

### List of topics in this lecture

- Wiener process is continuous in probability
  - Ornstein-Uhlenbeck Process (OU), Stokes' law, thermal excitations
  - Solution of particle velocity, colored noise, convergence to a white noise
  - Fluctuation-dissipation theorem, Maxwell-Boltzmann distribution
  - Solution of particle position
- 

### Recap

$dW/dt$  is a white noise (stationary stochastic process,  $R(t)$ , PSD)

Constrained Wiener process (Bayes theorem)

$$\rho(W(a+h)=x | W(a)=y_a \text{ and } W(a+2h)=y_b) \sim N\left(\frac{y_a+y_b}{2}, \frac{h}{2}\right)$$

### Wiener process is continuous in probability

Recall the continuity of a regular function  $f(t)$ .

Function  $f(t)$  is continuous at  $t$  if for any  $\varepsilon > 0$ ,

$|f(t+h) - f(t)| \geq \varepsilon$  is impossible when  $h$  is small enough.

### Theorem: (Continuity of $W(t)$ in probability)

Intuitively, for any  $\varepsilon > 0$ ,

$|W(t+h) - W(t)| \geq \varepsilon$  is almost impossible when  $h$  is small enough.

More precisely, for any  $\varepsilon > 0$ , we have

$$\lim_{h \rightarrow 0} \Pr(|W(t+h) - W(t)| \geq \varepsilon) = 0$$

Note: This property/condition is the definition of continuity in probability.

Proof of the theorem:

To prove the theorem, we need

Chebyshev-Markov inequality:

For a random variable  $X$ , we write  $E(|X|^\alpha)$  as

$$\begin{aligned} E(|X|^\alpha) &= \int |x|^\alpha \rho(x) dx \geq \int_{|x| \geq \varepsilon} |x|^\alpha \rho(x) dx \geq \\ &\geq \varepsilon^\alpha \int_{|x| \geq \varepsilon} \rho(x) dx = \varepsilon^\alpha \Pr(|X| \geq \varepsilon) \\ \Rightarrow \quad &\boxed{\Pr(|X| \geq \varepsilon) \leq \frac{1}{\varepsilon^\alpha} E(|X|^\alpha)} \end{aligned}$$

This is called the Chebyshev-Markov inequality.

Applying the Chebyshev-Markov inequality to  $X = W(t+h) - W(t)$  with  $\alpha = 2$ , we have

$$\begin{aligned} \Pr(|W(t+h) - W(t)| \geq \varepsilon) &\leq \frac{E(|W(t+h) - W(t)|^2)}{\varepsilon^2} \\ &= \frac{h}{\varepsilon^2} \rightarrow 0 \quad \text{as } h \rightarrow 0 \end{aligned}$$

Thus, the Wiener process  $W(t)$  is continuous in probability.

### **Ornstein-Uhlenbeck Process**

Consider the stochastic motion of a small particle in water (as Robert Brown observed the motion of pollen particles in water under a microscope)

For simplicity, we discuss the one-dimensional motion.

In the 3-dimensional motion, each dimension is described by this model.

Let

$X$  = position of the particle

$Y$  = velocity of the particle

$m$  = mass of the particle

Newton's second law (governing the motion)

$$m \frac{dY}{dt} = \text{viscous drag} + \text{Brownian force}$$

Stokes law (for the viscous drag)

$$\text{viscous drag} = -b Y$$

where  $b$  is the drag coefficient. For a spherical particle, the drag coefficient is

$$b = 6\pi \eta a$$

$a$  = radius of the particle

$\eta$  = viscosity of the fluid media

A short digression: Pollution particles **suspended** in air

When a solid ball is dropped in mid-air, it first accelerates, driven by the gravity. Then it reaches a constant velocity (called the terminal velocity or settling velocity) when the drag force balances the gravitational force.

The settling velocity satisfies

$$\underbrace{(6\pi\eta a)V_{\text{settling}}}_{\text{Drag force}} = \underbrace{\left(\frac{4}{3}\pi a^3 \rho_{\text{mass}}\right)g}_{\text{Gravity}}$$

$$\Rightarrow V_{\text{settling}} = \left(\frac{2\rho_{\text{mass}}g}{9\eta}\right)a^2 \propto a^2$$

where the air viscosity is  $\eta = 1.8 \times 10^{-4} \text{ g}(\text{cm})^{-1}\text{s}^{-1}$ .

