

## Lecture 2 - Brownian motion and the Langevin equation

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### Brownian motion:

Originally: random movement of pollen particles in a fluid

1827 - Robert Brown observes random irregular motion of pollen particles in water

1905 - Einstein provides a theory of random collisions from molecules  $\Rightarrow$  heat  $\approx$  molecular motion  
(Einstein did not know about Brown's exp.)

The random walk from the last lecture can be taken as the crudest modelling of Brownian motion. Can we do better?

### Langevin Equation (Paul Langevin 1908)

Let's try to make a bit more microscopic description of the dynamics of the Brownian particle. We assume that the mass of the Brownian particle  $m \gg m_{\text{atom}}$ , the mass of the atoms in the surrounding liquid.

The atoms then are bombarding the particle from all directions with each collision taking a time  $t_{\text{micro}}$  much smaller than the characteristic time scale of motion for the particle. We model then the impact of the fluid by a random force  $R(t)$  and the motion by a stochastic Newton eq:

(For simplicity of notation I'll do this in 1D, no essential physics is lost by doing this here)

$$m \frac{dv}{dt} = R(t)$$

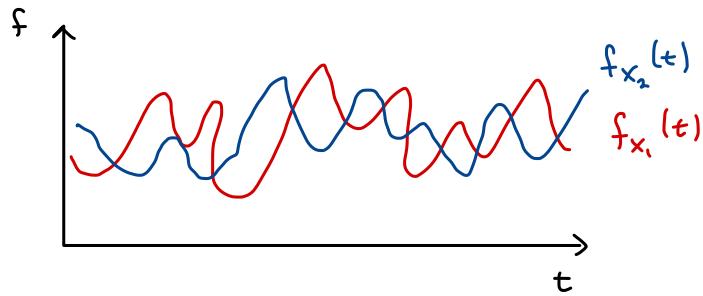
The random force  $R(t)$  is an example of what is often referred to as a stochastic process. Suppose  $X$  is a random variable. Any function of  $X$  is then also a random variable. This function can also depend on some parameter, say  $t$ , and we can denote it  $f(X, t)$ . Such a random function is called a stochastic process. With probability  $P(x)$ ,  $X$  takes the value  $x$ , and we get the sample function  $f(x, t) \equiv f_x(t)$ . We can take averages over the probability distribution to obtain

$$\langle f(X, t) \rangle = \int dx f_x(t) P(x)$$

and higher moments.

$$\langle f(X, t_1) f(X, t_2) \dots f(X, t_n) \rangle = \int dx f_x(t_1) \dots f_x(t_n) P(x)$$

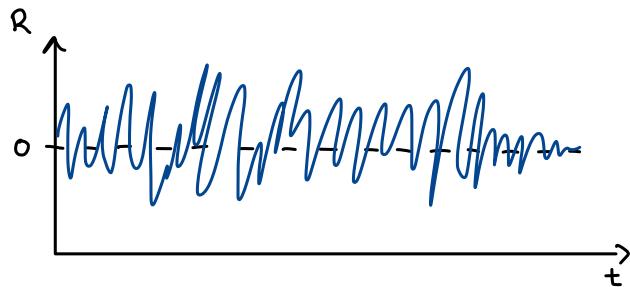
Visually we could imagine plotting different sample curves



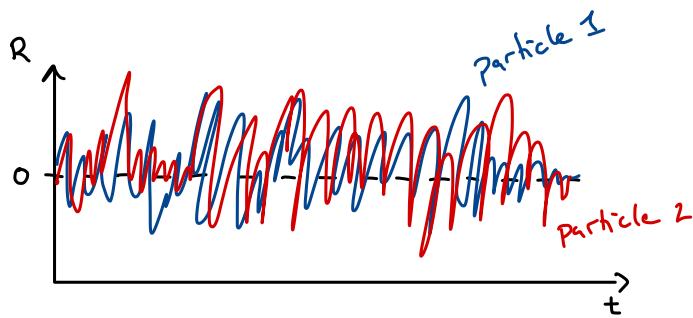
the curve  $\langle f(X(t)) \rangle$  is then the average curve

In the case of the Brownian motion the stochastic process is the random force  $R(t)$ , written without an explicit reference to the underlying random variable(s)  $X$ . What is this random variable in this case? In principle, there is nothing random going on. If we

knew the location and velocity of all particles in the fluid at some initial time, we could calculate exactly their effect on the Brownian particle. We could even imagine "integrating out" all the particles in the fluid to get the effective "random" force  $R(t)$  on the particle. It might look something (or nothing) like this



