

# Computer simulation of Brownian motion

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## Summary

### 1) Stochastic process

Consider a steady stochastic process  $Y(t)$  with  $\langle Y(t) \rangle = 0$ .

Fourier transformation

$$\tilde{Y}_T(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} Y_T(t) \quad (1)$$

Inverse Fourier transformation

$$Y_T(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tilde{Y}_T(\omega), \quad (2)$$

where

$$\begin{aligned} Y_T(t) &= Y(t) \quad (|t| \leq T/2) \\ Y_T(t) &= 0 \quad (|t| > T/2) \end{aligned} \quad (3)$$

The following equations can be derived.

I) Spectral density:

$$S_Y(\omega) = \lim_{T \rightarrow \infty} \frac{1}{T} |\tilde{Y}_T(\omega)|^2 \quad (4)$$

II) Auto-correlation function:

$$\varphi_Y(t) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-\infty}^{\infty} d\tau Y_T(\tau) Y_T(\tau + t) \quad (5)$$

III) Wiener–Khinchin theorem:

$$S_Y(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \varphi_Y(t) \quad (6)$$

$$\varphi_Y(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} S_Y(\omega) \quad (7)$$

## 2) Brownian motion and the Langevin equation

Suppose a Brownian spherical particle of radius  $a$  and mass  $m$  is moving in a liquid of viscosity  $\eta$  at a temporal velocity  $\mathbf{V}(t)$  under the influence of the random force  $\mathbf{F}_R(t)$  due to thermal fluctuation and the external force  $\mathbf{F}_{ext}(t)$  acting on the particle. The equation of motion for the Brownian particle can be given by

$$m \frac{d\mathbf{V}}{dt} = -\gamma \mathbf{V} + \mathbf{F}_R + \mathbf{F}_{ext}, \quad (8)$$

where  $\gamma = 6\pi\eta a$  (Stokes friction) and  $\mathbf{V} = \frac{d\mathbf{R}}{dt}$ . Assuming that the particle motion is over

dumped  $\frac{d\mathbf{V}}{dt} = 0$ , one yields the Langevin equation of the form

$$\frac{d\mathbf{R}(t)}{dt} = \frac{1}{\gamma} \mathbf{F}_R + \frac{1}{\gamma} \mathbf{F}_{ext} \quad (9)$$

with

$$\langle \mathbf{F}_R(t) \rangle = 0, \quad \langle \mathbf{F}_R(t) \cdot \mathbf{F}_R(t') \rangle = 2\tilde{D}\delta(t-t').$$

(10)

When the system is in equilibrium  $\mathbf{F}_{ext} = 0$ , the following results can be derived.

I) Auto-correlation function for  $\mathbf{V}(t)$ :

$$\varphi_V(t) = \frac{\tilde{D}}{\gamma} \exp\left(-\frac{\gamma}{m}t\right) \quad (11)$$

II) Fluctuation dissipation theorem:

$$\tilde{D} = \frac{3k_B T \gamma}{m} \quad (12)$$

III) Einstein relation, Stokes-Einstein relation:

$$D = \frac{k_B T}{\gamma} = \frac{k_B T}{6\pi\eta a} \quad (13)$$

When the particle is driven by an external force in x-direction  $\mathbf{F}_{ext} = F_0 \mathbf{e}_x$ , the following results can be derived.

IV) Steady drift velocity:

$$\lim_{t \rightarrow \infty} \langle V_x(t) \rangle = \frac{F_0}{\gamma} = \frac{DF_0}{k_B T} \quad (14)$$

$$\therefore D = \lim_{t \rightarrow \infty} \langle V_x(t) \rangle \frac{k_B T}{F_0} \quad (15)$$

### 3) Linear response theory and the Green-Kubo formula

I) Linear response theory (LRT):

$$H(t) = H_0, \quad \langle B \rangle_{H_0} = B_0 \quad (t < 0) \quad (16)$$

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$$H(t) = H_0 + H'(t), \quad \langle B \rangle_{H_0+H'} = B_0 + \langle \Delta B(t) \rangle_{H_0+H'} \quad (t \geq 0) \quad (17)$$

When  $H'(t) = -AF(t)$ ,

$$\langle \Delta B(t) \rangle_{H_0+H'} = \int_{-\infty}^t ds \Phi_{BA}(t-s)F(s) \quad (18)$$

$$\Phi_{BA}(t) = \frac{1}{k_B T} \langle B(\tau+t)\dot{A}(\tau) \rangle_{H_0} \quad (19)$$

II) Application of LRT to drift velocity:

$$A \equiv R_x(t), \quad B \equiv V_x(t), \quad \text{and} \quad H'(t) = -AF(t) = R_x F_0 \theta(t)$$

$$\begin{aligned} \langle \Delta B(t) \rangle_{H_0+H'} &= \langle V_x(t) \rangle_{H_0+H'} \\ &= \frac{F_0}{k_B T} \int_0^t ds \langle V_x(\tau+t)V_x(\tau) \rangle_{H_0} \\ &= \frac{F_0}{3k_B T} \int_0^t ds \langle \mathbf{V}(\tau+t) \cdot \mathbf{V}(\tau) \rangle_{H_0} \end{aligned} \quad (20)$$

$$\therefore D = \lim_{t \rightarrow \infty} \langle V_x(t) \rangle_{H_0+H'} \frac{k_B T}{F_0} = \frac{1}{3} \int_0^\infty ds \varphi_V(t) \quad (\text{Green-Kubo Formula}) \quad (21)$$