1 Nov 2012

III Langevin equation

3.1. Brownian motion

- $$\dot{v} + \gamma v = \Gamma(t) \quad \rightarrow \text{white noise force} \tag{3.1}$$

$$\langle \Gamma(t) \rangle = 0, \quad \langle \Gamma(t)\,\Gamma(t') \rangle = q\,\delta(t-t') \tag{3.2}$$

(q → to be derived from statistics)

The spectral density of the random force $\Gamma(t)$ is

$$S(\omega) = 2\int_{-\infty}^{\infty} e^{-i\omega\tau} \langle \Gamma(\tau)\,\Gamma(0)\rangle\, d\tau = 2q \tag{3.3}$$

↳ white noise. If $S(\omega)$ depends on ω, it is called coloured.

- If $v(0) = v_0$, then from (3.1)

$$v(t) = v_0 e^{-\gamma t} + \int_0^t e^{-\gamma(t-t')}\,\Gamma(t')\,dt' \tag{3.7}$$

$$\langle v(t_1)\, v(t_2)\rangle = v_0 e^{-\gamma t_1} \cdot v_0 e^{-\gamma t_2} + \int_0^{t_1} dt_1' \int_0^{t_2} dt_2'\, e^{-\gamma(t_1 - t_1')}\, e^{-\gamma(t_2-t_2')} \times$$

$$\times \underbrace{\langle \Gamma(t_1')\,\Gamma(t_2')\rangle}_{q\,\delta(t_1'-t_2')} = v_0^2 e^{-\gamma(t_1+t_2)} + q \int_0^{\min(t_1,t_2)} dt_1'\, e^{-\gamma(t_1+t_2-2t_1')}$$

$$= v_0^2 e^{-\gamma(t_1+t_2)} + \frac{q}{2\gamma}\left(e^{-\gamma|t_1-t_2|} - e^{-\gamma(t_1+t_2)} \right) \tag{3.8}$$

where (3.2) was used.

If $\gamma t_1 \gg 1$ or $\gamma t_2 \gg 1$,

$$\langle v(t_1)\, v(t_2)\rangle \simeq \frac{q}{2\gamma}\, e^{-\gamma|t_1-t_2|} \tag{3.10}$$

does not depend on v_0. At long times $\langle v(t)^2\rangle = \frac{q}{2\gamma}$ and the average energy

$$\langle E\rangle = \frac{1}{2} m \left(\frac{q}{2\gamma}\right) = \frac{mq}{4\gamma} \tag{3.11}$$

As $\langle E\rangle = \frac{1}{2} kT \rightarrow$

$$q = \frac{2\gamma kT}{m}. \tag{3.13}$$

to satisfy correct statistics

Mean-squared displacements (MSD)

$x(t=0) = x_0$, $v(t=0) = v_0$, the MSD

$$\langle (x(t)-x_0)^2 \rangle = \left\langle \left(\int_0^t v(\tau)\, d\tau \right)^2 \right\rangle = \int_0^t d\tau_1 \int_0^t d\tau_2 \underbrace{\langle v(\tau_1) v(\tau_2) \rangle}_{\text{Eq. (3.9)}}$$

We have using (3.9):

$$\int_0^t d\tau_1 \int_0^t d\tau_2 \, e^{-\gamma(\tau_1+\tau_2)} = \left[\frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right]^2 = \left(\frac{1-e^{-\gamma t}}{\gamma} \right)^2,$$

$$\int_0^t d\tau_1 \int_0^t d\tau_2 \, e^{-\gamma|\tau_1-\tau_2|} = \int_0^t d\tau_1 \left[\int_0^{\tau_1} d\tau_2 \, e^{-\gamma(\tau_1-\tau_2)} + \int_{\tau_1}^t d\tau_2 \, e^{+\gamma(\tau_1-\tau_2)} \right]$$

$$= \int_0^t d\tau_1 \left\{ e^{-\gamma\tau_1} \frac{1}{\gamma}\left(e^{\gamma\tau_1}-1\right) + e^{\gamma\tau_1} \frac{1}{\gamma}\left(e^{-\gamma\tau_1} - e^{-\gamma t}\right) \right\}$$

$$= \frac{1}{\gamma} \int_0^t d\tau_1 \left\{ 1 - e^{-\gamma\tau_1} + 1 - e^{\gamma\tau_1} e^{-\gamma t} \right\}$$