But that would be the force on one Brownian particle. Another Brownian particle somewhere else in the fluid would see a completely different force, so we would get



We can not really say anything useful about the individual paths the different particles take, but we can maybe say something about their statistics. Calculating the full distribution of  $R(t)$  is generally impossible, but we can use our intuition to say something about the first moments of the distribution. So, for example we expect

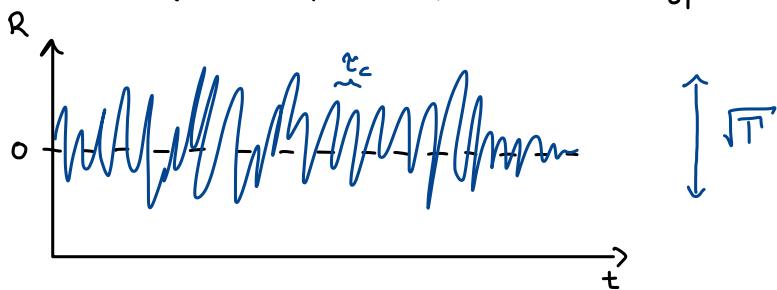
$$\langle R(t) \rangle = 0.$$

The force is equally likely to point in any direction and therefore averages to

zero. The next moment would be the auto-correlation function, which for a general random function  $Y(t)$  would be defined as

$$\begin{aligned} k(t, t') &= \langle [Y(t) - \langle Y(t) \rangle] [Y(t') - \langle Y(t') \rangle] \rangle \\ &= \langle Y(t) Y(t') \rangle - \langle Y(t) \rangle \langle Y(t') \rangle \end{aligned}$$

This tells us something about how long deviations from the mean remain correlated. Roughly speaking it tells us about the relevant time scales in the fluctuations of the force and their typical amplitudes:



When there is a single main time scale, this is called the auto-correlation time  $\tau_c$ .

For the random force  $R(t)$  we then need to specify  $\langle R(t) R(t') \rangle$ . The auto-correlation time  $\tau_c$  is the typical time scale for the particles of the fluid scattering of the Brownian particle. Since the fluid particles are much lighter and faster than the Brownian particle,  $\tau_c \rightarrow 0$  on the relevant time scale for the Brownian motion. We can then write

$$\langle R(t) R(t') \rangle = T \delta(t - t')$$

What about higher moments? In some calculations we don't need to know higher moments. Also, since the force arises from many particles we might make the additional assumptions that the process is Gaussian and therefore the first two moments

(the mean and the variance), fully determine the whole distribution. This assumption is commonly made.

Note: In making these assumptions we are sneaking in irreversibility and the arrow of time.

Anyway, we have now a stochastic differential equation to solve, namely

$$m \frac{dv}{dt} = R(t) \quad \left\{ \begin{array}{l} \langle R(t) \rangle = 0 \\ \langle R(t) R(t') \rangle = T \delta(t-t') \end{array} \right.$$

How do we do this?

To start with, we will just take expectation values and see what we get.

$$m \frac{d\langle v \rangle}{dt} = \langle R(t) \rangle$$

or

$$\langle v(t) \rangle = v_0 + \frac{1}{m} \int dt' \underbrace{\langle R(t') \rangle}_{=0} = v_0$$

Can this be correct?

No, at large times we should reach equilibration in which  $\langle v(t) \rangle = 0$ . So, what did we miss?

Inertia/friction/dissipation! We expect the liquid to resist the motion of the particle. There must therefore be a systematic part to the force from the atoms in addition to the random part.

This has to depend on velocity and if the velocity is in some sense small enough, then

$$F(t) = -\alpha v + R(t) \quad (\alpha > 0)$$

(6)

If in addition there is an external force  $F_{ext}$ , we obtain the Langevin equation

$$m \frac{dv}{dt} = -\alpha v + R(t) + F_{ext}$$

Note: For a macroscopic spherical particle the friction is given by Stokes law:  $\alpha = 6\pi\eta a$ , with  $\eta$  the viscosity and  $a$  the radius.

Note: The separation of the force from the liquid particles into friction and a random force is a typical separation of emergent macroscopic degrees of freedom and microscopic degrees of freedom. Often it is sufficient to introduce a few relevant macroscopic degrees of freedom to capture a large part of the collective motion of complex systems. This then leads to a hydrodynamic description such as diffusion from the first lecture. Compare this also to thermodynamics.

