## GOAL OF THE LECTURE(S)

We return to the stochastic differential equations (Langevin's equation) discussed earlier in connection with the Brownian motion. The problem is generalized to the dynamics of a particle in a potential in the presence of thermal fluctuations. The aim will be to find and explain what kind of noise should be added to the deterministic (mechanical) equation in order that the system would relax to equilibrium at a given temperature. We shall also show (though not quite precisely) that the resulting stochastic differential equation is equivalent to a probabilistic description through the Fokker-Planck equation.

## PRELIMINARIES

### Brownian motion in the overdamped limit

The Brownian motion was described earlier in terms of Langevin's equation

$$m\ddot{x} = -6\pi\tilde{\eta}a\,\dot{x} + X \tag{1}$$

where $x$, $m$ and $a$ are the position, mass and radius of the particle, respectively, $\tilde{\eta}$ is the viscosity of the medium, and $X$ is the random force resulting from thermal fluctuations.

Langevin's solution of (1) did not require much knowledge about $X$. Randomness meant that $\langle X\rangle = 0$, and it followed from the stationarity of the process that $\langle xX\rangle = 0$. It is also remarkable that the fact the particle moves in a medium of temperature $T$ entered the calculation only through the rewriting the left-hand side of (1) as $m\ddot{x} = m\ddot{x^2}/2 - m\dot{x}^2$ and replacing $\langle m\dot{x}^2\rangle$ by $k_BT$ (the average kinetic energy is given by the equipartition theorem).

Examining the derivation in more detail, one can also see that the $m\ddot{x^2}/2$ plays a role only in determining the relaxation to the long-time asymptote $\langle x^2\rangle = 2Dt$, thus the same asymptotics is obtained if this inertial term is neglected. Then the following question arises: Can we neglect the inertial term and consider the overdamped (túlcsillapított) motion of the particle

$$0 = -6\pi\tilde{\eta}a\,\dot{x} + X \tag{2}$$

and obtain the same $\langle x^2\rangle = 2Dt$ result? What do we have to assume in this case about the noise to imitate the fluctuations of a $T$-temperature heat bath?

### Motion in a potential

We shall address the above questions in a slightly more general setup. Let us imagine that the particle is attached to the origin ($x = 0$) by a spring, i.e. it is moving in a potential $U(x) = kx^2/2$. Then, equation (1) would have a term $-dU/dx = -kx$ on the right hand side, and the overdamped version of the equation of motion would have the following form

$$0 = -6\pi\tilde{\eta}a\,\dot{x} - kx + X \quad . \tag{3}$$

In this case, one may ask a more difficult question about the noise: What should be the properties of $X$ which ensure that the system relaxes to the thermal equilibrium, i.e. that the long-time limit of the probability that the particle is at $x$ is given by the Boltzmann distribution

$$P^e(x) = e^{-kx^2/2k_BT}/Z \tag{4}$$

where $Z$ is the normalizing factor (partition function)

$$Z = \int_{-\infty}^{\infty} dx\, e^{-kx^2/2k_BT} \quad . \tag{5}$$

Actually, the same question can be asked for a motion in a general potential $U(x)$ with the equation of motion and the equilibrium distribution being

$$0 = -6\pi\tilde{\eta}a\,\dot{x} - \frac{dU}{dx} + X \tag{6}$$

and

$$P^e(x) = e^{-U(x)/k_BT}/Z \quad , \quad Z = \int_{-\infty}^{\infty} dx\, e^{-U(x)/k_BT}. \tag{7}$$

## FORMULATION OF THE PROBLEM

Equation (6) can be written in the form

$$\dot{x}(t) = -\mu\frac{dU}{dx} + \eta(t). \tag{8}$$

where

$$\mu = \frac{1}{6\pi\tilde{\eta}a} \quad , \quad \eta(t) = \mu X(t) \quad . \tag{9}$$

The question is whether there are simple and practical realizations of $\eta(t)$ which brings the system to equilibrium

$$P^e(x) = e^{-U(x)/k_BT}/Z\,. \tag{10}$$

## BROWNIAN MOTION LIMIT

The equation of motion in this case ($U = 0$) is integrated easily

$$\dot{x} = \eta \quad \rightarrow \quad x(t) = \int_0^t \eta(\tau) d\tau \quad . \tag{11}$$

It follows then that we can calculate the averages

$$\langle x \rangle = \int_0^t \langle \eta(\tau) \rangle d\tau \quad , \tag{12}$$

$$\langle x^2 \rangle = \int_0^t \int_0^t d\tau d\tau' \langle \eta(\tau)\eta(\tau') \rangle \quad . \tag{13}$$

In order to obtain the known results for the Brownian motion, it is sufficient to assume that (1) the average of the random noise is zero and (2) the noise is independent at distinct time moments

$$\langle \eta(t) \rangle = 0 \quad , \quad \langle \eta(t)\eta(t') \rangle = 2D\delta(t - t') \tag{14}$$

where $\delta(t)$ is the usual delta-function and $D$ is the amplitude of the noise.