$$= \frac{1}{\gamma} \left\{ 2t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) - e^{-\gamma t} \cdot \frac{1}{\gamma}\left(e^{\gamma t}-1\right) \right\}$$

$$= \frac{1}{\gamma} \left\{ 2t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right\}$$

$$= \frac{2}{\gamma} \left\{ t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right\} = \frac{2t}{\gamma} - \frac{2}{\gamma^2}\left(1-e^{-\gamma t}\right) \quad (3.16)$$

to give:

$$\langle (x(t)-x_0)^2 \rangle = v_0^2 \frac{1}{\gamma^2}\left(1-e^{-\gamma t}\right)^2 + \frac{q}{2\gamma} \frac{2}{\gamma} \left[t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right] - \frac{q}{2\gamma} \frac{1}{\gamma^2}\left(1-e^{-\gamma t}\right)^2$$

$$\langle (x(t)-x_0)^2 \rangle = \left(v_0^2 - \frac{q}{2\gamma} \right) \frac{1}{\gamma^2}\left(1-e^{-\gamma t}\right)^2 + \frac{q}{\gamma^2} \left[t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right] \quad (3.17)$$

If we are to start from an average velocity, then $v_0^2 = \frac{q}{2\gamma}$, and

$$\langle (x(t)-x_0)^2\rangle = \frac{qt}{\gamma^2} - \frac{q}{\gamma^3}\left(1-e^{-\gamma t}\right)$$

$$\xrightarrow{\text{at } \gamma t \gg 1} \frac{q}{\gamma^2}t = \frac{2\gamma kT}{m\gamma^2}t = \frac{2kT}{m\gamma}t \equiv 2Dt \quad (3.18)$$

with $D = \frac{q}{2\gamma^2} = \frac{kT}{m\gamma}$ being the diffusion coefficient. (3.19)

- At this long time limit we can directly obtain from (3.1):

$$\gamma v = \Gamma(t) \;\rightarrow\; v(t) \simeq \frac{1}{\gamma}\Gamma(t)$$

$$\langle v(t_1)\, v(t_2)\rangle \simeq \frac{1}{\gamma^2}\langle \Gamma(t_1)\,\Gamma(t_2)\rangle = \frac{q}{\gamma^2}\delta(t_1-t_2) \quad (3.20)$$

$$\langle (x(t)-x_0)^2\rangle = \int_0^t d\tau_1 \int_0^t d\tau_2 \,\frac{q}{\gamma^2}\delta(\tau_1-\tau_2) = \frac{q}{\gamma^2}\int_0^t d\tau_1 = \frac{qt}{\gamma^2},$$

i.e. the same result (3.18).

- In 3 dimensions

$$\dot v_i + \gamma v_i = \Gamma_i(t), \quad i = 1,2,3; \quad (3.21)$$

$$\langle \Gamma_i(t)\rangle = 0, \qquad \langle \Gamma_i(t)\,\Gamma_j(t')\rangle = q\,\delta_{ij}\,\delta(t-t') \quad (3.22)$$

At long times

$$\langle E\rangle = \frac{1}{2}m\sum_i \langle v_i^2(t)\rangle = \frac{1}{2}m\cdot 3\cdot\frac{q}{2\gamma} = \frac{3mq}{4\gamma} \equiv \frac{3}{2}kT \quad (3.23)$$

from which the same $q = 2\gamma kT/m$ as in (3.13) follows.

$$\langle (\vec x(t)-\vec x_0)^2\rangle = \sum_i \langle (x_i(t)-x_{i0})^2\rangle = 3\cdot\frac{q}{\gamma^2}t \equiv \frac{6kT}{m\gamma}t \quad (3.24)$$

Stationary velocity distribution function

One way of doing this is to calculate all the moments of $v(t)$, and then obtain $C(u)$ from (2.21), and $W(v)$ is then its FT (2.22).

