will be replaced by  $x$ .

So, that accounts for the delta function integration that will be done then we substitute  $D$  equal to  $i\hbar$  upon  $m$  which  $i$  mentioned when we compared the diffusion equation and the Schrodinger equation and we substitute  $U$  equal to minus  $iV$  upon  $\hbar$ ; which also was apparent when we compared the Schrodinger and the diffusion equations.

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$$\begin{aligned}
 F / A : K(x, t; y) &= \lim_{n \rightarrow \infty} \int d\xi_1 \dots d\xi_n (2\pi Dt/n)^{-n/2} \\
 &\times \exp \left\{ -\frac{1}{2Dt/n} \sum_{k=1}^n (\xi_k - \xi_{k-1})^2 + \frac{t}{n} \sum_{k=1}^n U(\xi_k) \right\} \delta(x - \xi_n) \\
 K(x, t; y) &= \lim_{n \rightarrow \infty} \int d\xi_1 \dots d\xi_{n-1} \left( \frac{m}{2\pi i \hbar \varepsilon} \right)^{n/2} \\
 &\times \exp \left\{ \frac{i}{\hbar} \left[ \frac{m}{2\varepsilon} \sum_{k=1}^n (\xi_k - \xi_{k-1})^2 - \varepsilon \sum_{k=1}^n V(\xi_k) \right] \right\} \quad - (3)
 \end{aligned}$$

We abbreviate  $t$  by  $n$  as  $\varepsilon$ , which is the length of the time step and after doing all that we have this expression which is let us say equation number 3. This is what we have after making all those substitutions after taking care of whatever I have mentioned in this slide and doing the delta integration putting the values of  $D$ . And  $U$  in terms of their corresponding values in the Schrodinger equation and writing  $\varepsilon$  equal to  $t$  by  $n$  for priority.



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- with the provisos  $\xi_0 = y$  and  $\xi_n = x$ .
- We now call the integrals over  $\xi_1, \dots, \xi_{n-1}$  a sum over paths and write the integrand in continuum notation to get:

$$K(x,t;y) = \int_{\substack{\xi(0)=y \\ \xi(t)=x}} [D\xi] \exp\left\{\frac{i}{\hbar} S[\xi(\cdot)]\right\}$$



And then, we what we have is we know of course, because of the delta we had this assumption  $\xi_0$  is equal to  $y$  earlier. If you can recall that we had it here we have it there in the upper box the bright red box we have it;  $\xi_0$  is equal to  $y$  and because of the delta function we also have that  $\xi_n$  is equal to  $x$ .

So, both are taken care of and the integrals over  $\xi_1$  to  $\xi_{n-1}$  are now considered as integrations of over various paths. And, when we compactify the notation a bit we get this expression, where  $S$  now represents the classical action.

What is the and ended this expression the integration volume represents integration over all paths; that have these defining characteristics what  $\xi$  of 0 is equal to  $y$  and  $\xi$  of  $t$  is equal to  $x$ .


All the paths so, this integration has to be carried out over all the paths right. And all this integration is compactly written as  $D$  of  $\xi$  within the square bracket.

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$$K(x, t; y) = \int_{\substack{\xi(0)=y \\ \xi(t)=x}} [D\xi] \exp\left\{\frac{i}{\hbar} S[\xi(\cdot)]\right\} \quad \text{---(4)}$$