Indeed, using (14), one can see that equation (12) gives

$$\langle x \rangle = 0 \tag{15}$$

while equation (13) yields

$$\langle x^2 \rangle = 2Dt \quad . \tag{16}$$

Note that the diffusion coefficient $D$ is not determined in this description. So, it looks as if we would have lost something compared to the original Langevin description. This is not so, as will be demonstrated below for the case of oscillator in a heat bath [$U(x) = kx^2/2$]. The ammplitude of the noise has a well defined value in agreement with the Langevin description.

## LINEAR OSCILLATOR IN A HEATH BATH

The equation of motion is simple for the linear oscillator

$$\dot{x} = -\mu k x + \eta(t) \quad , \tag{17}$$

and the solution can be written (you can verify it by substitution) as

$$x(t) = x(0)e^{-\mu k t} + \int_0^t e^{-\mu k(t-\tau)} \eta(\tau) d\tau \quad , \tag{18}$$

where $x(0)$ is the initial ($t = 0$) value of $x$. Since $\langle \eta(t) \rangle = 0$, it follows from the above equation that, as expected, the average position of the particle relaxes to the mechanical equilibrium position

$$\begin{aligned} \langle x(t) \rangle &= x(0)e^{-\mu k t} + \int_0^t e^{-\mu k(t-\tau)} \langle \eta(\tau) \rangle d\tau \\ &= x(0)e^{-\mu k t} \rightarrow 0 \quad . \end{aligned} \tag{19}$$

Next we calculate the mean-square fluctuations $\langle x^2(t) \rangle$. If the system relaxes to equilibrium, the long-time limit of $\langle x^2(t \rightarrow \infty) \rangle = \langle x^2 \rangle_e$ should be given by the equilibrium distribution

$$\langle x^2 \rangle_e = \frac{1}{Z} \int_{-\infty}^{\infty} dx\, x^2\, e^{-kx^2/2k_B T} = k_B T/k \, . \tag{20}$$

When calculating $\langle x^2(t) \rangle$, one should square both sides of equation (18) and average the result over the noise. On the right-hand side, the cross terms are linear in $\eta$ so their average gives zero and only the following two terms remain

$$\begin{aligned} \langle x^2(t) \rangle &= x^2(0)e^{-2\mu k t} + \\ &\int_0^t \int_0^t d\tau d\tau' e^{-\mu k[(t-\tau)+(t-\tau')]} \langle \eta(\tau)\eta(\tau') \rangle \\ &= x^2(0)e^{-2\mu k t} + 2D \int_0^t d\tau e^{-2\mu k(t-\tau)} \quad . \end{aligned} \tag{21}$$

Using the delta correlation of the noise (14), the double integral on the right-hand side becomes a single integral which can be easily calculated and we obtain

$$\langle x^2(t) \rangle = x^2(0)e^{-2\mu k t} + \frac{D}{\mu k}\left(1 - e^{-2\mu k t}\right) . \tag{22}$$

We can see now that, in the large-time limit, the above expression converges to

$$\langle x^2(t \rightarrow \infty) \rangle = \frac{D}{\mu k} \, . \tag{23}$$

Since this limit should be equal to the equilibrium limit, we can compare the above result to (20) and obtain an equation relating the amplitude of the noise ($D$) and the temperature

$$\langle x^2(t \rightarrow \infty) \rangle = \langle x^2 \rangle_{eq} = \frac{D}{\mu k} = \frac{k_B T}{k} \, . \tag{24}$$

From the above equality it follows that the amplitude of the noise (which is the diffusion coefficient in the Brownian motion)

$$D = \mu k_B T = \frac{k_B T}{6\pi\tilde{\eta}a} \tag{25}$$

is given by the same expression as in the original Langevin theory.

So far we have used only limited features of the noise given in (14) and obtained agreement with the Brownian motion results and with some of the known results for the linear oscillator. It remained a question whether any noise satisfying (14) would produce for example the full equilibrium distribution $P^e(x)$. We shall show below that if we add the feature of "gaussianity" to the noise then $P^e(x) \sim \exp\left[-U(x)/k_BT\right]$ emerges as the long-time limit of the distribution for any potential $U(x)$.