For large times (see (3.7))

$$v(t) \simeq \int_0^\infty e^{-\gamma(t-t')}\,\Gamma(t')\,dt' = \left| t-t' = \tau \right|$$

$$= \int_t^\infty e^{-\gamma\tau}\,\Gamma(t-\tau)\,d\tau \simeq \int_0^\infty e^{-\gamma\tau}\,\Gamma(t-\tau)\,d\tau$$

To calculate the moments of $v(t)$, we need moments of $\Gamma(t)$:

$$\langle \Gamma(t_1)\dots\Gamma(t_n)\rangle = 0\,, \quad \text{if } n = \text{odd}$$

$$\langle \Gamma(t_1)\dots\Gamma(t_{2n})\rangle = q^n \sum_{\mathcal{S}} \delta(t_{i_1}-t_{i_2})\,\delta(t_{i_3}-t_{i_4})\dots\delta(t_{i_{n-1}}-t_{i_n}) \qquad (3.4)$$

$\mathcal{S}$ – all decompositions into pairs, $(2n)!/2^n n!$ of them.

Therefore,

$$\langle v(t)^{2n+1}\rangle = 0$$

$$\langle v(t)^{2n}\rangle = \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \dots \int_0^\infty d\tau_{2n}\; e^{-\gamma(\tau_1+\dots+\tau_{2n})} \langle \Gamma(t-\tau_1)\dots\Gamma(t-\tau_{2n})\rangle$$

$$= q^n \sum_{\mathcal{S}} \int_0^\infty d\tau_1 \dots e^{-\gamma(\tau_1+\dots)}\, \delta(\tau_{i_1}-\tau_{i_2})\dots\delta(\tau_{i_{n-1}}-\tau_{i_n})$$

~~Each integral gives the same contribution of~~ All integrals split into pairs, each pair giving the same contribution of

$$\int_0^\infty d\tau_1 \int_0^\infty d\tau_2\; e^{-\gamma(\tau_1+\tau_2)}\,\delta(\tau_1-\tau_2) = \int_0^\infty d\tau_1\, e^{-2\gamma\tau_1} = \frac{1}{2\gamma}(1) = \frac{1}{2\gamma}$$

$$\hookrightarrow \langle v(t)^{2n}\rangle = \frac{(2n)!}{2^n n!}\left(\frac{q}{2\gamma}\right)^n \equiv M_{2n} \qquad (3.28)$$

(n – # of pairs). The characteristic function

$$C(u) = 1 + \sum_{n=1}^\infty \frac{(iu)^n}{n!} \underbrace{M_n}_{\langle v(t)^n\rangle} = 1 + \sum_{j=1}^\infty \frac{(iu)^{2j}}{(2j)!} M_{2j}$$

$$= 1 + \sum_{j=1}^\infty \frac{(iu)^{2j}}{(2j)!}\,\frac{(2j)!}{2^j j!}\left(\frac{q}{2\gamma}\right)^j = 1 + \sum_{j=1}^\infty \frac{1}{j!}\left(\frac{(iu)^2}{2}\,\frac{q}{2\gamma}\right)^j =$$

$$= 1 + \sum_{j=1}^{\infty} \frac{1}{j!}\left(-\frac{q u^2}{4\gamma}\right)^j \equiv \exp\left[-\frac{q u^2}{4\gamma}\right] \qquad (3.29)$$

$$\int_{-\infty}^{\infty} e^{-px^2 - qx}\,dx = \sqrt{\frac{\pi}{p}}\, e^{q^2/4p}$$

and ~~the~~

$$W(v) = \frac{1}{2\pi}\int_{-\infty}^{\infty} C(u)\, e^{-iuv}\,du = \frac{1}{2\pi}\int \exp\left[-iuv - \frac{q}{4\gamma}u^2\right]du$$

$$= \sqrt{\frac{\gamma}{\pi q}}\exp\left(-\frac{\gamma v^2}{q}\right) \equiv \sqrt{\frac{m}{2\pi kT}}\exp\left(-\frac{mv^2}{2kT}\right) \qquad (3.30)$$

It is indeed the Maxwell distr. of $q = \frac{2kT\gamma}{m}$.

3.2. Ornstein – Uhlenbeck process

- It is a system of Langevin eqs:

$$\dot{\xi}_i + \sum_{j=1}^{N} \gamma_{ij}\, \xi_j = \Gamma_i(t), \qquad i = 1, \dots, N \qquad (3.31)$$

$$\langle \Gamma_i(t) \rangle = 0, \quad \langle \Gamma_i(t)\Gamma_j(t') \rangle = q_{ij}\,\delta(t-t'), \quad q_{ij} = q_{ji} \qquad (3.32)$$

- Wiener process: if $\gamma_{ij} = 0$:

$$\dot{\xi}_i = \Gamma_i(t)$$

- Solving (3.31)–(3.32) subject to initial conditions

$$\xi_i(0) = x_i \qquad (3.33)$$

In the matrix form:

$$\dot{\xi} + \gamma\xi = \Gamma(t)$$

Homogeneous eq. → solution $\quad \xi^h(t) = e^{-\gamma t} c \equiv G(t)\, c$, where c – constants (a vector), $G(t)$ – Green's f., satisfying $G_{ij}(0) = \delta_{ij}$.