Consider budesonide, a drug used in treating asthma. It has  $\rho_{\text{mass}} = 1.26 \text{ g/cm}^3$ .

For a ball of 0.1 mm in diameter

$$a = 50 \text{ }\mu\text{m} \quad \Rightarrow \quad V_{\text{settling}} = 38 \text{ cm/s}$$

For a ball of 10  $\mu\text{m}$  in diameter (PM<sub>10</sub> particles)

$$a = 5 \text{ }\mu\text{m} \quad \Rightarrow \quad V_{\text{settling}} = 0.38 \text{ cm/s}$$

For a ball of 2.5  $\mu\text{m}$  in diameter (PM<sub>2.5</sub> particles)

$$a = 1.25 \text{ }\mu\text{m} \quad \Rightarrow \quad V_{\text{settling}} = 0.024 \text{ cm/s}$$

With this tiny settling velocity, it takes more than 1 hour for a 2.5  $\mu\text{m}$  particle to descend 1 meter with respect to the surrounding air.

Remark:

Small pollution particles are more dangerous for two reasons:

- They stay in air much longer (virtually forever)
- They can pass the filtration system of human body to enter the lung and the circulatory system.

End of digression

Thermal excitations (Brownian force)

We model the Brownian force as a white noise.

$$\text{Brownian force} = q \frac{dW}{dt}$$

where the coefficient  $q$  is to be determined later.

The governing equation

$$m dY = \underbrace{-bY dt}_{\text{dissipation}} + \underbrace{q dW}_{\text{fluctuation}}$$

$$dX = Y dt$$

Remark:

Both the viscous drag and the Brownian force on the particle are results from the particle colliding with surrounding fluid molecules: the viscous drag is the mean and the Brownian force is the fluctuation. As a result, the fluctuation coefficient ( $q$ ) and the dissipation coefficient ( $b$ ) are related by the fluctuation-dissipation theorem.

Four goals of the discussion

- 1) Solve for  $Y(t)$
- 2) Show that
  - A)  $Y(t)$  is a colored noise and
  - B)  $Y(t)$  converges to a white noise as  $m$  converges to zero (when the effect of inertia is negligible)
- 3) Relate  $q$  to  $b$  (fluctuation-dissipation theorem)
- 4) Study the behavior of  $X(t)$

Goal #1: We solve for  $Y(t)$ .

For mathematical convenience, we divide the equation by  $m$

$$dY = -bY dt + q dW$$

$$\Rightarrow dY = -\beta Y dt + \gamma dW, \quad \beta = \frac{b}{m}, \quad \gamma = \frac{q}{m}$$

We use the integrating factor method. Multiply by  $e^{\beta t}$

$$e^{\beta t} dY + \beta e^{\beta t} Y dt = \gamma e^{\beta t} dW$$

$$\Rightarrow d(e^{\beta t} Y(t)) = \gamma e^{\beta t} dW$$

$$\Rightarrow e^{\beta t} Y(t) - Y(0) = \int_0^t \gamma e^{\beta s} dW(s) \equiv G(t)$$

where the integral  $G(t)$  is defined as the limit of Riemann sum.

$$\Delta s = \frac{t}{N}, \quad s_j = j \Delta s, \quad dW_j = W(s_{j+1}) - W(s_j)$$

$$G(t) = \lim_{N \rightarrow \infty} \sum_{j=0}^{N-1} \gamma e^{\beta s_j} dW_j$$

Recall that the sum of independent Gaussians (normal RVs) is a Gaussian.

$\{dW_j, j = 0, 1, \dots, N-1\}$  are independent Gaussians.

$\Rightarrow G(t)$  is a Gaussian.

The mean and variance of  $G(t)$  are

$$E(G(t)) = \lim_{N \rightarrow \infty} \sum_j \gamma e^{\beta s_j} E(dW_j) = 0$$

$$\begin{aligned} \text{var}(G(t)) &= \lim_{N \rightarrow \infty} \sum_j (\gamma e^{\beta s_j})^2 \text{var}(dW_j) = \lim_{N \rightarrow \infty} \sum_j (\gamma e^{\beta s_j})^2 \Delta s \\ &= \int_0^t (\gamma e^{\beta s})^2 ds = \gamma^2 \int_0^t e^{2\beta s} ds = \frac{\gamma^2}{2\beta} (e^{2\beta t} - 1) \end{aligned}$$

Caution:

$ds$  in integral comes from  $\Delta s$  in Riemann sum, which comes from  $\text{var}(dW)$ .