Solving the Langevin equation

$$m \ddot{v} = -\alpha v + R(t) + F_{ext}$$

Let's first take  $F_{ext}=0$  and look again at the average:

$$m \frac{d}{dt} \langle v \rangle = -\alpha \langle v \rangle$$

$$\Rightarrow \langle v(t) \rangle = v_0 e^{-\gamma t} \quad \text{with} \quad \gamma = \frac{\alpha}{m}$$

This makes sense!  $\tau_v = 1/\gamma$  velocity relaxation time

Note: Now we have the relevant time scale to compare with the auto-correlation time  $\tau_c$  of  $R(t)$ , i.e., we need  $\tau_c \ll \tau_v$ .

Now that we have an equation that makes sense we can attempt to obtain a more general solution. For now, imagine the Langevin equation is well defined and we can think of solving it for a given sample function  $R(t)$ . Here the notation is a little bit imprecise.

If we write  $R(t)$  as  $R(\mathbb{X}, t)$  to be explicit about it being a stochastic process, we can imagine solving the equation for a given sample function  $R(x, t)$  where  $\mathbb{X}$  takes the value  $x$ . In our notation, which is not explicit about the random variable,  $R(t)$  stands for both  $R(\mathbb{X}, t)$  and  $R(x, t)$ .

That, or we are a bit sloppy about what we mean by integration.

Let's worry about that later and just integrate (everything is in fact well defined). we obtain:

$$v(t) = e^{-\gamma t} v_0 + \int_0^t e^{-\gamma(t-s)} \frac{1}{m} [R(s) + F_{ext}(s)] ds \quad (8)$$

as we can verify by inspection

$$\begin{aligned} m \frac{dv}{dt} &= -\gamma m \left[ e^{-\gamma t} v_0 + \int_0^t e^{-\gamma(t-s)} \frac{1}{m} [R(s) + F_{ext}(s)] ds \right] + R(t) + F_{ext}(t) \\ &\stackrel{v(t)}{=} \alpha v(t) + R(t) + F_{ext}(t) \quad \checkmark \end{aligned}$$

We can use this solution now to calculate averages

and velocity correlators, as well as the position

$$x(t) = x_0 + \int_0^t v(s) ds$$

For now we take  $F_{ext} = 0$ .

What more do we expect?

In equilibrium we expect thermalization, and thus

$$\frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} k_B T$$

Using (\*) we have

$$\begin{aligned} \langle (\delta v(t))^2 \rangle &= \langle [v(t) - e^{-\gamma t} v_0]^2 \rangle \\ &= \frac{1}{m^2} \int_0^t ds \int_0^t ds' e^{-\gamma(2t-s-s')} \underbrace{\langle R(s) R(s') \rangle}_{T \delta(s-s')} \\ &= \frac{T}{m^2} \int_0^t e^{-2\gamma(t-s)} ds \\ &= \underbrace{\frac{T}{2m^2 \gamma}}_{\cancel{\text{---}}} \left[ 1 - e^{-2\gamma t} \right] \xrightarrow{t \rightarrow \infty} \cancel{\frac{T}{2m^2 \gamma}} \end{aligned}$$

In order for everything to come together, this requires

$$\frac{T}{2m^2 \gamma} = \frac{k_B T}{m} \quad \text{or}$$

$$T = 2\gamma m k_B T$$

This is a great and deep result, so let's make sure we understand it and that it makes sense.

\*  $T \propto \langle R^2 \rangle$  the higher the temperature the larger the fluctuations, or randomness in the force  $R$  ( $\langle R^2 \rangle \propto T$ )

\*  $T \propto \gamma$  Fluctuation  $\leftrightarrow$  dissipation

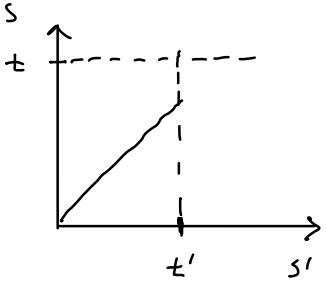
Equilibrium requires a fine balance between fluctuations and dissipation.

This is a general result, sometimes referred to as  
The fluctuation-dissipation theorem.

We will see it in many guises during this course.