Then

$$G(t) = e^{-\gamma t} = 1 - \gamma t + \frac{1}{2}\gamma^2 t^2 - \dots \qquad (3.37)$$

The particular solution: assume $c = c(t)$:

$$\xi(t) = G(t)\, c(t), \quad \dot{\xi} = \dot{G}c + G\dot{c} = -G\gamma c + G\dot{c}$$

$$\hookrightarrow (-\cancel{G\gamma c} + G\dot{c}) + \cancel{\gamma G c} = \Gamma \;\rightarrow\; G\dot{c} = \Gamma$$

But $\quad G^{-1} = e^{+\gamma t} \equiv G(-t) \qquad (3.40)$

$$\dot{C} = G(-t)\,\Gamma(t), \quad C(t) = \int_0^t G(-\tau)\,\Gamma(\tau)\,d\tau$$

~~const. vector~~

Final solution:

~~$\xi(t) = G(t)C + \int_0^t G(-\tau)\Gamma(\tau)d\tau$.~~

$$\xi(t) = G(t)\,C + G(t)\int_0^t G(-\tau)\,\Gamma(\tau)\,d\tau$$

$$= G(t)\,C + \int_0^t G(\underbrace{t-\tau}_{t'})\,\Gamma(\tau)\,d\tau = G(t)C + \int_0^t G(t')\,\Gamma(t-t')\,dt'$$

Initial: $\xi(0) = X = G(0)\,C = C \;\rightarrow$

$$\xi_i(t) = G_{ij}(t)\,X_j + \int_0^t G_{ij}(t')\,\Gamma_j(t-t')\,dt' \qquad (3.43)$$

where summation convention is applied.

- <u>Calculation of moments</u>

$$M_i(t) = \langle \xi_i(t) \rangle = G_{ij}(t)\,X_j \qquad (3.44)$$

$$\sigma_{ij}(t) = \langle (\xi_i - \langle \xi_i \rangle)(\xi_j - \langle \xi_j \rangle) \rangle$$

$$= \int_0^t dt_1 \int_0^t dt_2\, G_{ik}(t_1)\,G_{je}(t_2)\,\underbrace{\langle \Gamma_k(t-t_1)\,\Gamma_e(t-t_2)\rangle}_{q_{ke}\,\delta(t_1-t_2)}$$

$$= \int_0^t dt_1\, G_{ik}(t_1)\,G_{je}(t_1)\,q_{ke} \qquad (3.45)$$

$\sigma_{ij}(t)$ satisfies the equation:

$$\dot{\sigma}_{ij} = G_{ik}(t)\,G_{je}(t)\,q_{ke} \;\rightarrow\; \dot{\sigma} = G(t)\,q\,G(t) \quad (G = G^T) \qquad (*)$$

~~$\ddot{\sigma}_{ij} = \dot{G}_{ik}(t)\,G_{je}(t)\,q_{ke} + G_{ik}(t)\,\dot{G}_{je}(t)\,q_{ke}$~~

$$\ddot{\sigma} = \dot{G}qG + Gq\dot{G} = -\gamma G q G - G q G \gamma = -\gamma\dot{\sigma} - \dot{\sigma}\gamma$$

$$\ddot{\sigma}_{ij} = -\gamma_{ik}\,\dot{\sigma}_{kj} - \dot{\sigma}_{ik}\,\gamma_{kj} = -\gamma_{ik}\,\dot{\sigma}_{kj} - \gamma_{jk}\,\dot{\sigma}_{ki}$$

Integrating:

$$\dot{\sigma}_{ij}(t) - \underbrace{\dot{\sigma}_{ij}(0)}_{= q_{ij} \text{ from } (*)} = -\gamma_{ik}\,\sigma_{kj} - \gamma_{jk}\,\sigma_{ki} + \gamma_{ik}\underbrace{\sigma_{kj}(0)}_{0} + \gamma_{jk}\underbrace{\sigma_{ki}(0)}_{0}$$

from (3.[illegible]

↳ $$\dot{\sigma}_{ij} = -\gamma_{ik}\sigma_{kj} - \gamma_{jk}\sigma_{ki} + q_{ij} \qquad (3.46)$$

- If real parts of eigenvalues of γ are positive, $G(t) \to 0$ at $t \to \infty$.