This works well for  $t > 0$  in  $\int_0^t \gamma e^{\beta s} dW(s)$ .

For  $t < 0$ , increments  $\{dW_j, j = 0, 1, \dots, N-1\}$  are backwards in time and are no longer independent. The situation with  $dW$  is different from that of a regular ODE.

We will discuss the case of  $t < 0$  later. For the time being, we work with  $t > 0$ .

Summary:

$$G(t) \equiv \int_0^t \gamma e^{\beta s} dW(s) \sim N\left(0, \frac{\gamma^2}{2\beta} (e^{2\beta t} - 1)\right) \quad \text{for } t > 0$$

In the above, we just derived a theorem.

Theorem:

$$\int_0^L f(t) dW(t) \sim N\left(0, \int_0^L f(t)^2 dt\right)$$

Now we write out  $Y(t)$

$$e^{\beta t} Y(t) - Y(0) = G(t)$$

$$\Rightarrow Y(t) = e^{-\beta t} Y(0) + e^{-\beta t} G(t) \quad \text{for } t > 0$$

When  $Y(0)$  is fixed,  $Y(t)$  is a Gaussian with mean and variance given by

$$E(Y(t)|Y(0)) = e^{-\beta t} Y(0) \quad \text{for } t > 0$$

$$\text{var}(Y(t)|Y(0)) = e^{-2\beta t} \text{var}(G(t)) = \frac{\gamma^2}{2\beta} (1 - e^{-2\beta t}) \quad \text{for } t > 0$$

Summary:

$$(Y(t)|Y(0) = y_0) \sim N\left(e^{-\beta t} y_0, \frac{\gamma^2}{2\beta} (1 - e^{-2\beta t})\right) \quad \text{for } t > 0$$

As  $t$  increases,  $Y(t)$  relaxes to the equilibrium.

$$E(Y(t)) = e^{-\beta t} Y(0) \rightarrow 0 \quad \text{as } t \rightarrow +\infty$$

$$\text{var}(Y(t)) = \frac{\gamma^2}{2\beta} (1 - e^{-2\beta t}) \rightarrow \frac{\gamma^2}{2\beta} \quad \text{as } t \rightarrow +\infty$$

For large  $t$ ,  $Y(t)$  reaches an equilibrium Gaussian distribution.

$$Y(\text{large } t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right)$$

Goal #2: we show that

A)  $Y(t)$  is a colored noise and

B)  $Y(t)$  converges to a white noise as  $m$  converges to zero.

We assume that the equilibrium has been reached long time ago and  $Y(t)$  is already a stationary process. Under this assumption,  $Y(t)$  has the equilibrium distribution.

$$Y(t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right) \quad \text{for all } t$$

Goal #2A: We show that  $Y(t)$  is a colored noise.

We calculate the autocorrelation function.

$$R(t) \equiv E(Y(t)Y(0))$$

We use the law of total expectation.

$$E(Z_1) = E(E(Z_1|Z_2))$$

We select  $Z_1 = Y(t) Y(0)$  and  $Z_2 = Y(0)$ . We consider the case of  $t > 0$ .

$$E(Y(t)Y(0)) = E(E(Y(t)Y(0)|Y(0))) = E(Y(0) \cdot E(Y(t)|Y(0)))$$

$$\text{using } E(Y(t)|Y(0)) = e^{-\beta t} Y(0) \text{ for } t > 0 \text{ and } Y(t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right) \text{ for all } t$$

$$= E(Y(0) \cdot e^{-\beta t} Y(0)) = e^{-\beta t} E(Y(0)^2) = \frac{\gamma^2}{2\beta} e^{-\beta t} \quad \text{for } t > 0$$

$$\Rightarrow R(t) = \frac{\gamma^2}{2\beta} e^{-\beta t} \quad \text{for } t > 0$$