### Velocity correlator

An object of great interest is the velocity correlator

$$\begin{aligned} c(t, t') &\equiv \langle v(t)v(t') \rangle - \langle v(t) \rangle \langle v(t') \rangle \\ &= \frac{1}{m^2} \int_0^t ds \int_0^{t'} ds' e^{-\gamma(t-s)-\gamma(t'-s')} \langle R(s)R(s') \rangle \\ &\quad t > t': \frac{\pi}{m^2} e^{-\gamma(t+t')} \int_0^{t'} ds e^{+2\gamma s} \\ &\quad = \frac{\pi}{m^2} e^{-\gamma(t+t')} \frac{1}{2\gamma} [e^{2\gamma t'} - 1] \\ &\quad \begin{matrix} t, t' \rightarrow \infty \\ \xrightarrow{(t-t') \text{ finite}} \end{matrix} \frac{\pi}{2\gamma m^2} e^{-\gamma(t-t')} \end{aligned}$$


or

$$\begin{aligned} c(t, t') &= \frac{\pi}{2\gamma m^2} e^{-\gamma|t-t'|} = c(|t-t'|) \\ &\quad \begin{matrix} t, t' \rightarrow \infty \\ |t-t'| \text{ finite} \end{matrix} \end{aligned}$$

Note that this only depends on  $t-t'$ !

We expect this since at long times we reach an equilibrium steady state (time independent)

Note: If we integrate this result

$$\int_{-\infty}^{\infty} C(t) dt = \int_{-\infty}^{\infty} \frac{\pi}{2\gamma m^2} e^{-\gamma |t|} dt = \frac{\pi}{\gamma^2 m^2} = \frac{2k_B T}{\gamma m}$$

or  $\frac{1}{\alpha} = \frac{1}{\gamma m} = \frac{1}{2k_B T} \int_{-\infty}^{\infty} C(t) dt$

Fluctuation-dissipation

Friction coefficient  
related to correlation  
function.

General!  
C

## Position

Let's now calculate the position

$$\begin{aligned}
 x(t) &= x_0 + \int_0^t v(s) ds \\
 &= x_0 + \int_0^t ds \left[ e^{-\gamma s} v_0 + \int_0^s ds' e^{-\gamma(s-s')} \frac{1}{m} R(s') \right] \\
 &= x_0 + \frac{v_0}{\gamma} (1 - e^{-\gamma t}) + \frac{1}{m} \int_0^t ds \int_0^s ds' R(s') e^{-\gamma(s-s')}
 \end{aligned}$$

and

$$\langle x(t) \rangle = x_0 + \frac{v_0}{\gamma} (1 - e^{-\gamma t})$$

What about correlations?

Can calculate things like:

$$\langle x(t) x(t') \rangle - \langle x(t) \rangle \langle x(t') \rangle$$

$$= \frac{1}{m^2} \int_0^t \int_0^{s_1} ds_1 \int_0^{t'} \int_0^{s_2} ds_2 e^{-\gamma(s_1-s'_1)} e^{-\gamma(s_2-s'_2)} \langle R(s'_1) R(s'_2) \rangle$$

For example, taking  $t=t'$ , and then  $t \gg 1$

$$\langle (\delta x(t))^2 \rangle \rightarrow 20t \quad \text{with}$$

$$D = \frac{k_B T}{\gamma m}$$

Diffusion coefficient

## Some mathematical details on stochastic differential equations and integration

The Langevin equation that we wrote down is an example of the slightly more general Langevin type of equation

$$\frac{dx}{dt} = a(x(t); t) + b(x(t); t) \eta(t)$$

where  $a$  and  $b$  are general functions. The stochastic process  $\eta(t)$  satisfies

$$\begin{aligned}\langle \eta \rangle &= 0 \\ \langle \eta(t) \eta(t') \rangle &= \delta(t-t')\end{aligned}$$

Because of the delta function, the Langevin equation is not well defined.

In fact, the derivative  $\dot{\eta}(t)$  does not exist at any time since  $\eta(t)$  is discontinuous at every time. However, the integral of  $\eta(t)$  is continuous (but not differentiable), and therefore we can introduce a new stochastic

process

$$w(t) = \int_0^t \eta(t') dt'$$

This is a well defined stochastic process that is sometimes called a Wiener process. This Wiener process is a Gaussian process that satisfies

$$\langle w(t) \rangle = 0$$

$$\langle w(t) w(t') \rangle = \min(t, t')$$

and in particular  $\langle w^2(t) \rangle = t$ .