## GAUSSIAN NOISE AND STOCHASTIC DIFFERENTIAL EQUATIONS

In order to understand the stochastic differential equations, we have to imagine that we are trying to solve them on a computer. This means that we have to discretize the equations. In the simplest discretization scheme, we obtain the value of $x$ at time $t+\varepsilon$ from the following iteration

$$x(t+\varepsilon) = x(t) - \mu\frac{dU}{dx}\varepsilon + \eta_\varepsilon(t) \quad , \tag{26}$$

where the deterministic part of $x$'s increment $-\mu dU/dx\,\varepsilon$ is understandable and is given. The task is to understand what to write for the stochastic part, $\eta_\varepsilon(t)$.

As before, one assumes that $\langle\eta_\varepsilon(t)\rangle = 0$ and, furthermore, the values of $\eta_\varepsilon(t)$ at different $t$-s are assumed to be independent of each other. The amplitude of the noise is expected to be proportional to $D$ but due to discretization, the proportionality constant is not quite obvious. We can, however, determine the amplitude by considering again the case without external potential, which should be the just the discretized version of the Brownian motion

$$x(t+\varepsilon) = x(t) + \eta_\varepsilon(t) \quad . \tag{27}$$

After $n$ steps when the elapsed time is equal to $n\varepsilon$, the position of the particle given by

$$x(t+n\varepsilon) = x(t)+\eta_\varepsilon(t)+\eta_\varepsilon(t+\varepsilon)+...+\eta_\varepsilon(t+(n-1)\varepsilon) \quad . \tag{28}$$

Thus the average of the mean square displacement of the particle is found to be

$$\begin{aligned}&\langle[x(t+n\varepsilon)-x(t)]^2\rangle = \\ &\langle[\eta_\varepsilon(t)+\eta_\varepsilon(t+\varepsilon)+...+\eta_\varepsilon(t+(n-1)\varepsilon)]^2\rangle = \\ &\langle\eta_\varepsilon^2(t)\rangle + \langle\eta_\varepsilon^2(t+\varepsilon)\rangle + ... + \langle\eta_\varepsilon^2(t+(n-1)\varepsilon)\rangle = \\ &\langle\eta_\varepsilon^2\rangle n \quad .\end{aligned} \tag{29}$$

Since the elapsed time is $n\varepsilon$, the mean square displacement of the Brownian motion should be

$$\langle[x(t+n\varepsilon)-x(t)]^2\rangle = 2Dn\varepsilon \quad . \tag{30}$$

Thus the comparison of (30) and (29) gives us the amplitude of the discretized noise

$$\langle\eta_\varepsilon^2\rangle = 2D\varepsilon \quad . \tag{31}$$

It is important to observe here that the magnitude of $\eta_\varepsilon$ is $\sqrt{\varepsilon}$. And this is what should be compared with the increment coming from the deterministic part in (26) which is proportional to $\varepsilon$.

As we shall see below, if we assume that the noise (of average zero and of amplitude $2D\varepsilon$) is Gaussian, then we can prove that this noise drives the system to equilibrium at temperature $T$, and the time-evolution of probability distribution satisfies the appropriate Fokker-Planck equation.

The assumption of gaussianity means that the stochastic increment $\eta_\varepsilon$ in the iteration (26) is drawn, independently in every step, from the probability distribution

$$P_G(\eta_\varepsilon) = \frac{1}{\sqrt{4\pi D\varepsilon}}e^{-\eta_\varepsilon^2/4D\varepsilon} \quad . \tag{32}$$

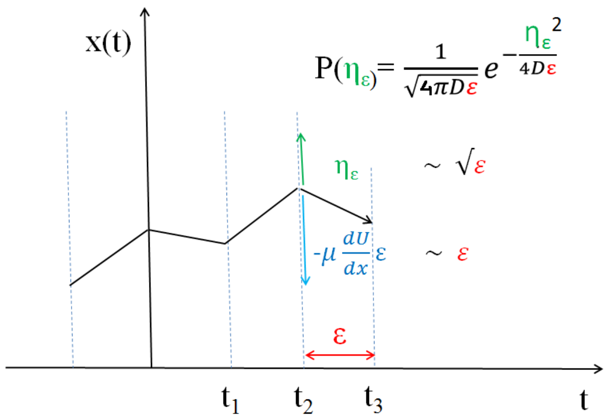


FIG. 1: Random, $\eta_\varepsilon$, and deterministic, $-\mu(dU/dx)\varepsilon$, components of the coordinate increment.

