

Physics through Computation Thinking

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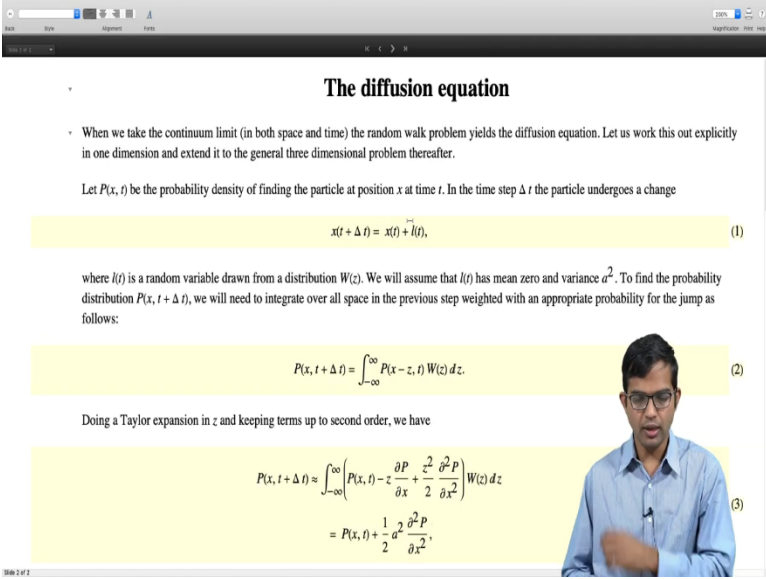
Lecture 48

Random Walks 5

Hello everyone. So, we have looked at how random walks can give us, you know some very simple discrete random walks, can give us a lot of insight into how these diffusive motion happens. And then we also saw how the diffusion equation itself is something that you can be motivated from the random walk point of view. Then we managed to make contact between these two.

So, what I want to do now is, in this module, so quickly I will show you some more arguments around this theme. It is something that we have already seen. But I want to give you some more details.

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The diffusion equation

- When we take the continuum limit (in both space and time) the random walk problem yields the diffusion equation. Let us work this out explicitly in one dimension and extend it to the general three dimensional problem thereafter.

Let $P(x, t)$ be the probability density of finding the particle at position x at time t . In the time step Δt the particle undergoes a change

$$x(t + \Delta t) = x(t) + l(t), \quad (1)$$

where $l(t)$ is a random variable drawn from a distribution $W(z)$. We will assume that $l(t)$ has mean zero and variance a^2 . To find the probability distribution $P(x, t + \Delta t)$, we will need to integrate over all space in the previous step weighted with an appropriate probability for the jump as follows:

$$P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - z, t) W(z) dz. \quad (2)$$

Doing a Taylor expansion in z and keeping terms up to second order, we have

$$\begin{aligned} P(x, t + \Delta t) &\approx \int_{-\infty}^{\infty} \left(P(x, t) - z \frac{\partial P}{\partial x} + \frac{z^2}{2} \frac{\partial^2 P}{\partial x^2} \right) W(z) dz \\ &= P(x, t) + \frac{1}{2} a^2 \frac{\partial^2 P}{\partial x^2} \end{aligned} \quad (3)$$

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So, how did we, so to speak derive this we said, instead of having a used know discrete motion, suppose your position could change continuously, and let us allow time also to change continuously. So, then we allow you know the amount by which your particle moves to the right or to the left to be a random variable, $l(t)$, with where which was known to have a certain mean which is 0 and a variance a^2 . That is all is known about it. And some distribution w of this, some reasonable distribution.

And we did not impose any special forms for this distribution. And then you were able to do just a Taylor expansion of this probability $x(t, t+\Delta t)$, in terms of $x - z$. And then we assume that you know this the last jump from $x - z$ to to x , could happen in you know for all values of z from $-\infty$ to $+\infty$ were theoretically allowed.

