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Lecture – 10 Derivation of Drift-Diffusion Equations

(Refer Slide Time: 00:15)

So, when we derive this Diffusion Equation, if you remember if you recall what we said was that I draw my step lengths. So, I wrote down an evolution for the position of the random walker at time t plus delta t plus some step l of t, but the step sizes were drawn from a distribution which has 0 mean and some constant variance, right. So, the 0th moment was 1, the first moment was 0 and the second moment was a square.

(Refer Slide Time: 01:17)

Now, you could have a particle undergoing diffusion even when this mean is nonzero. And if this mean is nonzero, what you would have is the net drift term. So, if the mean is nonzero, you would have a net drift term when in addition to sort of doing random things overall if you look for large enough, the particle is moving net in some direction it has some drift velocity. So, it has some drift velocity.

So, it could happen if these individual steps of the random walk have a nonzero mean or for example, if you apply some sort of an external force. So, for example, if you have charged ions or charged proteins or whatever and you apply an electric field, and the electric field will tend to push the ion in certain direction depending on where how you apply negative field.

So, if you have a net force then again you will have some sort of a net drift and I can write this drift velocity let us call this v d. This drift velocity is in general proportional to the force

that you apply and the constant of proportionality you can write either in terms of a mobility or in terms of a friction coefficient. So, mu is called the mobility, gamma is called the friction coefficient.

So, you apply an external force that causes the particle to move in some direction with a certain velocity which is called the drift velocity, and the drift velocity is proportional to the force. Is this what you generally encounter in a general set up is the velocity proportional to the force?

Student: No.

No, right; so, this is a slightly special case and we will do deal with that over the next lectures when we do hydrodynamics.

(Refer Slide Time: 03:25)

So, this is a special regime of low Reynolds numbers low Reynolds numbers which may or may not make sense to you, but which we will define. So, this happens when you can neglect inertial forces so, when you can neglect inertial forces

So, the acceleration term is not important in Newton's laws. Generally that is the regime in which biological systems operate, we will calculate how to quantify the biological medium in which this object. These proteins, these organisms are undergoing random walks and that characterization happens to this quantity called the Reynolds number and we will see in what sort of regimes is this is this approximation with the velocity is proportional to the force valid. But for the time being, let us take this as a given that the drift velocity is proportional to the force, the larger the force you apply the larger the velocity with which it moves, ok.

(Refer Slide Time: 04:33)

So, if this is my velocity v d then in a time t it has moved in time t, in time t it has moved an amount which is let us say if delta t, in time delta t it has moved an amount v d delta t right, all right. So, given this I will now try to re derive the diffusion equations. So, this is my setup I have a net drift velocity due to some force that causes the particles to take in time delta t to be shifted by an amount v d times delta t and now I am now trying to re derive the diffusion equation.

So, let us start off with this x of t plus delta t is x of t plus l of t and then ls are still going to be drawn from a distribution chi, and chi except now the moments will change somewhat. What is the zeroth moment going to be?

Student: (Refer Time: 05:20).

Will this change?

Student: No.

No right, because that is just a normalization that is always true. Will the first moment change?

Student: (Refer Time: 05:26).

Yes, what will it be?

Student: (Refer Time: 05:30).

Hm?

Student: (Refer Time: 05:37) mu.

Mu, no; why mu?

Student: (Refer Time: 05:45).

Yes you were saying.

(Refer Slide Time: 05:49)

Student: v into t.

v into t, right that is the distance it is moved on an average in a single step, and the second moment is still assumed to be a square, ok; so, it is still constant, ok. So, that is the difference from this un biased random walks; so, this is what is called the biased random walk ah. So, now, I will do the same thing as before.

So, I still write my rho of x what we are writing x t plus delta t, right and I will assume expand this and then I will substitute for these moments. So, I will just write it rho of x comma t integral chi z t z minus del rho del x integral z chi z d z, right and plus half del 2 rho del x 2 integral z square chi z d z, right.

So, this is exactly what we did last class for the unbiased diffusion, except in the last class we had have thrown away this term because the first moment was 0. We took on biased random walks where the mean was the first moment was 0 in this case I have some finite first moment. So, I need to take into account out of that. And this of course. so, this is one, this is one, this is v d times delta, let us just call it v delta delta t and this is a square, right ok.