We emphasize again that the magnitude of the stochastic increment is proportional to $\sqrt{\varepsilon}$ while the deterministic part of the increment is $-\mu dU/dx\,\varepsilon \sim \varepsilon$ as shown in Fig.1. This means that the practical discretization is not entirely trivial. For small $\varepsilon$, the noise is dominant and one needs large number of steps for the deterministic part to play a role. For large $\varepsilon$, on the other hand, the deterministic part is dominating and it takes again a large number of steps for the noise to be felt and for the equilibrium distribution to emerge.

## DERIVATION OF THE FOKKER-PLANCK EQUATION

(*The details of this section are not required at the exam*).

In order to see how the Gaussian noise discussed above drives the system to equilibrium, we need to write down the time evolution of the probability distribution $P(x,t)$ defined as the probability of the particle being at $x$ at time $t$. Then one should look at the $t \to \infty$ limit of $P(x,t)$ and a stationary thermal distribution at temperature $T$ should be observed. We shall carry out the above program only for the case of quadratic potential $U(x) = kx^2/2$ but the same calculation with slightly increased difficulties in technicalities goes through for the general potential $U(x)$ as well.

The discretized Langevin equation given by equation (26) with $-\mu dU/dx = -\mu kx \equiv -\lambda x$ (to simplify notation we introduce here $\lambda \equiv \mu k$)

$$x(t+\varepsilon) = x(t) - \lambda x(t)\varepsilon + \eta_\varepsilon(t) \quad . \tag{33}$$

The path of the particle generated by the iteration is not deterministic due to the noise $\eta_\varepsilon(t)$ term. The equation governing the probability $P(x,t)$ can be derived using the Chapman-Kolmogorov equation which we shall also write in a time-discretized form

$$P(x,t+\varepsilon) = \int_{-\infty}^{\infty} W(x,y;\varepsilon)P(y,t)dy \tag{34}$$

where $W(x,y;\varepsilon)$ is the probability that particle moves to $x$ by the time $t+\varepsilon$ provided it started at $y$ at time $t$. In order that the iteration (33) would move the particle from $y$ to $x$ in time $\varepsilon$, the noise term should have just the right value satisfying the equation (33) with $x(t+\varepsilon) \equiv x$ and $x(t) \equiv y$:

$$x = y - \lambda y\varepsilon + \eta_\varepsilon(t) \quad . \tag{35}$$

The probability of the above $\eta_\varepsilon(t)$ is given by (32) with $\eta_\varepsilon(t)$ replaced by the solution of (35). Thus $W(x,y;\varepsilon)$ is obtained as

$$\begin{aligned} W(x,y;\varepsilon) &= P_G(\eta_\varepsilon = x - y + \lambda y\varepsilon) \\ &= \frac{1}{\sqrt{4\pi D\varepsilon}} e^{-[x-y+\lambda y\varepsilon]^2/4D\varepsilon} \quad . \end{aligned} \tag{36}$$

Substituting the above $W(x,y;\varepsilon)$ into equation (34) and expanding the left-hand side of the equation to first order in $\varepsilon$, one finds

$$P(x,t) + \partial_t P(x,t)\varepsilon = \int_{-\infty}^{\infty} \frac{e^{-[x-y+\lambda y\varepsilon]^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} P(y,t)dy\,. \tag{37}$$

We should now expand the integral on the right-hand side to order $\varepsilon$, as well. To do this, let's make the following change in the integration variable

$$z = y(1-\lambda\varepsilon) - x \quad , \tag{38}$$

resulting in

$$\begin{aligned} P\ &(x,t) + \frac{\partial P(x,t)}{\partial t}\varepsilon \\ &= \frac{1}{1-\lambda\varepsilon}\int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} P\left[\frac{z+x}{1-\lambda\varepsilon}, t\right] dz\,. \end{aligned} \tag{39}$$

The expansion to order $\varepsilon$ is somewhat tedious. As a first step, we replace $1/(1-\lambda\varepsilon)$ by $1+\lambda\varepsilon$ which is correct to order $\varepsilon$

$$\begin{aligned} P\ &(x,t) + \frac{\partial P(x,t)}{\partial t}\varepsilon \\ &= \int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} P\left[z(1+\lambda\varepsilon) + x(1+\lambda\varepsilon), t\right] dz \\ &+ \lambda\varepsilon \int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} P\left[z+x, t\right] dz\,, \end{aligned} \tag{40}$$

where we set in $P\left[z(1+\lambda\varepsilon=0) + x(1+\lambda\varepsilon=0), t\right]$ in the last integral since $\varepsilon$ is multiplying this integral. We should also set $\varepsilon \to 0$ in the Gaussian which we know yields a delta function $\delta(z)$ and, consequently, this last term simplifies to $\lambda\varepsilon P(x,t)$, and we have

$$\begin{aligned} P\ &(x,t) + \frac{\partial P(x,t)}{\partial t}\varepsilon \\ &= \int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} P\left[z(1+\lambda\varepsilon) + x(1+\lambda\varepsilon), t\right] dz \\ &+\lambda\varepsilon P(x,t)\ . \end{aligned} \tag{41}$$