And of course, there is weight associated with all these jumps. So typically you think of $w(z)$ to be a sharply peaked function. So, the possibility of you know very large positive or negative jumps are usually very minimal. But the key point here is that, you don't give any special forms for $w(z)$. It is a very very generic distribution function.

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(1)

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where $l(t)$ is a random variable drawn from a distribution $W(z)$. We will assume that $l(t)$ has mean zero and variance a^2 . To find the probability distribution $P(x, t + \Delta t)$, we will need to integrate over all space in the previous step weighted with an appropriate probability for the jump as follows:

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$$\begin{aligned} P(x, t + \Delta t) &\approx \int_{-\infty}^{\infty} \left(P(x, t) - z \frac{\partial P}{\partial x} + \frac{z^2}{2} \frac{\partial^2 P}{\partial x^2} \right) W(z) dz \\ &= P(x, t) + \frac{1}{2} a^2 \frac{\partial^2 P}{\partial x^2} \Delta t, \end{aligned}$$

where we have used the fact that $W(z)$ is normalized, has mean zero and variance a^2 . Taking Δt to be small we have

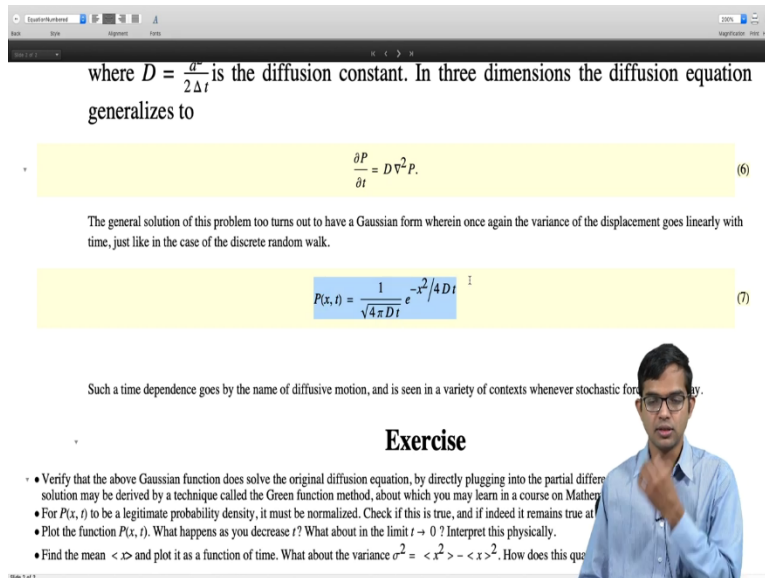
$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t$$

using which we get the diffusion equation

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And then we do a Taylor expansion. And then we see that one of these terms will drop out, because we have chosen $l(t)$ to have a mean 0. And then we make contact with, you know an alternate way of getting at $P(x, t + \Delta t)$. So, it also can be thought as $P(x, t + \frac{\partial P}{\partial t} \Delta t)$, using which we get the diffusion equation in 1D and then we generalize this to get a diffusion equation in 3D.

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where $D = \frac{a^2}{2\Delta t}$ is the diffusion constant. In three dimensions the diffusion equation generalizes to

$$\frac{\partial P}{\partial t} = D \nabla^2 P. \quad (6)$$

The general solution of this problem too turns out to have a Gaussian form wherein once again the variance of the displacement goes linearly with time, just like in the case of the discrete random walk.

$$P(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} \quad (7)$$

Such a time dependence goes by the name of diffusive motion, and is seen in a variety of contexts whenever stochastic forces are at play.

Exercise

- Verify that the above Gaussian function does solve the original diffusion equation, by directly plugging into the partial differential equation. A solution may be derived by a technique called the Green function method, about which you may learn in a course on Mathematical Physics.
- For $P(x, t)$ to be a legitimate probability density, it must be normalized. Check if this is true, and if indeed it remains true at all times.
- Plot the function $P(x, t)$. What happens as you decrease t ? What about in the limit $t \rightarrow 0$? Interpret this physically.
- Find the mean $\langle x \rangle$ and plot it as a function of time. What about the variance $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. How does this quantity depend on time?