From the definition of auto-correlation function,  $R(t)$  is an even function of  $t$ :

$$\begin{aligned} R(-t) &\equiv E(Y(s-t)Y(s)) \quad \text{for all } s \\ &= E(Y(0)Y(t)) = R(t) \end{aligned}$$

Therefore, we obtain

$$R(t) = \frac{\gamma^2}{2\beta} \exp(-\beta |t|) \quad \text{for } t \in (-\infty, +\infty)$$

The corresponding power spectrum density is

$$s(\xi) = \frac{\gamma^2}{2\beta} F[\exp(-\beta |t|)] = \frac{\gamma^2}{2\beta} \cdot \frac{2\beta}{\beta^2 + 4\pi^2 \xi^2} = \frac{\gamma^2}{\beta^2 + 4\pi^2 \xi^2}$$

(Homework problem)

In conclusion,  $Y(t)$  is a colored noise.

Goal #2B: We show that  $Y(t)$  converges to a white noise as  $m \rightarrow 0$   
(when the effect of inertia is negligible).

A simplified story:  $m \rightarrow 0$  (while  $b$  and  $q$  stay unchanged)

Recall that  $\beta = \frac{b}{m}$ ,  $\gamma = \frac{q}{m}$ .

$$R(t) = \frac{\gamma^2}{2\beta} \exp(-\beta |t|) = \frac{q^2}{m^2} \cdot \frac{m}{2b} \exp\left(-\frac{b}{m} |t|\right) = \frac{q^2}{b^2} \cdot \underbrace{\frac{b}{m}}_{1/h} \cdot \underbrace{\frac{1}{2} \exp\left(-\frac{b}{m} |t|\right)}_{f(t)}$$

$$= \frac{q^2}{b^2} \cdot \frac{1}{h} f\left(\frac{t}{h}\right), \quad h \equiv \frac{m}{b}, \quad f(u) \equiv \frac{1}{2} \exp(-|u|)$$

$f(u)$  given above is a density function. For a density function, we have

$$\lim_{h \rightarrow 0} \frac{1}{h} f\left(\frac{t}{h}\right) = \delta(t)$$

As  $m \rightarrow 0$ , we have  $h \equiv m/b \rightarrow 0$  and

$$R(t) = \frac{q^2}{b^2} \cdot \frac{1}{h} f\left(\frac{t}{h}\right) \rightarrow \frac{q^2}{b^2} \cdot \delta(t)$$

Therefore,  $\lim_{m \rightarrow 0} Y(t)$  is a white noise.

The real story:

Mathematically, the limit above is rigorous.

In physics, the situation is a bit complicated. Coefficients  $m$ ,  $b$  and  $q$  are all related. We cannot make  $m \rightarrow 0$  without changing  $b$  and  $q$ .

Consider a spherical particle. The mass of the particle is

$$m = \frac{4\pi}{3} \rho_{\text{mass}} a^3$$

where  $\rho_{\text{mass}}$  is the mass density and  $a$  the radius of particle.

In physics,  $m \rightarrow 0$  is achieved by  $a \rightarrow 0$ .

We need to consider the effect of radius  $a$  on coefficients  $b$  and  $q$ .

$$m = \frac{4\pi}{3} \rho_{\text{mass}} a^3 = O(a^3) \rightarrow 0$$

$$b = 6\pi \eta a = O(a) \rightarrow 0$$

$$h \equiv \frac{m}{b} = O(a^2) \rightarrow 0$$

$$q = \sqrt{2k_B T b} = O(\sqrt{a}) \rightarrow 0 \quad (\text{we will derive this shortly})$$

$$\frac{q^2}{b^2} = O(a^{-1}) \rightarrow \infty$$

$$a \frac{q^2}{b^2} = O(1) \quad \text{independent of } a.$$

Consider  $\sqrt{a} Y(t)$ . We have



$$R_{\sqrt{a}Y}(t) = aR_Y(t) = \left( a \frac{q^2}{b^2} \right) \cdot \frac{1}{h} f\left(\frac{t}{h}\right) \rightarrow \left( a \frac{q^2}{b^2} \right) \cdot \delta(t) \quad \text{as } a \rightarrow 0$$

$\Rightarrow \sqrt{a}Y(t)$  is a white noise.

In physics, as radius  $a \rightarrow 0$ ,  $Y(t)$  converges to a white noise of magnitude  $\frac{1}{\sqrt{a}}$ .