For large times: from (3.45):

$$\sigma_{ij}(\infty) = \int_0^\infty G_{ik}(t)\, G_{je}(t)\, q_{ke}\, dt \qquad (3.47)$$

For small times $t \geq 0$:

$$M_i(t) = \langle \xi_i(t) \rangle = G_{ij}(t)\, x_j = \left(\delta_{ij} - \gamma_{ij} t + \frac{1}{2}\gamma_{ik}\gamma_{kj} t^2 - \ldots\right) x_j$$

$$= x_i - \gamma_{ij} x_j t + \frac{1}{2}\gamma_{ik}\gamma_{kj} x_j \cdot t^2 - \ldots \qquad (3.48)$$

$$\sigma_{ij}(t) = \int_0^t dt_1 \left[\delta_{ik} - \gamma_{ik} t_1 + \frac{1}{2}\gamma_{ik}\gamma_{kj} t_1^2 - \ldots\right]\left[\delta_{je} - \gamma_{je} t_1 + \frac{1}{2}\gamma_{jj'}\gamma_{j'e} t_1^2 - \ldots\right] q_{ke}$$

$$= q_{ij} t + \int_0^t dt_1 \left\{ -\gamma_{ik} q_{kj} t_1 - q_{ie}\gamma_{je} t_1 + O(t_1^2) \right\}$$

$$= q_{ij} t - \frac{1}{2}\left(\gamma_{ik} q_{kj} + \gamma_{jk} q_{ik}\right) t^2 + \ldots \qquad (3.49)$$

↳ q_{ij} determines the motion of the variance;
γ_{ij} — " — " — mean.

- <u>Wiener process</u>: $\sigma_{ij}(t) = q_{ij} t$ for $\forall t \geq 0$. (3.50)
- Higher order moments vanish for n = odd; for n = even they are proportional to $t^{n/2}$ for small times.

- <u>Correlation function</u>

$$K_{ij}(\tau, t) = \langle \xi_i(t+\tau)\, \xi_j(t) \rangle \qquad (3.53)$$

Write solution (3.43) for $x_j \to \xi_j(t)$ as the initial value:

$$\xi_i(t+\tau) = G_{ij}(\tau)\, \xi_j(t) + \int_t^{t+\tau} G_{ij}(t-t')\, \Gamma_j(t')\, dt', \quad \tau \geq 0 \qquad (3.54)$$

Here τ – propagation time),

Then,

$$K_{ij}(\tau,t) = G_{ik}(\tau)\,\langle \xi_k(t)\,\xi_j(t)\rangle + \int_t^{t+\tau} G_{ik}(t-t')\,\underbrace{\langle \Gamma_k(t')\,\xi_j(t)\rangle}_{\text{uncorrelated } t'\geq t}\,dt'$$

$$= G_{ik}(\tau)\,\langle \xi_k(t)\,\xi_j(t)\rangle = G_{ik}(\tau)\,K_{kj}(0,t) \qquad (3.55a)$$

This is a <u>regression theorem.</u>

For $\tau \leq 0$:

$$K_{ij}(\tau,t) = \langle \xi_i(t+\tau)\,\xi_j(t)\rangle = \langle \xi_i(t-|\tau|)\,\xi_j(t-|\tau|+|\tau|)\rangle$$

$$= \langle \xi_j(t-|\tau|+|\tau|)\,\xi_i(t-|\tau|)\rangle = K_{ji}(|\tau|, t-|\tau|)$$

or since

$$\xi_j(t-|\tau|+|\tau|) = G_{js}(|\tau|)\,\xi_s(t-|\tau|) + \int_{t-|\tau|}^{t} dt'\,G_{js}(t-|\tau|+t')\,\Gamma_s(t')\,dt',$$

then

$$K_{ij}(\tau,t) = G_{js}(|\tau|)\,\langle \xi_s(t-|\tau|)\,\xi_i(t-|\tau|)\rangle =$$

$$= G_{js}(|\tau|)\,K_{si}(0, t-|\tau|)$$

$$= G_{js}(|\tau|)\,K_{is}(0, t-|\tau|) \qquad (3.55b)$$

- <u>Correlation function of the stationary state</u>

If Re of γ_{ij} eigenvalues >0, then there exists a stationary state at $t\to\infty$. For $\tau\geq 0$:

$$K_{ij}(\tau,\infty) = K_{ij}(\tau) = G_{is}(\tau)\,\langle \xi_s(\infty)\,\xi_j(\infty)\rangle = G_{is}(\tau)\,\sigma_{sj}(\infty) \qquad (3.56a)$$