And then I claim that the general solution for the diffusion equation is just the Gaussian of this form. And this is where the connection, the contact between you know this continuous version of the problem and the binomial distribution. So, we just saw that that there is a way to make connection between the binomial distribution which comes from say, you know, thinking of a scenario where you are repeatedly tossing coins and taking, using the sterling approximation, we saw that there is a way to see that this is a Gaussian distribution.

So here what I want to do here is, so I am claiming that this is the this is the solution of a partial differential equation. Partial differential equations in general are messy problems to solve. But it turns out that there is a solution available for the diffusion equation. So, you can in fact go ahead and do a full brute force approach to solve this problem using the Greens function method and so on. But here what I want to do is, actually just quickly verify that this result holds.

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$$P(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} \quad (7)$$

Such a time dependence goes by the name of diffusive motion, and is seen in a variety of contexts whenever stochastic forces are in play.

Exercise

- Verify that the above Gaussian function does solve the original diffusion equation, by directly plugging into the partial differential equation. The exact solution may be derived by a technique called the Green function method, about which you may learn in a course on Mathematical Methods.
- For $P(x, t)$ to be a legitimate probability density, it must be normalized. Check if this is true, and if indeed it remains true at all times.
- Plot the function $P(x, t)$. What happens as you decrease t ? What about in the limit $t \rightarrow 0$? Interpret this physically.
- Find the mean $\langle x \rangle$ and plot it as a function of time. What about the variance $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. How does this quantity vary with t ? Plot it.

Solution

Integrate $\left[\frac{1}{\sqrt{4\pi Ds t}} \text{Exp} \left[\frac{-x^2}{4Ds t} \right], \{x, -\infty, \infty\} \right]$

And we can in fact use mathematica to help us with this. So, what I want to do is, first of all, I will just do, I want to check that in deed this is a legitimate probability density. So, it must be normalized. So of course, you can do this integration by hand. But this is an opportunity for us to exploit you know some features of mathematica. So, what I will do is, I will use the Integrate

function. So, I can just do $\int \frac{1}{\sqrt{4\pi Ds t}} e^{-\frac{x^2}{4Ds t}}$. D for diffusion in constant and x going from $-\infty$ to $+\infty$.

So, so, this normalization must be equal to 1, at any given, at any point of time. It's this whole function is evolving as a function of time. But at any given time, the particle better be somewhere. That is what it means. The probability of finding your particle at position x at time t, is this. That means that at every time t, the particle better be somewhere. So, that is why, if you integrate this, it has to go to 1. No matter what time is. That is the key point here.

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Exercise

- Verify that the above Gaussian function does solve the original diffusion equation, by directly plugging into the partial differential equation. The exact solution may be derived by a technique called the Green function method, about which you may learn in a course on Mathematical Methods.
- For $P(x, t)$ to be a legitimate probability density, it must be normalized. Check if this is true, and if indeed it remains true at all times.
- Plot the function $P(x, t)$. What happens as you decrease t ? What about in the limit $t \rightarrow 0$? Interpret this physically.
- Find the mean $\langle x \rangle$ and plot it as a function of time. What about the variance $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. How does this quantity vary with time? Plot it.

Solution

In[95]:=

$$\text{Integrate}\left[\frac{1}{\sqrt{4 \pi D s t}} \text{Exp}\left[\frac{-x^2}{4 D s t}\right], \{x, -\infty, \infty\}\right]$$

Out[95]=

$$\text{ConditionalExpression}\left[\sqrt{\frac{1}{D s t}} \sqrt{D s t}, \text{Re}\left[\frac{1}{D s t}\right]\right]$$

So, if I hit shift enter for this integrate, then you will see that, so here it goes. It did complete the integration. So, but the, so what you see is this conditional expression. So, it is it is giving you the answer $\frac{1}{\sqrt{D s t}} \sqrt{D s t}$. Because mathematica does not make any assumptions about what D, s and t are.

