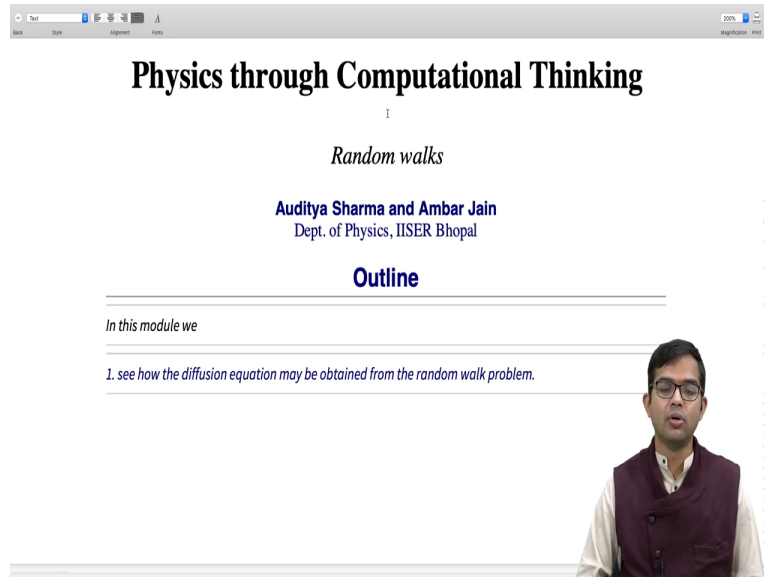


Physics through Computational Thinking
Dr. Auditya Sharma & Dr. Ambar Jain
Department of Physics
Indian Institute of Science Education and Research, Bhopal
Lecture 45
Random Walks 2

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The screenshot shows a presentation slide with the following content:

- Title: **Physics through Computational Thinking**
- Subtitle: *Random walks*
- Authors: **Auditya Sharma and Ambar Jain**, Dept. of Physics, IISER Bhopal
- Section: **Outline**
- Text: *In this module we*
- List item: *1. see how the diffusion equation may be obtained from the random walk problem.*

A video inset in the bottom right corner shows a man with glasses and a maroon vest speaking.

Hi guys. So, we started our discussion of Random Walks in the previous module and so now we want to see how random walks are connected to the diffusion equation. So, I have already made a sort of a comment in passing that you know this result that the average distance covered after N steps is the typical distance is like \sqrt{N} . And so, this is in fact, true of you know diffusive motion. And so the general terminology for these kinds of motions is diffusive motion as opposed to ballistic motion.

So, if, typically you are taking N steps and moving as an order of N then it is called ballistic motion. And if it is going as \sqrt{N} it is called diffusive motion. There are, of course, you know based on this terminology, there are other kinds of random walk motions where you can have some diffusive behaviour or super diffusive behaviour. These are all you know more sort of sophisticated phenomena which do happen by the way, where people are interested in this but the main.

So, the landmark points in some sense are ballistic motion and then with respect to ballistic, you compare and you see that random walks give you \sqrt{N} behaviour. And so, in this module we are going to see how this connection between random walks which I described last time, discrete random walk and how one can make a contact to a differential equation, which partial differential equation which is actually that of diffusive motion. That is the agenda for this module.

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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

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

Okay, so what is the procedure? We must take a continuum limit. So, you can in principle take a continuum limit in x and in t . So, we will do this particular case and you are free to play with in all four possibilities. We already did the discrete in space, discrete in time problem. You can keep time discrete and keep make space continuous or you can make space discrete and time continuous. Or you can make both of them continuous like we are about to do now.

So, let $P(x, t)$ be the probability density of finding the particle at position x at time t . So, now it is a probability density. So, you have to integrate in some region in time to get a probability. So in the time step, Δt , the particle undergoes a change, if it were located at $x(t)$, it is going to be at $x(t) + l(t)$ after this small interval of time Δt has elapsed. And now but the key point is that $l(t)$ is a stochastic random variable. It is drawn from some distribution W of z .

So, we will just assume that this random variable $l(t)$, this distribution has mean 0 and variance \bar{a}^2 . You are not going to assume anything specific about the nature of distribution. Let us say that it has some mean 0 and variance \bar{a}^2 . To find the probability distribution, $P(x, t + \Delta t)$. So, initially it had a certain probability distribution.

Now, you can still ask what is a probability density of your particle being at x at time $t + \Delta t$ we will need to integrate over all space in the previous step right. So, we could have arrived at the position from anywhere. Theoretically, it is possible. Of course, it is more likely that it has moved into that region from a nearby point but you have to take care of all possibilities. So, you will have to integrate over all space weighted with an appropriate probability for the jump as follows.

So, you have, suppose it were at some positive $x - z$ at time t . The probability that it were at $x - z$ at step t . $W(z)$. So, this $W(z)$ comes from now it is telling you that your random variable, the length of this random variable could be anything basically. So, we are taking it to go from minus infinity all the way up to plus infinity. Although it is unphysical to make this a very broad distribution.