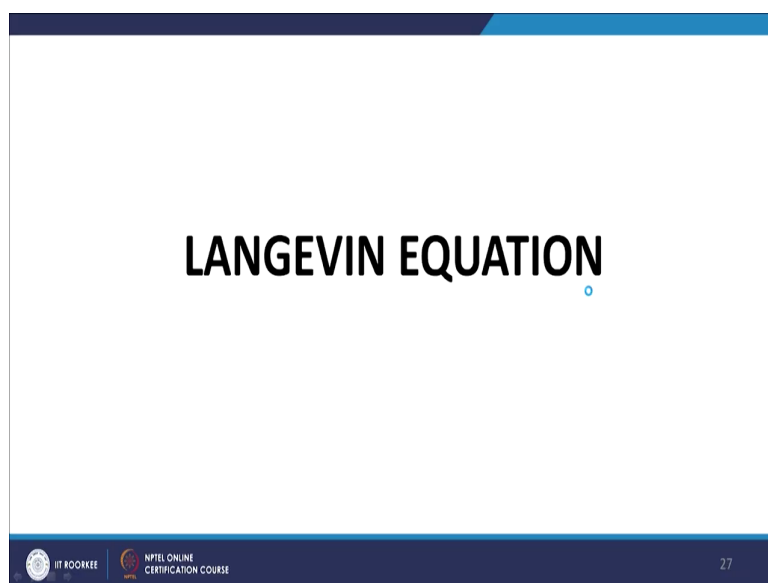
$$S[\xi(\cdot)] = \int_0^t ds \left[ \frac{1}{2} m \left( \frac{d\xi}{ds} \right)^2 - V(\xi(s)) \right] \quad \text{---(5)}$$

**$S$  is the classical action. The above eqs are the Feynman path integral.**



And as far as the classical action is concerned if you look at what we had earlier this expression if you simplify this expression a bit you find that it is nothing but the, classical action that we have in terms of the Lagrangian. And this is nothing, but the kinetic energy the first term, the second term is nothing but the potential energy. So, the action is nothing but the, time integral of the Lagrangian as we normally expect in nonrelativistic classical and quantum mechanics right.

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So, that is our Feynman path integral. This is our Feynman path integral; in fact, this equation let us call it equation 4. Equation 4 and equation 5 together constitute the framework of path integration that is extended and that is applied in quantum mechanics and in quantum field theory.  $S$  is the action and this represents the path integral which is either the kernel or the green function right.

Now, we come back to our discussion on the Langevin equation I had given an introduction to the Langevin equation. Actually, this is the dynamical equation we had you see that the diffusion equation also represents the motion of a Brownian particle in a fluid, but that represents it from the perspective of the probabilities the conditional probabilities. Here we have a direct equation manifesting itself as the dynamical equations the Newtonian equation of the representing the dynamics of the Brownian particle.

So, let us now explore that in detail, let us start with a very simple straightforward situation. Where, we assume that the force that is impacted or that is that applies on the Brownian particle due to collisions of the particle with the molecules of the fluid is totally random, we do not know anything about it and we model it simply as a magnified or a scaled white noise where under root gamma is the scaling factor.

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**INTRODUCTION**

- Consider the simplest SDE of a Brownian particle acted on by a purely random force. Its EOM has the form:
- $m \frac{dv}{dt} = \sqrt{\Gamma} \eta(t)$  where the factor  $\sqrt{\Gamma}$  relates to the strength of the impulse acting on the particle as a result of its collisions with the molecules.


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So, we can write the dynamical equation as the force equation the force on the left hand side  $m$ ; mass into acceleration is equal to the applied force which is given by  $\eta$  sorry under root gamma  $\eta$   $t$ .  $\eta$   $t$  is the white noise or the factor that captures the stochasticity of the force the randomness embedded in the force, randomness embedded in the collisions when the particles collide with the Brownian particles.

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## PROPERTIES OF $\eta(t)$

- We assume that:
- Each collision is practically instantaneous.
- Successive collisions are uncorrelated.
- The collision force varies rapidly.
- The collisions do not have any preferred direction.
- whence  $\eta(t)$  can be approximated by a delta correlated, Markov, Gaussian white noise so that:
- $\langle \eta(t) \rangle = 0$  and  $\langle \eta(t) \eta(t') \rangle = \delta(t - t')$



We make certain assumptions. We make that the assumptions that each collision is for a very short period of time and as a result of which we can assume it to be instantaneous. And we can we also make the assumption that successive collisions are random; in other word they are uncorrelated with each other there is no significant association no significant memory between various collisions.