And we know of course that, both D, s and t are real and positive. So, it makes no sense to think of a diffusion coefficient which is not positive or not real. So, for sure D s is positive and real. And also time, there is no negative time in this problem. So, we think of a random walker starts this is motion at a certain time. And that time is 0.

And then as a function of time, how does this probability distribution vary. That is the question we are studying. So, for for sure we know both D s and t are real and positive. Therefore real part of $\frac{1}{D s}$ is definitely greater than 0. Therefore, this answer is actually nothing but 1. So, this is the reassuring result, which is what we already expect.

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Find the mean $\langle x \rangle$ and plot it as a function of time. What about the variance $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. How does this quantity vary with time? Plot it.

Solution

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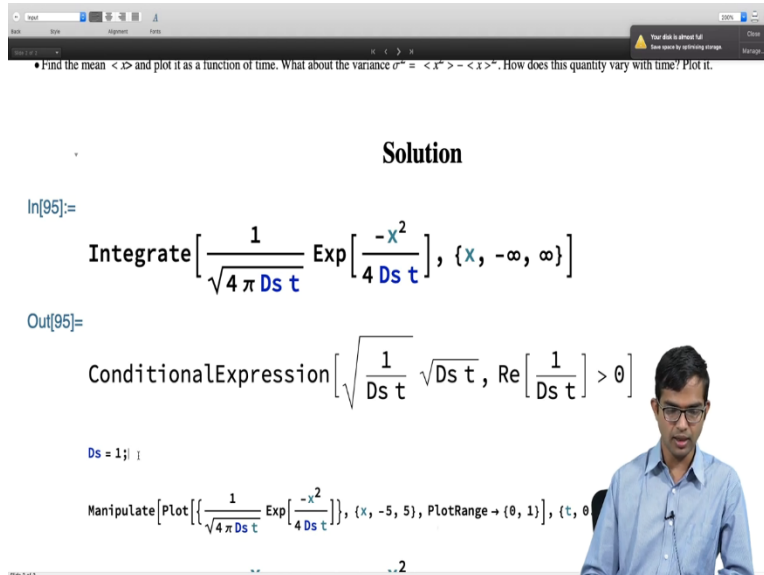
$$\text{Integrate}\left[\frac{1}{\sqrt{4 \pi D s t}} \text{Exp}\left[\frac{-x^2}{4 D s t}\right], \{x, -\infty, \infty\}\right]$$

Out[95]=

$$\text{ConditionalExpression}\left[\sqrt{\frac{1}{D s t}} \sqrt{D s t}, \text{Re}\left[\frac{1}{D s t}\right] > 0\right]$$

DS = 1;

Manipulate[Plot[{{ $\frac{1}{\sqrt{4 \pi D s t}} \text{Exp}\left[\frac{-x^2}{4 D s t}\right]}$ }}, {x, -5, 5}, PlotRange -> {0, 1}], {t, 0, 1}]

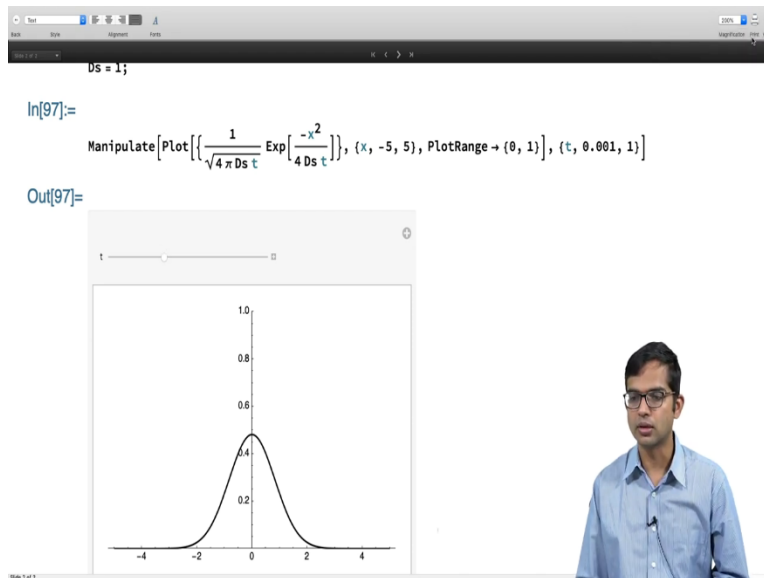


DS = 1;