So, again if I take this term to this side rho of x t plus delta t minus rho x t I divide by delta t, what I get is del rho del t what I get is del rho del t right then what I have over here is equal to minus v del rho del x plus d del 2 rho del x 2, all right. So, when you have a nonzero mean for these step lengths, in addition to the standard diffusion term d delta rho del x 2, here this additional will drift term which is minus v times del rho del x, ok.

(Refer Slide Time: 08:13)

So, this is called the drift diffusion equations; so, this is called the drift diffusion equation or the advection diffusion equation it has multiple names. So, just for sake of interest, you can derive this in multiple ways the drift diffusion equation or the diffusion equation. I will just show you one more way just because I will use this formalism in a different context.

(Refer Slide Time: 08:47)

So, let us say I take a 1D random walk, right; so, let us say I take a 1D random walk, right. So, you have a line and you have a random walker which can only move left or right on this line. Let us say that the probability it takes a step and let us say I have some step length which I will call as delta x let us say.

So, it takes equal steps; so, steps of length delta x right, each step has size delta x. It can hop to the right with a probability p and it can hop to the left to the probability q, ok. That is the only two possibilities that it can have which means that I my p plus q is equal to 1 at every time instant it can must either hop to the right or it must hop to the left.

So, I can now write the time evolution of the probabilities that what is the probability for this random walker to be at position x at time t plus delta t, all right. So, if it needs to be at position x at time t plus delta t at time t that is one step before, it could have been in only 1 of 2 positions right, x minus delta x or x plus delta x.

So, it could have been in x minus delta x comma t or it could have been in x plus delta x comma t, all right. If it was here if it was at x minus delta x then with what probability will it come to x?

Student: P.

P right, because it has to take a hop to the right. So, p times this plus if it was at this position, it would have to take a hop to the left which means q, right. So, it can be either here x minus delta x or x plus delta x, if it was here it hops to the right it is probability if it was here it hops to the left with that probability, ok.

Now, let me expand these terms in Taylor series. So, P x comma t plus delta t is equal to P of x comma t right, since I am writing delta let me just write delta ok, plus delta t del P del t, all right. P of x minus delta x comma t is P of x comma t minus delta x del P del x plus half delta x square delta 2 p del x 2, right. And, similarly for P x plus delta x comma t that is P of x square t plus delta x del P del x plus half delta x square del 2 P del x 2, ok.

Now, this x minus delta x term comes with a p small p. So, let me write the small p throughout small p, small p, small p, this one comes with a q. So, q, q, q and now let me put this back into this equation. This P x of t which is on the left hand side and this p plus q into P x of t will cancel of course, because p plus q is 1. So, there will be no p x of t.

(Refer Slide Time: 12:31)

So, on the left hand side I will have a delta t del P del t is equal to this is a minus sign that is a plus sign. So, minus let me call this p minus q delta x del P del x and then a plus this is again a p plus q which is 1; so, plus half delta x square del 2 P del x 2, ok. I bring this delta t down, I bring this delta t down so, this is what I have.

Now, this is exactly the same form as the drift diffusion equation that I have. Once I identify the proper forms of the velocity and the diffusion coefficient. So, that velocity is; obviously, from this term. So, the velocity is p minus q delta x by delta t. The diffusion constant is again length square over time so, delta x square by 2 delta t.

So, the moment you have a random walk where it is more likely to hop in one direction versus the other, the translates automatically into a velocity a net velocity which is proportional to the difference between these two to the difference between these two probabilities, ok. If p was equal to q you would have unbiased random walk, the velocity would be 0 and I would come back to my standard diffusion equation in the absence of drift, ok. This is just another alternate way of thinking about this from the language of random walks, ok.

Once I have this; so, once I have so, once I do that of course, I come back to this drift diffusion equation. And, since I have this let me just write down what is therefore, the flux or the current. What is the conserved current in this case then what is J? Remember we talked about the continuity equation which says that in the absence of any sources or sinks del rho del t is equal to minus divergence of J right, which means in a 1D case its minus del J del x in 1D, ok. So, given that what is the current in this case then?

Student: (Refer Time: 15:02) v.

This is v times rho right, the current is v times rho minus D del rho del x such that you still satisfy the continuity equation, which is good to write down the expression for the current as well, ok good.

(Refer Slide Time: 15:39)

So, I had the diffusion equation last class; now, we have derived the drift diffusion equation del rho del t is equal to minus v in del rho del x plus D del 2 rho del x square.