So, typically one is thinking of you know in the case of the discrete random walk, we say it is either $+$ or -1 . It is a bimodal distribution. But you can have other kinds of distribution. So, it is not as you will see. The main results of this discussion will actually not depend too much on the precise form of this distribution. It will just get washed out.

However, I mean perhaps there is some pathological distribution you can come up with and you can try to mess up this analysis. But the main point here is that it is not really of interest. Physicists world if you think of it as a distribution which is a reasonable distribution. You can take $l(t)$ to be sort of peaked around a certain mean and that mean is 0 here. It is equally likely to be going to the right or to the left and it has a spread around it. It has a variance \bar{a}^2 .

So, the typical distance it covers in one step is actually a . Equal to the right or to the left. Okay,

so if you do this, then you have
$$P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - z, t) W(z) dz$$

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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.

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

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

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

Now, if you do a Taylor expansion in z and keeping terms up to second order, you can write this

as
$$\int_{-\infty}^{\infty} P(x, t) \left(1 - z \frac{\partial}{\partial x} + \frac{z^2}{2} \frac{\partial^2}{\partial x^2} \right) W(z) dz$$
. So, I am just doing a Taylor expansion and keeping terms up to second order. Yeah, so next you must invoke some features of this distribution $W(z)$. It has mean 0 and variance a^2 .

Now, if you take Δt to be small, right so that is coming in a moment but first of all, let us see that you know this second term actually vanishes. Why does it vanish? It vanishes because $\frac{\partial P}{\partial x}$ comes out and then the mean of z is actually just 0. So, there is no contribution from the second term, only the this square term comes in. So, in some sense, we are keeping this $P(x, t)$ of course and then we are keeping the next the lowest order which survives because this first order term will vanish. And so that is the Taylor expansion that we are doing.

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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:

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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

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

And so taking Δt to be small, you can also argue that $P(x, t + \Delta t)$ is actually you know

connected to $\partial P / \partial t$. So, $P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t$. So, I have so two independent ways of doing this difference. Now, on the one hand, this argument using W gave us this quantity. It is $1/2 a^2 \partial^2 P / \partial x^2$.

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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:

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

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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

$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t \quad (4)$$

using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2},$$

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$$P(x, t + \Delta t) \approx \int_{-\infty}^{\infty} \left(P(x, t) - z \frac{\partial P}{\partial x} + \frac{z^2}{2} \frac{\partial^2 P}{\partial x^2} \right) W(z) dz \quad (3)$$

$$= P(x, t) + \frac{1}{2} a^2 \frac{\partial^2 P}{\partial x^2},$$

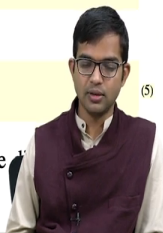
where we have used the fact that $W(z)$ is normalized, has mean zero and variance a^2 . Taking Δt to be small we have

$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t \quad (4)$$

using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}, \quad (5)$$

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



And so, if I equate these two different ways of getting this difference then I have $\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}$
 where $D = \frac{a^2}{2\Delta t}$. So, for some reason, Mathematica has changed the font here but it is okay.

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

$$P(x, t + \Delta t) \approx \int_{-\infty}^{\infty} \left(P(x, t) - z \frac{\partial P}{\partial x} + \frac{z^2}{2} \frac{\partial^2 P}{\partial x^2} \right) W(z) dz \quad (3)$$

$$= P(x, t) + \frac{1}{2} a^2 \frac{\partial^2 P}{\partial x^2},$$


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

$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t \quad (4)$$

using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}, \quad (5)$$

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

$$\frac{\partial P}{\partial t} = D \nabla^2 P.$$


So, in three dimensions, this is something that generalizes automatically. So, this is what is called the diffusion equation. It is a partial differential equation involving a second order

derivative in space and that is just a first order derivative in time. $\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}$ and this D is connected to the variance of this distribution W. And in three dimensions, this generalizes automatically to this expression. $\frac{\partial P}{\partial t} = D \nabla^2 P$. And there is another diffusion constant associated with this as well.

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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

$$P(x, t + \Delta t) - P(x, t) \approx \frac{\partial P}{\partial t} \Delta t \quad (4)$$

using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}, \quad (5)$$

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

$$\frac{\partial P}{\partial t} = D \nabla_1^2 P. \quad (6)$$

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

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

And the general solution of this problem turns out to be a Gaussian distribution. So, it is very closely related to the homework exercise that you should have hopefully done based on the earlier module where I asked you to take the limit using Stirling's approximation and show that the binomial distribution goes to the Gaussian distribution. And so, indeed you can show that this

P, the solution to the diffusion equation is this Gaussian equation. $\frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$.