Now, the tricky part of the derivation is to expand $P\left[z(1+\lambda\varepsilon) + x(1+\lambda\varepsilon)\right]$ around $z=0$. The Gaussian becomes a delta function $\delta(z)$ in the limit of $\varepsilon \to 0$ and only the $z \approx 0$ range is relevant in $P$. Then the terms up to order $\varepsilon$ must be collected.

The term coming from setting $z = 0$ in $P\left[z(1+\lambda\varepsilon) + x(1+\lambda\varepsilon)\right]$ yields $P\left[x(1+\lambda\varepsilon), t\right]$ once it is recognized that the remaining integral of the Gaussian just gives 1. To order $\varepsilon$, this term can be written as

$$P(x,t) + \varepsilon\lambda x\frac{\partial P}{\partial x}\,. \tag{42}$$

The next term is zero

$$\left.\frac{\partial P}{\partial z}\right|_{z=0} \int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} z(1+\lambda\varepsilon)dz = 0\,, \tag{43}$$

since the integrand is an odd function of $z$.

The $3^{rd}$ term of the expansion is given by

$$\frac{1}{2}\left.\frac{\partial^2 P}{\partial z^2}\right|_{z=0} \int_{-\infty}^{\infty} \frac{e^{-z^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} z^2(1+\lambda\varepsilon)^2 dz\,. \tag{44}$$

The above integral is proportional to $\varepsilon$, and is given by $2D\varepsilon$. In addition, one should note that the argument of $P$ is $z(1+\lambda\varepsilon)+x(1+\lambda\varepsilon)$, thus

$$\left.\frac{\partial^2 P}{\partial z^2}\right|_{z=0} = \left.\frac{\partial^2 P}{\partial x^2}\right|_{z=0} , \tag{45}$$

and, furthermore, the $\partial^2 P/\partial x^2$ is multiplied by $2D\varepsilon$ thus, to order $\varepsilon$, its argument $x(1+\lambda\varepsilon)$ can be replaced by $x$. Thus the $3^{rd}$ term of the expansion is reduced to

$$\varepsilon D \frac{\partial^2 P}{\partial x^2} , \tag{46}$$

All the higher order terms in the expansion by $z$ yield terms proportional higher then first power of $\varepsilon$ (try to show it!). Collecting now the order $\varepsilon$ terms (42) and (46), and substituting them into equation (41) yields, at the end, the following Fokker-Planck equation

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial \lambda x P(x,t)}{\partial x} + D\frac{\partial^2 P(x,t)}{\partial x^2} \quad , \tag{47}$$

Had we carried out the calculation for a general $U(x)$ then the $\lambda x = \mu k x = \mu \partial U/\partial x$ part in the first term on the right hand side would also be $\mu \partial U(x)/\partial x$, and then the general equation would be

$$\frac{\partial P(x,t)}{\partial t} = \mu \frac{\partial}{\partial x}\left(\frac{\partial U}{\partial x} P(x,t)\right) + D\frac{\partial^2 P(x,t)}{\partial x^2} \quad . \tag{48}$$

The stationary solution of the above equation can be obtained by setting $\partial P(x,t)/\partial t$ to zero

$$0 = \mu \frac{d}{dx}\left(\frac{dU}{dx} P^{(e)}(x)\right) + D\frac{d^2 P^{(e)}(x)}{dx^2} \quad . \tag{49}$$

The derivation of $P^{(e)}(x)$ from the above equation is straightforward but uses an argument that no probability current can be present in equilibrium. Instead of the derivation, I just suggest to verify by substitution that the above equation is solved by the function

$$P^{(e)}(x) = Ce^{-\mu U(x)/D} \tag{50}$$

where $C$ is a normalization constant. If we remember now that $D$ and $\mu$ are not independent of each other but, according to (25), they are related by $D = \mu k_B T$, the final result for the stationary distribution function is obtained as the equilibrium Boltzmann distribution

$$P^{(e)}(x) = \frac{1}{Z} e^{-U(x)/k_B T} \quad . \tag{51}$$

Even if we did not prove everything in full generality, we have seen (1) how a stochastic differential equation with a special type of additive noise yields relaxation to equilibrium, (2) how the noise can be handled and put on the computer.