Lecture 9

In the last lecture ...

Chain rule:

$$\frac{d f(x,t)}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial t}$$

$$\Rightarrow \dot{f} + (\underline{v} \cdot \underline{\nabla}) f$$

convective derivative

(or is it $\underline{\nabla}(\underline{v} f)$?)

In K-M expansion:

$$\frac{\partial^n}{\partial x^n} \int (\Delta x)^n \, G(x+\Delta x | x) \, P(x,t) \, d\Delta x$$

$$\Rightarrow \frac{\partial^n}{\partial x^n}\left(D^{(n)}(x) \, P(x,t) \right)$$

(definitely under $\frac{\partial}{\partial x}$)

We have seen the Smoluchowski equation in harmonic potential (for O-U process)

What if the force $f(x)$ is arbitrary: $f = -\dfrac{\partial V(x)}{\partial x}$

SDE
(overdamped limit) $\gamma \dot{x} = f(x) + \sqrt{2kT\gamma}\,\xi(t)$

will derive soon...

via K.-M. expansion:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P(x,t)\right) + \frac{1}{2}\frac{2kT\gamma}{\gamma^2} P'' \quad (*)$$

$$= -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P\right) + \frac{kT}{\gamma}\frac{\partial^2 P}{\partial x^2}$$

diffusion in $\forall$ force.

$D = \dfrac{kT}{\gamma} \equiv \dfrac{1}{2}\sigma^2$

Write it in an alternative equivalent form:

$$\frac{\partial P}{\partial t} = -\nabla J(x,t)$$

where the "flux" or "current of probability"

in multi-dimensions: $\mathrm{div}\,\underline{J}$

$$\boxed{J = \underbrace{-D\frac{\partial P}{\partial x}}_{\text{"Fick's Law"}} + \frac{f(x)}{\gamma} P(x,t)}$$

$D = \frac{kT}{\gamma}$

Another equivalent form:

$$\boxed{J(x,t) = -D\, e^{-\beta V(x)} \frac{\partial}{\partial x}\left[e^{\beta V(x)} P(x,t) \right]}$$

In all cases, we see a general "flux" $\underline{J} = \rho \underline{v}$, and Continuity equation: $\dot{P} = -\operatorname{div} \underline{J}$ for conserved field

$\int P\, dx = 1$

What if we have an x-dependent noise: $\sigma(x)$?

$$dx = \mu(x,t)\, dt + \sigma(x,t)\, dW$$

Then we "probably" would still have following Itoh's maths!

$$\boxed{\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big(\mu(x,t) P \Big) + \frac{1}{2} \frac{\partial^2}{\partial x^2} \Big(\sigma^2(x,t) P \Big)}$$

from K.-M. expansion.

However, we shall (soon) see, that in physics, we could have:

$$\frac{1}{2} \sigma^2(x) \frac{\partial^2 P}{\partial x^2} \quad \text{or} \quad \frac{1}{2}\sigma(x) \frac{\partial}{\partial x} \left(\sigma(x) \frac{\partial P}{\partial x} \right)$$

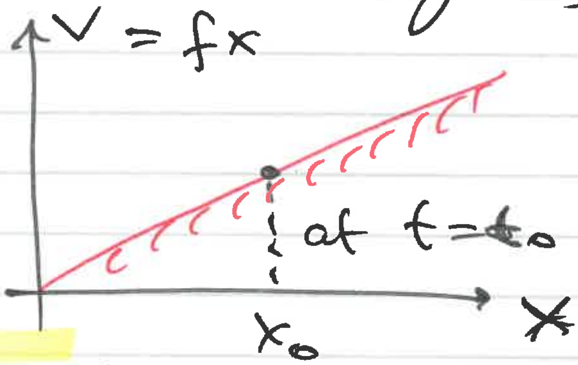
To finish the O-U section:

two examples:

1) Diffusion in constant force

e.g. sedimentation under gravity

$$\dot{p} = \frac{f}{\gamma} p' + D p''$$



$$\Downarrow$$

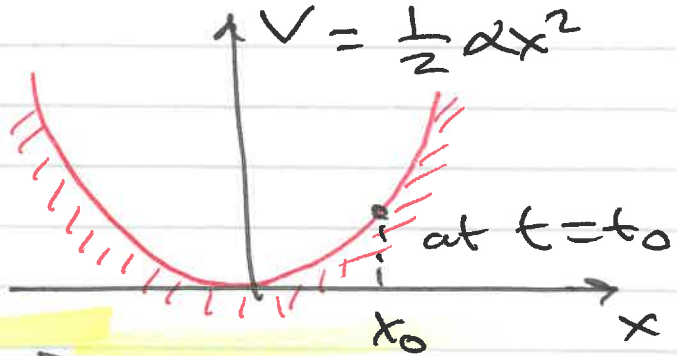
$$P(x,t) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left[-\frac{\left(x - x_0 + \frac{f}{\gamma}(t-t_0)\right)^2}{4D(t-t_0)}\right]$$