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using which we get the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}, \quad (5)$$

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 grows 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

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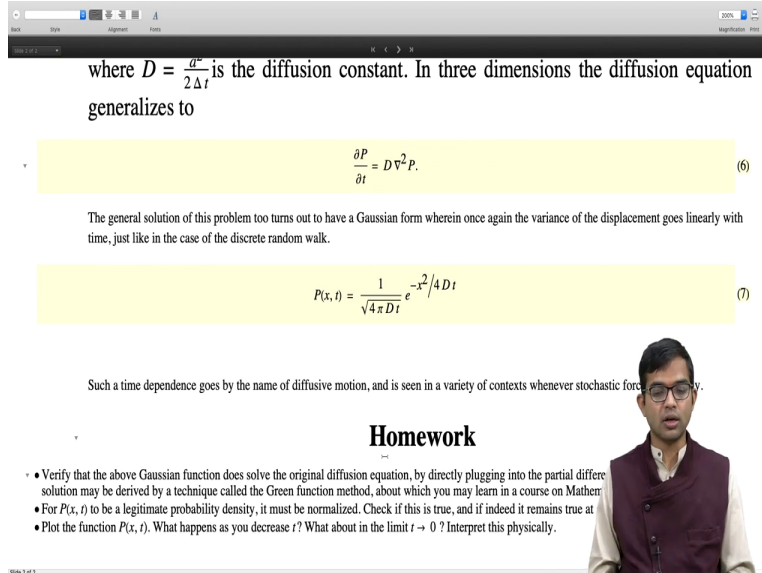
Homework



So, whenever you have a dependence of this kind. The distribution of the position at time t going in this form in a Gaussian way and particularly, the important point is that the denominator has Dt . So, the variance is directly proportional to time. That situation is called diffusive motion.

And it is seen in a lot of context you know not which apparently appear to be not, nothing to do with random walks or anything like that. And even in such context, these kinds of Gaussian forms come about. And so then some analysis will reveal that indeed there is some underlying random walk behaviour involved.

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where $D = \frac{d^2}{2\Delta t}$ 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 involved.

Homework

- Verify that the above Gaussian function does solve the original diffusion equation, by directly plugging into the partial differential equation. The 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.

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So, you have some homework now to do and what you have to do is first of all just simply plug this equation in. I am claiming that this is the solution of this but I have not told you how to find the solution. So, one way to believe me is to convince yourself by you know just plugging this in and verifying for yourself. So in other words, do not really believe me but actually verify for yourself. That is homework one.

And in fact, there is a way to systematically solve for this problem which you might see in a somewhat more advanced course on math methods of or elsewhere there is a Green function technique involved that is one way of solving for this. There must be other ways as well. So, it is possible to go from the differential equation to the solution but here I am asking you to just take the solution which I am claiming is the solution and verify. That is one of them.

Second is to check that this is legitimate probability density. So, integrating over all time or all space, both ways you should check this and it should be normalized. And sorry it is over all times. It is over all space. At any given time, the particle has to be at any position in space. And as a function of time, it is if the whole probability distribution will change but it is not clear if we integrate over time, we are going to get something. So, it is it is an integration over space.

Okay and then final thing to do is to make a plot of this and check for yourself what happens as you, if you keep on decreasing time. That is an interesting question to address and what about in the limit of t going to 0? Is there something very special that will happen. So, this is something for you to interpret graphically and think about. That is homework.

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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.

Homework

- 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.

Remarkable Generality

The linear dependence of the variance of the displacement with time turns out to be very general, and holds regardless both are discrete or continuous. It also works for a range of distributions of the walker at each step. Again, it is independent effects. The reason for this remarkable universality is rooted in a very deep theorem called the central limit theorem of a large number of independent random variables has a Gaussian distribution, independent of the precise details constituent random variables in question.

And so, one comment about this is that there is a very remarkable generality associated with these results. The main result I have said before and I am emphasizing again is that the typical distance covered in you know N steps actually goes as \sqrt{N} and in time t , whether it is continuous or whether it is discrete time, discrete space. It does not matter. None of these things count. It is just simply this kind of random walk behaviour will give you \sqrt{t} or \sqrt{N} dependence. And this is that is why there is generic terminology associated with it and it is called diffusive motion.

And why does it appear in so many contexts and so there is a deep theorem in stochastic probability theory which is called the central limit theorem. So, which says basically that if you take the sum of a large number of random variables. No matter what the details are of each of these random variables and what the distributions are of these individual random variables, the

sum is going to actually get a, give you a bell shaped curve. The distribution of the sum is going to approach the Gaussian distribution. The limit of very large number of random variables.

So, there is a rigorous proof for this. It is possible you might encounter it if you take math code on probability theory. But it has very important consequences in lots of areas in physics, in financial systems it has in certain kind of biological problems and all kinds of other fields.

And it has, it is one of the favourite theorems of Probabilists and it also appears, for example, in error analysis. These kinds of ideas. So, it has widespread use and you will encounter it whether you approach it with knowledge or without it, you are going to encounter it in lots of cases.

The bell distribution is an ubiquitous distribution and hopefully this discussion will help us you know whenever we encounter it in the future, we should hark back to this discussion and say that, oh okay we had actually have a reasonable understanding of it. That is the goal of this module. Thank you.