While  $w(t)$  is not differentiable, infinitesimal increments are well defined.

That is

$$dw(t) = w(t+dt) - w(t) = \int_t^{t+dt} \eta(t') dt'$$

and

$$\langle dw(t) \rangle = \int_t^{t+dt} \langle \eta(t') \rangle dt' = 0$$

$$\langle (dw(t))^2 \rangle = \int_t^{t+dt} dt' \int_t^{t+dt} dt'' \langle \eta(t') \eta(t'') \rangle = dt$$

Note: The fact that, schematically,  $(dw)^2 \sim dt$  means that usual differential calculus may not work directly as usual. Care must be taken, for example, when changing variables.

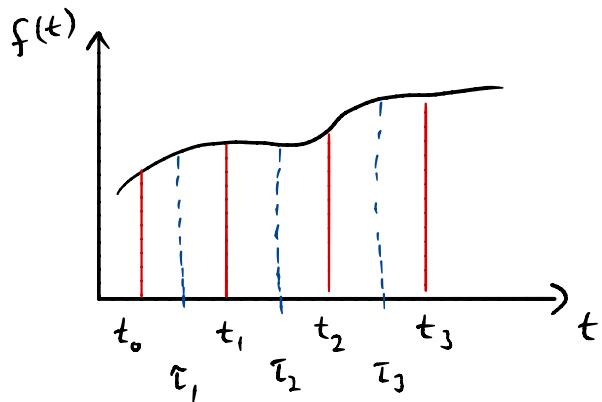
With this, we should think of the general Langevin equation as a short hand for the more well defined

$$dx(t) = a(x(t); t) dt + b(x(t); t) dw(t)$$

We can formally integrate this equation to find

$$x(t) = x_0 + \int_0^t a(x(t'); t') dt' + \int_0^t b(x(t'); t') dw(t')$$

Note: Compare with our calculation with the Langevin equation earlier in this lecture. This looks good, but there is one more complication. Namely, the last integral is not uniquely defined. Remember how usual integrals are defined by dividing an interval into small segments



$$\int f(t) dt = \lim_{n \rightarrow \infty} \sum_{i=1}^n f(\tilde{t}_i) (t_i - t_{i-1})$$

Two main choices of discretization exist (limits implied)

$$\text{Ito: } \tau_i = t_{i+1} : I_I = \sum_{i=0}^{n-1} f(t_i) \Delta w(t_i)$$

$$\text{Stratonovich: } \tau_i = t_i : I_S = \sum_{i=0}^{n-1} f(t_{i+1}) \Delta w(t_i)$$

When  $f(t) = b(x(t); t)$  depends on the solution  $x(t)$ , it also depends implicitly on the stochastic variable  $dW(t)$ . For small  $\Delta w(t_i)$  we can expand

$$f(t_{i+1}) = f(t_i) + \alpha \Delta w'(t_i) + \dots$$

where  $\Delta'$  is a different realization of the Wiener process.  
we now get

$$\left\langle \lim_{\Delta w \rightarrow 0} I_I \right\rangle = \left\langle \int_0^t f(\epsilon') dW(t') \right\rangle = 0$$

but

$$\begin{aligned} \left\langle \lim_{\Delta w \rightarrow 0} I_S \right\rangle &= \left\langle \int_0^t f(\epsilon') dW(t') \right\rangle + \int_0^t \int_0^t \alpha(t'') \langle dW(t') dW(t'') \rangle \\ &= \int_0^t \alpha(t') dt' \end{aligned}$$

using  $\langle dW(t) dW(t') \rangle = \delta(t-t') dt$ .

This last expression is generally not zero.

In the Langevin equation taking the average of the term

$$\left\langle \int_0^t b(x(t'), t') dW(t') \right\rangle = \int_0^t \langle b(x(t'); t') dW(t') \rangle$$

the Ito description allows us to take  $\langle b dW(t) \rangle = 0$  and think of  $b(x(t); t)$  and  $dW$  as independent processes. For this reason, the Ito

prescription is often simpler to use. The Stratonovich prescription is, however, sometimes more convenient.

Note: In our calculations we most of the time didn't need to worry about this since  $b$  was a constant and therefore not a random process. Instead we only got terms like  $\langle R(t) R(t') \rangle$  which we know how to deal with. Otherwise we used the Ito prescription