Then, we also make the assumption that the force that results due to the collision acts for a very short period of time and therefore, varies very rapidly. Then another important property that we have is, that the collisions do not have any preferred direction; in other words even ah the Brownian particle encounters a similar collision pattern when viewed from any point of reference in the 3- dimensional space.

So, these are some fundamental assumptions that we make, and under these assumptions we can approximate  $\eta(t)$  as a delta correlated white noise as a delta correlated Gaussian white noise. And therefore, we have the 2 fundamental properties the average of  $\eta(t)$  you know over an ensemble is 0, and the autocorrelation functions of  $\eta(t)$  are also delta functions, there the  $\eta(t)$  is delta correlated in time.

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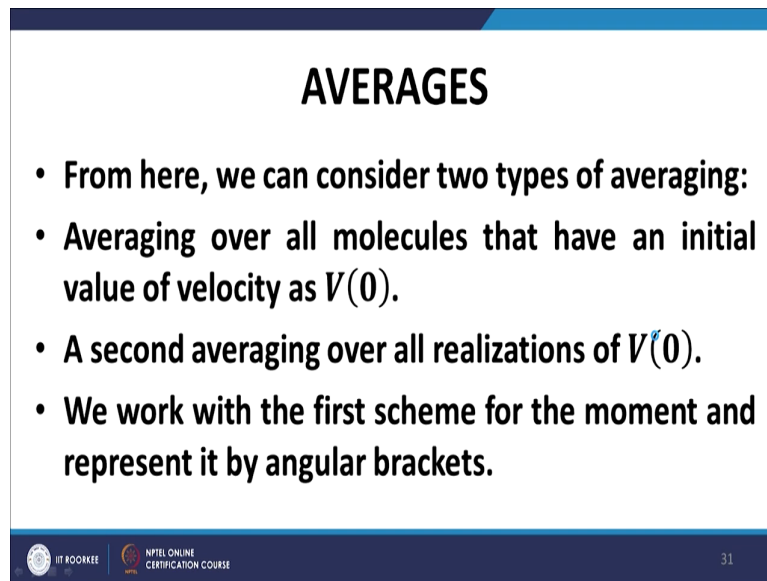
## SOLUTION

- The solution of
- $m \frac{dv}{dt} = \sqrt{\Gamma} \eta(t)$  takes the form:
- $V(t) = \underline{V(0)} + \frac{\sqrt{\Gamma}}{m} \int_0^t dt' \eta(t')$



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What is the solution of this equation? The solution of this equation is relatively straightforward. You can write it in the form  $V$  of  $t$  is equal to  $V_0$  plus under root gamma upon  $m$  where,  $m$  is the mass of the particle in integral 0 to  $t$   $dt'$  dash  $\eta(t)$  dash and so, this it is a straightforward see inhomogeneous first order equation. So, if we do not have much problem in writing down its solution.

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## AVERAGES

- From here, we can consider two types of averaging:
- Averaging over all molecules that have an initial value of velocity as  $V(0)$ .
- A second averaging over all realizations of  $V(0)$ .
- We work with the first scheme for the moment and represent it by angular brackets.

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Now, from here we have we have certain interesting feature, certain interesting inferences that we can draw. The first thing is averaging can be done in two ways; first one way of averaging would be that we average over all particles in that in the ensemble all particles we average over which have the initial velocity of  $V_{naught}$  or  $V_0$ .

The other way of averaging would be a second averaging, where we also average over all possible realizations of  $V_{naught}$ . So, for the moment we will stick to the first case of averaging in other words, we average over all particles of the ensemble that have the initial velocity of  $V_{naught}$ . So, let us do that.