→ at $t = t_0$ this is $\delta(x - x_0)$

→ drift velocity $u = f/\gamma$

2) Diffusion in harmonic well

$$\dot{p} = \frac{\alpha}{\gamma}(x p)' + D p''$$



$$\Downarrow$$

$$P(x,t) = \frac{1}{\sqrt{2\pi kT\, S(t)/\alpha}} \exp\left[-\frac{\alpha}{2}\frac{\left(x - x_0 e^{-\frac{\alpha}{\gamma}(t-t_0)}\right)^2}{kT\, S(t)}\right]$$

with $\boxed{S(t) = 1 - e^{-\frac{2\alpha}{\gamma}(t-t_0)}}$

Convection Diffusion

(or advection, etc. ...)

There is a background flow with velocity $u(x)$, diffusion on top of that...

Recall $\dfrac{\partial P(x,t)}{\partial t} = -\dfrac{\partial}{\partial x} J(x,t)$

$$J = -D e^{-\beta V(x)} \frac{\partial}{\partial x}\left(e^{\beta V(x)} P(x,t)\right) + \underline{\qquad}$$

Now, when $u(x)$ is present: extra flux $u \cdot P$

$$\frac{\partial P}{\partial t} = D \underline{\nabla}\left(e^{-\beta V} \underline{\nabla}\left[e^{\beta V} \cdot P\right]\right) - \underline{\nabla}(\underline{u} \cdot P)$$

Or re-write:

$$\frac{\partial P}{\partial t} + \underline{\nabla}\left(\underline{u}(x) \cdot P\right) = \text{"old r.h.s."}$$

$$= -\frac{\partial}{\partial x}\left(\frac{f(x)}{\gamma} P\right) + D \frac{\partial^2 P}{\partial x^2}$$

r.h.s. of Smoluchowski

if div $\underline{u} = 0$

convective derivative

$$\boxed{\frac{\partial P}{\partial t} + (\underline{u} \cdot \underline{\nabla}) P} = \ldots\ldots$$

Many implications, since $u(x)$ adds to the potential $V(x)$

$$\frac{\partial P}{\partial t} = -\nabla\left(\left(\frac{f(x)}{\gamma} + u(x)\right)P\right) + D\frac{\partial^2 P}{\partial x^2}$$

New structure emerging.

What if $u = \text{const}$:

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

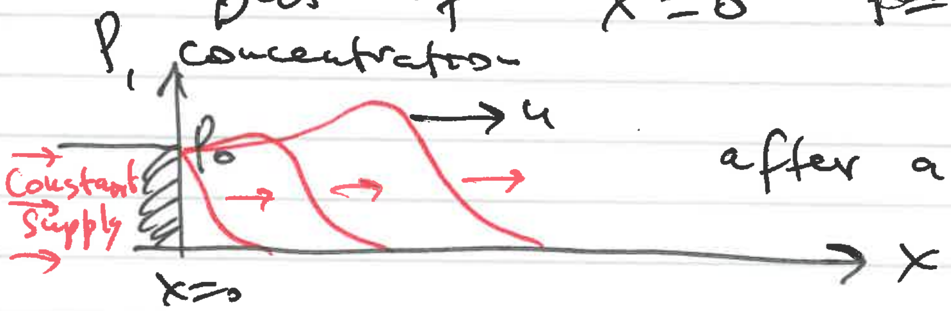
Similar to diffusion under constant force.

So if $t=0$ $P = \delta(x)$

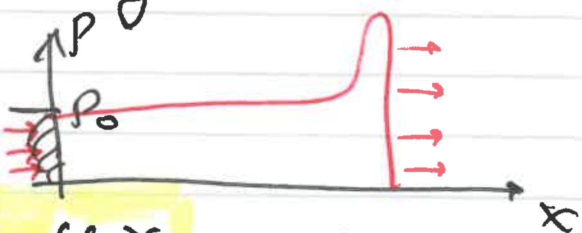
easy!

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

But if $x=0$ $P=P_0$ (Boundary Condition)



after a long time



$$P(x,t) = \tfrac{1}{2}P_0\left[\mathrm{Erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right) + e^{\frac{u\cdot x}{D}}\,\mathrm{Erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right)\right]$$

"Dispersivity" parameter