For $\tau\leq 0$:

$$K_{ij}(\tau,\infty) = K_{ij}(-|\tau|) = G_{js}(|\tau|)\,\sigma_{si}(\infty) \equiv K_{ji}(|\tau|) \qquad (3.56b)$$

$$\hookrightarrow \quad K_{ij}(\tau) = K_{ji}(-\tau) \qquad (3.57)$$

This is valid for any stationary process:

$$K_{ij}(\tau,t) = \text{does not depend on } t = \langle \xi_i(t+\tau)\,\xi_j(t)\rangle \xrightarrow{t\to t-\tau}$$

$$\to \langle \xi_i(t-\tau+\tau)\,\xi_j(t-\tau)\rangle = \langle \xi_j(t-\tau)\,\xi_i(t)\rangle \equiv K_{ji}(-\tau).$$

Solution by FT (Rice's method)

$$\tilde{\xi}_i(\omega) = \int e^{-i\omega t}\, \xi_i(t)\, dt \qquad (3.58)$$

$$\tilde{\Gamma}_i(\omega) = \int e^{-i\omega t}\, \Gamma_i(t)\, dt$$

Then:

$$\xi_i(t) = \int \tilde{\xi}_i(\omega)\, e^{i\omega t}\, d\omega \left(\frac{1}{2\pi}\right)$$

$$\dot{\xi}_i(t) = \int \tilde{\xi}_i(\omega)\, i\omega\, e^{i\omega t}\, d\omega \left(\frac{1}{2\pi}\right)$$

↳ eqs. (3.31) transform into:

$$i\omega\, \tilde{\xi}_i(\omega) + \gamma_{ij}\, \tilde{\xi}_j(\omega) = \tilde{\Gamma}_i(\omega)$$

$$(\delta_{ij}\, i\omega + \gamma_{ij})\, \tilde{\xi}_j(\omega) = \tilde{\Gamma}_i(\omega) \rightarrow \tilde{\xi}(\omega) = (i\omega \mathbb{1} + \gamma)^{-1}\, \tilde{\Gamma}(\omega) \qquad (3.59)$$

Spectral density matrices are introduced via:

$$\langle \tilde{\xi}_j(\omega)\, \tilde{\xi}_k^*(\omega') \rangle = \pi\, S_{jk}^{(\xi)}(\omega)\, \delta(\omega - \omega') \qquad (3.60)$$

$$\langle \tilde{\Gamma}_j(\omega)\, \tilde{\Gamma}_k^*(\omega') \rangle = \pi\, S_{jk}^{(\Gamma)}(\omega)\, \delta(\omega - \omega')$$

~~Note: in the book π is used instead of 1/π~~

Here

$$\langle \tilde{\Gamma}_j(\omega)\, \tilde{\Gamma}_k^*(\omega') \rangle = \int dt\, dt'\, e^{-i\omega t} e^{i\omega' t'} \underbrace{\langle \Gamma_j(t)\, \Gamma_k(t') \rangle}_{q_{jk}\, \delta(t-t')}$$

$$= q_{ik} \underbrace{\int dt\, e^{-i(\omega - \omega')t}}_{2\pi\, \delta(\omega - \omega')} = q_{ik}\, \delta(\omega - \omega')\, 2\pi,$$

which means that

$$S_{jk}^{(\Gamma)}(\omega) = 2 q_{jk} \qquad (3.62)$$

Using (3.59), we get:

$$\langle \tilde{\xi}_j(\omega)\, \tilde{\xi}_k^*(\omega') \rangle = (i\omega \mathbb{1} + \gamma)^{-1}_{jj'}\, \langle \tilde{\Gamma}_{j'}(\omega)\, \tilde{\Gamma}^*_{k'}(\omega') \rangle\, (-i\omega \mathbb{1} + \gamma)^{-1}_{kk'}$$

$$= 2\pi\, \delta(\omega - \omega')\, q_{j'k'}\, (\gamma + i\omega \mathbb{1})^{-1}_{jj'}\, (\gamma - i\omega \mathbb{1})^{-1}_{kk'},$$

$$\hookrightarrow\quad S_{jk}^{(\xi)}(\omega) = 2\, (\gamma + i\omega \mathbb{1})^{-1}_{jj'}\, q_{j'k'}\, (\gamma - i\omega \mathbb{1})^{-1}_{kk'} \qquad (3.63)$$