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### AVERAGE OF $V(t)$

- $\langle V(t) \rangle = V(0) + \frac{\sqrt{\Gamma}}{m} \left\langle \int_0^t dt' \eta(t') \right\rangle$
- $= V(0) + \frac{\sqrt{\Gamma}}{m} \int_0^t dt' \langle \eta(t') \rangle$
- $= V(0)$  *since*  $\langle \eta(t') \rangle = 0$

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The average of we represented by angular brackets as usually, the case we have  $V(t)$  is equal to  $V(0)$  plus this thing now the always  $V(0)$  is not stochastic, it is deterministic. So, no problem under root to gamma upon m is also; it is a number it is a constant. So, it can be taken outside the averaging process and the averaging is confined to the integral of  $\eta(t)$ .

Now, integral is in essence a sum. Integral represents a sum and, because the integral represents a sum and expectation the expectation operates in such a way that the expectation of a sum is equal to the sum of the expectations. We can take the expectation operator inside the integral and we can write it in the form which is given in the second equation.

But, the average of  $\eta(t)$  is over the realization in the assemble are 0. And therefore, what we find is that the average velocity at time t is equal to the initial velocity  $V(0)$ . In this particular model the average velocity at time t is equal to the initial velocity  $V(0)$ ; not to



this does not seem in any way counter intuitive, but we carry on the analysis to understand more about this model.

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**AVERAGE OF  $V^2(t)$**

- $\langle V^2(t) \rangle = V^2(0) + \frac{\Gamma}{m^2} \left\langle \int_0^t dt_1 dt_2 \eta(t_1) \eta(t_2) \right\rangle + \langle \text{CROSS TERM} \rangle$
- Now,  $\langle \text{CROSS TERM} \rangle = 0$
- since the cross term contains  $\langle \eta(t') \rangle = 0$

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Let us work out the average of  $V$  square  $t$ .  $V$  square  $t$  when you work at the average the first term will; obviously, be  $V$  square of 0 the square of the initial velocity which again being deterministic is a number it is a constant and therefore, averaging over this make no difference to it.

ah Now, we have 2 more terms in this. Let us go back a bit this is the equation for  $V$   $t$ . So, when we do the when we work out  $V$  square, what do we have? We have  $V$  square of  $t$  is equal to  $V$  square of 0 plus  $\frac{\Gamma}{m^2}$   $\frac{\Gamma}{m^2}$  integral this into integral the same expression with a different integration a variable plus we have a term that

comprises of  $V_0$  and that comprises of this expression. That comprises of  $V_0$  and this expression.

Now, let us call this the cross term. So, we have  $V_0$  that is one term. We have the product of these in this expression twice over. So, that is the second term and we have a cross term. Now look at the cross term, when you look at the cross term what does it comprises of? It comprises of  $V_0$  which is deterministic, it comprises of  $\sqrt{\gamma}$  upon  $m$  which is constant, and it comprises of this integral one time.

Now, this when you take the average as we have done just now just in the previous case, when you take the average over  $\eta t$  dash this average vanishes. So, in other words what I am trying to say is, that the average of the cross term, when I work out this average of the square of  $V_t$ , the average of the cross term will vanish will be 0. And therefore, we have two terms; one is  $V^2$   $V$  square of  $V_0$   $V$  square the square of the initial velocity and the second term is  $\gamma$  upon  $m$  square of the noise twice over let us go back now.

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- **Also**
- $\left\langle \int_0^t dt_1 dt_2 \eta(t_1) \eta(t_2) \right\rangle = \int_0^t dt_1 dt_2 \langle \eta(t_1) \eta(t_2) \rangle$
- $\int_0^t dt_1 dt_2 \delta(t_1 - t_2) = \int_0^t dt_1 = t$
- $\langle V^2(t) \rangle = V^2(0) + \left( \frac{\Gamma t}{m^2} \right)$
- **is unbounded in time and hence, unphysical.**