Goal #3: We relate fluctuation coefficient  $q$  to drag coefficient  $b$

To connect  $b$  and  $q$ , we need the Maxwell-Boltzmann distribution

Maxwell-Boltzmann distribution

$$\rho(Y = y) \propto \exp\left(\frac{-\text{Energy}(Y = y)}{k_B T}\right)$$

where

$\rho(y)$  is the equilibrium distribution of velocity  $Y$ ,

$k_B$  is the Boltzmann constant and

$T$  is the absolute temperature.

Maxwell-Boltzmann distribution is a universal law applicable to all thermodynamic systems. In our system,  $y$  = velocity and

$$\text{Energy}(Y = y) = \frac{1}{2} m y^2$$

The Maxwell-Boltzmann distribution gives us

$$\rho(Y = y) \propto \exp\left(\frac{-\text{Energy}}{k_B T}\right) = \exp\left(\frac{-\frac{1}{2} m y^2}{k_B T}\right)$$

writing it into the form of a Gaussian  $\exp\left(\frac{-y^2}{2\sigma^2}\right)$

$$= \exp\left(\frac{-y^2}{2\left(\frac{k_B T}{m}\right)}\right) \sim N\left(0, \frac{k_B T}{m}\right)$$

We have two equilibrium distributions:

- The equilibrium dictated by the Maxwell-Boltzmann distribution is

$$Y(t) \sim N\left(0, \frac{k_B T}{m}\right)$$

- The equilibrium derived from the Ornstein-Uhlenbeck Process is

$$Y(t) \sim N\left(0, \frac{\gamma^2}{2\beta}\right) \quad \text{for all } t$$

Comparing these two equilibrium distributions, we obtain

$$\frac{\gamma^2}{2\beta} = \frac{k_B T}{m}$$

$$\text{Recall that } \beta = \frac{b}{m}, \quad \gamma = \frac{q}{m}.$$

$$\implies \frac{q^2}{m^2} \cdot \frac{m}{2b} = \frac{k_B T}{m}$$

$$\implies q^2 = 2k_B T b$$

Therefore, we conclude

$$q = \sqrt{2k_B T b}$$

This is called the fluctuation dissipation relation (theorem).

With the fluctuation dissipation relation, the governing equation becomes.

$$m dY = \underbrace{-bY dt}_{\text{dissipation}} + \underbrace{\sqrt{2k_B T b} dW}_{\text{fluctuation}}$$

Remark:

Now all coefficients in the governing equation are determined.

Goal #4: we study the behavior of  $X(t)$ .

First, we solve for  $X(t)$ .

$$Y(t) = e^{-\beta t} Y(0) + e^{-\beta t} G(t) \quad \text{for } t > 0, \quad G(t) \equiv \int_0^t \gamma e^{\beta s} dW(s)$$

$$X(t) - X(0) = \int_0^t Y(\tau) d\tau = \int_0^t \left( e^{-\beta \tau} Y(0) + e^{-\beta \tau} G(\tau) \right) d\tau$$

$$\begin{aligned}
 &= \int_0^t \left( e^{-\beta\tau} Y(0) + e^{-\beta\tau} \int_0^\tau \gamma e^{\beta s} dW(s) \right) d\tau \\
 &= \frac{1}{\beta} (1 - e^{-\beta t}) Y(0) + \gamma \int_0^t \int_0^\tau e^{-\beta\tau} e^{\beta s} dW(s) d\tau \\
 &\quad \text{Change the order of integration} \\
 &= \frac{1}{\beta} (1 - e^{-\beta t}) Y(0) + \gamma \int_0^t \left( \int_s^t e^{-\beta\tau} d\tau \right) e^{\beta s} dW(s) \\
 &= \frac{1}{\beta} (1 - e^{-\beta t}) Y(0) + \underbrace{\frac{\gamma}{\beta} \cdot \int_0^t (1 - e^{-\beta(t-s)}) dW(s)}_{G_2(t)}
 \end{aligned}$$

$G_2(t) \equiv \int_0^t (1 - e^{-\beta(t-s)}) dW(s)$  is a sum of independent Gaussians.

$\implies G_2(t)$  is a Gaussian.

Therefore,  $(X(t) - X(0))$  is a Gaussian. We will look into it in more detail.