3.3. Non-linear Langevin Equation, One variable

$$\dot{\xi} = h(\xi,t) + g(\xi,t)\,\Gamma(t) \qquad (3.67)$$

$$\langle \Gamma(t)\rangle = 0, \qquad \langle \Gamma(t)\Gamma(t')\rangle = 2\delta(t-t') \qquad (3.68)$$

If h, g do not depend on time, one can divide by $g(\xi)$:

$$\frac{\dot{\xi}}{g(\xi)} = \frac{h(\xi)}{g(\xi)} + \Gamma(t) \Rightarrow \quad \eta = \eta(\xi): \quad \dot{\eta} = \frac{\dot{\xi}}{g(\xi)} \to \eta = \int^{\xi} \frac{d\xi'}{g(\xi')}$$

$$\hookrightarrow \quad \dot{\eta} = f(\eta) + \Gamma(t) \qquad (3.69)$$

For t-dependent h and g there are difficulties.

- Example

$$\dot{\xi} = a\xi\Gamma(t), \quad \xi(0) = x \qquad (3.72)$$

$$\frac{\dot{\xi}}{\xi} = a\Gamma(t) \rightarrow \quad \xi(t) = x\exp\left(a\int_0^t \Gamma(t')\,dt'\right) \qquad (3.73)$$

The following derivation implies a general colour noise

$$\langle \Gamma(t)\Gamma(t')\rangle = \Phi(t-t')$$

Then,

$$\langle \xi(t)\rangle = x\left\langle \exp\left[a\int_0^t \Gamma(t')dt'\right]\right\rangle =$$

$$= x\left\{ 1 + a\int_0^t \langle \Gamma(t')\rangle dt' + \frac{a^2}{2!}\int_0^t dt_1 \int_0^t dt_2 \langle \Gamma(t_1)\Gamma(t_2)\rangle + \dots \right.$$

$$\left. + \frac{a^{2n}}{(2n)!}\int_0^t dt_1 \dots \int_0^t dt_{2n} \langle \Gamma(t_1)\dots\Gamma(t_{2n})\rangle + \dots \right\}$$

$\Gamma(t)$ is Gaussian:

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

$$\langle \Gamma(t_1)\dots\Gamma(t_{2n+1})\rangle = 0$$

$$\langle \Gamma(t_1)\dots\Gamma(t_{2n})\rangle = \underbrace{\sum_{S}}_{\text{over distinct pairs}} \Phi(t_{i_1}-t_{i_2})\dots\Phi(t_{i_{2n-1}}-t_{i_{2n}})$$

$(2n)!/2^n n!$

$$\hookrightarrow \langle \xi(t) \rangle = x\left\{1 + \frac{a^2}{2!}\int_0^t dt_1 \int_0^t dt_2\, \Phi(t_1-t_2) + \dots + \frac{a^{2n}}{2n!}\left(\int_0^t dt_1\int_0^t dt_2\, \Phi(t_1-t_2)\right)^n + \dots\right.$$

$$= x \sum_{n=0}^{\infty} \frac{a^{2n}}{(2n)!}\frac{(2n)!}{2^n n!}\left(\int dt_1 \int dt_2\, \Phi\right)^n$$

$$= x \exp\left[\frac{a^2}{2}\int_0^t dt_1 \int_0^t dt_2\, \Phi(t_1-t_2)\right] \qquad (3.75)$$