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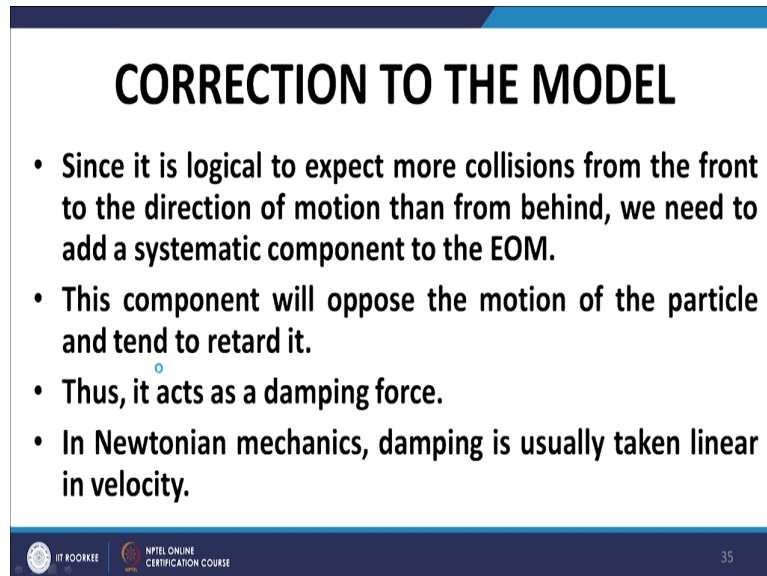
Yes. So, so the second term let us analyze the second term. We have integral dt 1 dt 2 eta t 1 eta t 2 the average of this. Now, as I mentioned because the integral is nothing but, a sum we can take this integral we can take this averaging I am sorry inside the integral and we can write it as an integral 0 to t dt 1 d 2 and the averaging between eta t 1 and eta t 2. Now, this is nothing but the autocorrelation function and which we have assumed to be a delta correlation.

So, putting that delta correlation here, and doing the t 2 integration we get this is equal to 0 to t 1 and integral dt 1 which is equal to t. So, what do we end up with? We end up with the average of V square t being equal to V square 0 plus gamma t upon m square. Now this has a problem with it. The problem is that as t tends to infinity this expression gets unbounded.

The second part is unbounded as t increases the average value of V square t also increases and without any restriction without any bound which is physically not correct which is unphysical.

Therefore, some modification somewhere down the line has to be made with the model that we started with, what did what was the model that we started with just to have a look so, so that we can proceed further? This was the model that we started with, but this model has led us to and physically incompatible result.

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## CORRECTION TO THE MODEL

- Since it is logical to expect more collisions from the front to the direction of motion than from behind, we need to add a systematic component to the EOM.
- This component will oppose the motion of the particle and tend to retard it.
- Thus, it acts as a damping force.
- In Newtonian mechanics, damping is usually taken linear in velocity.

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So, now we modify this model. The modification that we the modification that we propose to look at; so, far we have assumed that when the Brownian particle is moving is hit by a particular molecule it; obviously, moves in a say its hit from the left hand side it moves tends to move towards the right hand side due to the impact.

Notwithstanding the fact that, it continues to move to the right hand side due to the impact, the symmetry of the way of the collisions does not get disturbed. In other words, the number of collisions occurring from the front or and the number of collisions occurring from the back

continue to remain the same continue to be equal in fact, at the level of the averages; equal at the level of averages notwithstanding the fact, that the particle is moving in the forward direction.

However, in practice it does not happen in that way, in practice if the particle is moving in the forward direction it will encounter more collisions; it will encounter more collisions from the front rather than collisions from the side from which it is moving away. In other words, from the front collisions would be more compared to collisions from the back side if it moves in a forward direction.

So, what will happen? As the particle moves forward as the particle moves forward it will experience a greater force greater restoring force greater force that will tend to push it backwards, because the number of collisions from the forward side would be more.

And therefore, the on the average the collisions being more from the forward side, they will tend to push it backwards. And as a result it will face a drag a damping sort of thing which would tend to reduce its movement reduce its speed as it move forward, due to an initial collision in from the back from the left hand side from the back side.

So, that being the case we need to incorporate a damping term or viscous term. This impact can also be related to the viscosity of the fluid and a damping or a viscous term needs to be incorporated in order to account for this and that is precisely what we are going to do now after the break.

Thank you.