In[97]:=

$$\text{Manipulate}\left[\text{Plot}\left[\left\{\left\{\frac{1}{\sqrt{4 \pi D s t}} \text{Exp}\left[\frac{-x^2}{4 D s t}\right]\right\}\right\}, \{x, -5, 5\}, \text{PlotRange} \rightarrow \{0, 1\}\right], \{t, 0.001, 1\}\right]$$

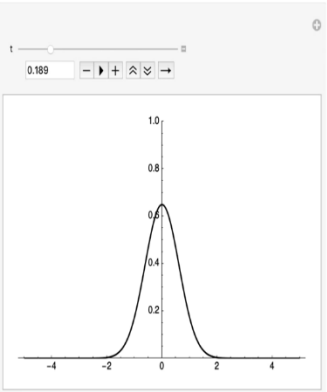
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In[97]:=

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Manipulate[Plot[{{ $\frac{1}{\sqrt{4 \pi D_s t}}$  Exp[ $-\frac{x^2}{4 D_s t}$ ] }}, {x, -5, 5}, PlotRange -> {0, 1}], {t, 0.001, 1}]
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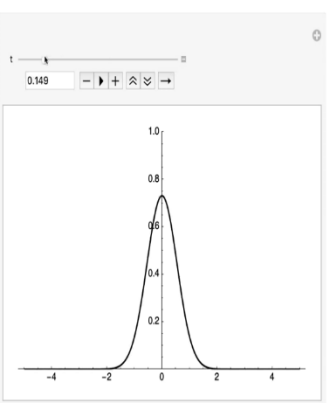


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In[97]:=

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Manipulate[Plot[{{ $\frac{1}{\sqrt{4 \pi D_s t}}$  Exp[ $-\frac{x^2}{4 D_s t}$ ] }}, {x, -5, 5}, PlotRange -> {0, 1}], {t, 0.001, 1}]
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Out[97]=



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So, next what I want to do is, so this is another question here. So, what about, what is the nature of this function? If I were to plot this, is there some special forms this text? It is something that you already probably know it. And this is what is called a Gaussian. So, let me do that. I am going to choose D_s to be 1 for purposes of this exploration. And then I will use the Manipulate command.

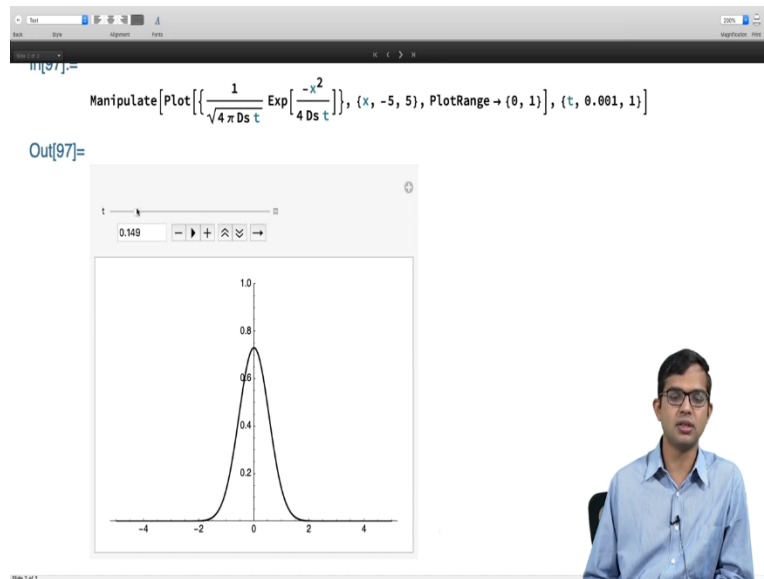
I will use the Manipulate command to allow t to go from 0.001, all the way up to 1. So, if I use, so if I see, if I put t to be some relatively small number, like $t = 0.3$ for example. Or 0.5 or so on.

