

Supplemental note for Week 4 Part 1

ver. 20170416-01

Ryoichi Yamamoto

1 Average and variance of the cumulative impulse $\Delta\mathbf{W}_i$

Let us start with the Langevin equation

$$m \frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) + \mathbf{F}(t), \quad (\text{F2})$$

where the random force $\mathbf{F}(t)$ satisfies the following conditions

$$\langle \mathbf{F}(t) \rangle = \mathbf{0} \quad (\text{F3})$$

$$\langle \mathbf{F}(t)\mathbf{F}(0) \rangle = 2k_B T \zeta \mathbf{I} \delta(t), \quad (\text{F4})$$

with $\mathbf{0} \equiv (0, 0, 0)$ and $\mathbf{I} \equiv \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

We now discretize the time t using an increment Δt , such that $t_i \equiv i\Delta t$, and define the cumulative impulse during the interval $t_i \leq t \leq t_{i+1} = t_i + \Delta t$, as

$$\Delta\mathbf{W}_i \equiv \int_{t_i}^{t_{i+1}} dt \mathbf{F}(t). \quad (\text{F8})$$

From Eq.(F3), it is straightforward to show

$$\langle \Delta\mathbf{W}_i \rangle = \int_{t_i}^{t_{i+1}} dt \langle \mathbf{F}(t) \rangle = \mathbf{0}. \quad (\text{F10})$$

Also from Eq.(F4), for $j \neq i$

$$\langle \Delta\mathbf{W}_i \Delta\mathbf{W}_{j \neq i} \rangle = \int_{t_i}^{t_{i+1}} dt \int_{t_j}^{t_{j+1}} dt' \langle \mathbf{F}(t)\mathbf{F}(t') \rangle \quad (1)$$

$$= 2k_B T \zeta \mathbf{I} \int_{t_i}^{t_{i+1}} dt \int_{t_j}^{t_{j+1}} dt' \delta(t - t') \quad (2)$$

$$= \mathbf{0}, \quad (3)$$

where $\mathbf{0} \equiv \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$.

For $j = i$

$$\langle \Delta\mathbf{W}_i \Delta\mathbf{W}_i \rangle = \int_{t_i}^{t_{i+1}} dt \int_{t_i}^{t_{i+1}} dt' \langle \mathbf{F}(t)\mathbf{F}(t') \rangle \quad (4)$$

$$= 2k_B T \zeta \mathbf{I} \int_{t_i}^{t_{i+1}} dt \int_{t_i}^{t_{i+1}} dt' \delta(t - t') \quad (5)$$

$$= 2k_B T \zeta \Delta t \mathbf{I}. \quad (6)$$

Combining Eqs.(3) and (6), we obtain

$$\langle \Delta\mathbf{W}_i \Delta\mathbf{W}_j \rangle = 2k_B T \zeta \Delta t \mathbf{I} \delta_{ij}. \quad (\text{F11})$$

2 Distribution of $\Delta\mathbf{W}_i$

Here we further divide Δt into n segments ($n \gg 1$) of a very small time span ϵ , *i.e.*, $\Delta t \equiv n\epsilon$, and define a new cumulative impulse over ϵ

$$\mathbf{W}_i^m \equiv \int_{t_i+(m-1)\epsilon}^{t_i+m\epsilon} dt \mathbf{F}(t), \quad (7)$$

where $1 \leq m \leq n$.

Repeating the same procedure performed in the previous section, the following conditions are derived.

$$\langle \mathbf{W}_i^m \rangle = \mathbf{0} \quad (8)$$

$$\langle \mathbf{W}_i^m \mathbf{W}_j^l \rangle = 2k_B T \zeta \epsilon \mathbf{I} \delta_{ij} \delta_{ml} \quad (9)$$

Eqs.(8) and (9) show that the mean and variance of the random numbers $W_{\alpha,i}^m$ ($\alpha \in x, y, z$) are zero and $2k_B T \zeta \epsilon$, respectively.

From Eq.(F8) and (7), we should notice that

$$\Delta \mathbf{W}_i = \mathbf{W}_i^1 + \mathbf{W}_i^2 + \dots + \mathbf{W}_i^n. \quad (10)$$

Therefore, from the central limit theorem Eqs.(D7)-(D9) introduced in Part 3 of Week 2, one realizes that the $\Delta W_{\alpha,i}$ should be drawn from a *Gaussian* distribution, with average and variance equal to zero and $2k_B T \zeta \Delta t$, respectively, regardless of the distribution of the $W_{\alpha,i}^m$.