You see that it is a Gaussian. And who spread keeps on you know it is expanding as a function of time. So, as I reduce my t and take it to the in the limit of t going to 0, you know mathematica does not like to plot this anymore.

But what is going on here? You see that at any given time t , I have already shown that this normalization holds. Does not matter what t is. But in the limit of t going to 0, this whole function keeps on shrinking. And in fact at time $t = 0$, it becomes what is called as Dirac delta function. Where in fact you know for sure that your particle is at at 0. It is not, there is no spread in its probability distribution.

And so, and as you allow it to evolve, what what happens is just this very very narrowly peaked function, becomes broader and broader and broader. But it always remains a Gaussian. So, that is the interesting feature of this diffusion equation. So, that was the second exploration that we wanted to do.

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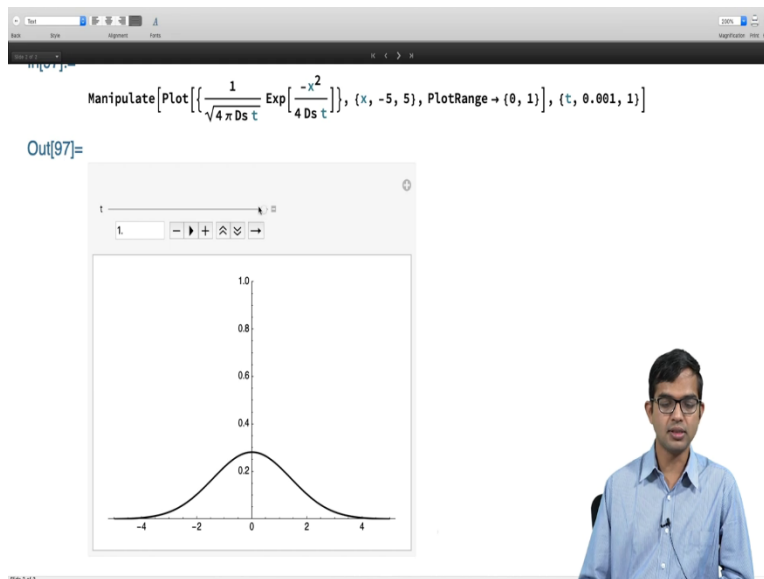
And then third one is also something that just by looking at this already we have some idea, what is going on here. So, the question is, what about the nature of this spread, as a function of time? So, you see clearly that the chances of, you know, where the particle is located, it becomes

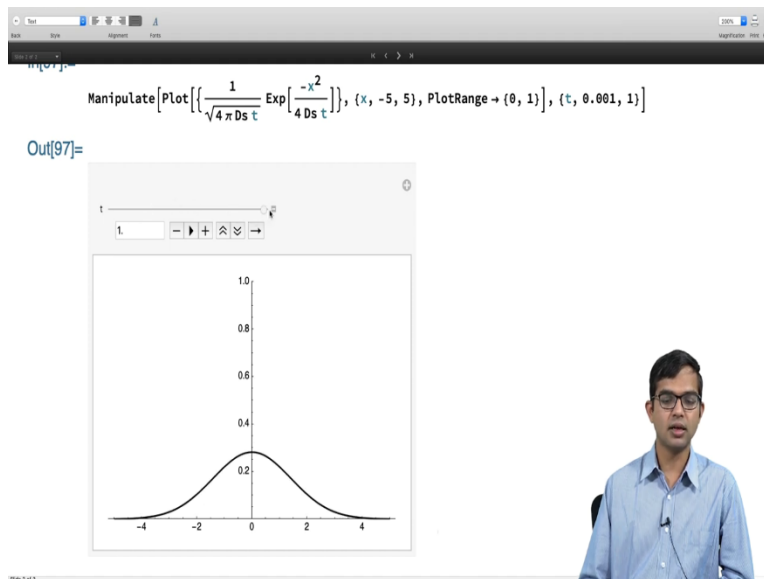
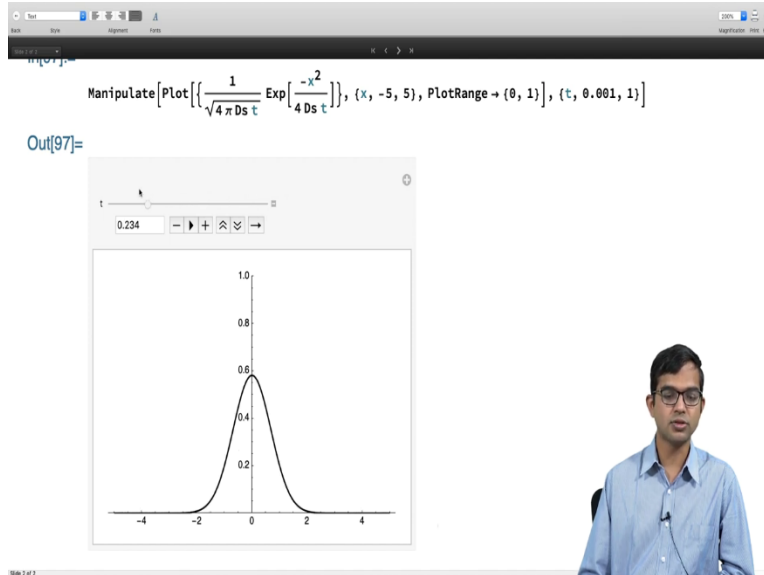
broader and broader and broader. So, although the mean always remains 0, it is actually, I told you before, that the mean does not carry as much information in this problem as the variance does.

In fact, the most likely place for your particle is not at the mean, after if you spend the time t , the particle is very likely to be somewhere, which is proportional to \sqrt{t} . Plus plus on the plus side or the minus side, that you cannot say. But a typical distance between the origin and your particle, if a time t has elapsed, will go as \sqrt{t}

That is that is why the variance or the standard deviation is more important factor in this case, rather than the mean. So, that is also something that is not a surprise, but it is something that we can verify with the help of visualization here.

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Now, let us see what happens, check this. Let us look at the variance itself. Using integrate, we can actually do the mean. So, mean of this function is simply given by $\int_{-\infty}^{+\infty} x P(x)$. Once again it gives me a conditional expression. And it is 0 if real part of t is greater than 0. Indeed real part of t is greater than 0, because t is just time. And therefore, the average position of your particle, no matter what the time is, is always 0.

And then finally, I will just look at the variance turns out to be $\int_{-\infty}^{+\infty} x^2 P(x)$ in this case, because the average position x is 0. And we already know that this quantity is linear in time. It is in fact going to be $2t$. You can check this. So, the $\langle x^2 \rangle$ for the Gaussian distribution as a function of time goes as is goes linearly in t and in fact it is precisely $2t$. So, as you can also qualitatively see here.

As a function of time it is the width of this Gaussian distribution is a measure of its σ^2 . And so the longer, the more the time that elapses, greater is the width. And in fact, it is precisely linear in time, with the factor being 2 in this case. All of which is something that you should verify.

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generalizes to

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OK. So, you should also do this exercise of plugging in this whole function, $P(x,t)$ into into this equation here. $\partial P/\partial t$ on the one hand. On the left hand side. And $D \nabla^2 P$. So, $\nabla^2 P$ is also something, it is a vector second order differential that you have to take. So, you should take it appropriately and check for yourself that what you get on the right hand side is the same on the left hand side.

So that is something that I am leaving it open for you as an exercise. But the other thing things I have already shown you how to visualize these different quantities and show you it what it physically means. What is this spread and how it goes as a function of time. So, that is what this module was about. Thank you.