If $\Phi = 2\delta(t-t')$, then

$$\int_0^t dt_1 \int_0^t dt_2\, 2\delta(t_1-t_2) = 2\int_0^t dt_1 = 2t$$

$$\hookrightarrow \langle \xi(t) \rangle = x \exp(a^2 t) \qquad (3.76)$$

- Average of $\langle \xi(t)^n \rangle$ can also be calculated:

$$\langle [\xi(t)]^n \rangle = x^n \left\langle \exp\left(an \int_0^t \Gamma(t')dt'\right)\right\rangle$$

$$= x^n \sum_{k=0}^{\infty} \frac{(an)^{2k}}{(2k)!}\left[\int dt_1 \int dt_2\, \Phi(t_1-t_2)\right]^k = x^n \exp\left[\frac{(an)^2}{2}\int_0^t dt_1 \int_0^t dt_2\, \Phi(t_1-t_2)\right]$$

and for the δ-correlated noise

$$\langle [\xi(t)]^n \rangle = x^n \exp[(an)^2 t] \qquad (3.78)$$

- <u>n-th centred moment</u> (δ-correlated noise)

$$\tilde{M}_n(t) = \langle [\xi(t) - x]^n \rangle = x^n \left\langle \left[\exp\left(a\int_0^t \Gamma(t')dt'\right) - 1\right]^n \right\rangle$$

$$= x^n \sum_{\nu=0}^{n} \binom{n}{\nu} \underbrace{\exp\left((a\nu)^2 t\right)}_{\text{here we used (3.78)}} (-1)^{n-\nu}$$

$$= x^n \sum_{\nu=0}^{n} \binom{n}{\nu}(-1)^{n-\nu} \sum_{m=0}^{\infty} \frac{(a^2 t)^m}{m!} \nu^{2m}$$

$$= x^n \sum_{m=0}^{\infty} \frac{(a^2 t)^m}{m!} \sum_{\nu=0}^{n} \binom{n}{\nu} \nu^{2m} (-1)^{n-\nu}$$

The $m=0$ term vanished:

$$\sum_{\nu=0}^{n}\binom{n}{\nu}(-1)^{n-\nu} = \sum_{\nu=0}^{n}\binom{n}{\nu}1^{\nu}(-1)^{n-\nu} = (1-1)^n = 0$$

$$\hookrightarrow \tilde{M}_n(t) = x^n \sum_{m=1}^{\infty}\frac{(a^2t)^m}{m!}\underbrace{\left[\sum_{\nu=0}^{n}\binom{n}{\nu}\nu^{2m}(-1)^{n-\nu}\right]}_{S_{nm}} \qquad (3.80)$$

Here

$$S_{nm} = \left(\frac{d}{dy}\right)^{2m}(e^y-1)^n\Big|_{y=0} = \left(\frac{d}{dy}\right)^{2m}\sum_{\nu=0}^{n}\binom{n}{\nu}e^{\nu y}(-1)^{n-\nu}\Big|_{y=0}$$

$$= \sum_{\nu=0}^{n}\binom{n}{\nu}\nu^{2m}e^{\nu y}(-1)^{n-\nu}\Big|_{y=0} \equiv \sum_{\nu=0}^{n}\binom{n}{\nu}\nu^{2m}(-1)^{n-\nu}, \text{ i.e. correct.}$$

Therefore,

$$S_{nm} = \left(\frac{d}{dy}\right)^{2m}(e^y-1)^n\Big|_{y=0} = \left(\frac{d}{dy}\right)^{2m}\underbrace{\left(y+\frac{y^2}{2!}+\frac{y^3}{3!}+\dots\right)^n}_{y^n + \dots y^{n+1}+\dots}\Big|_{y=0}$$

~~If $2m<n$, then (because of $y=0$ in the end), $S_{nm}=0$, i.e. $S_{n,m}=0$.~~ We are interested in the small t behaviour, i.e. smallest possible t^m term in (3.80). We need to find for the given n the smallest possible non-zero m. Two cases:

(a) <u>$n \Rightarrow$ even</u>

$$\tilde{M}_{2n}(t) = x^{2n}\sum_{m=1}^{\infty}\frac{(a^2t)^m}{m!}S_{2n,m},$$

$$S_{2n,m} = \left(\frac{d}{dy}\right)^{2m}\left(y+\frac{y^2}{2}+\dots\right)^{2n}\Big|_{y=0} = \left(\frac{d}{dy}\right)^{2m}y^{2n}\left[1+\frac{y}{2}+\dots\right]^{2n}\Big|_{y=0}$$

For small y:

$$1+\frac{y}{2}+\dots \simeq e^{y/2} \to \left(1+\frac{y}{2}+\dots\right)^{2n} \simeq \left(e^{y/2}\right)^{2n} = e^{ny}$$

$$= 1 + yn + \frac{1}{2}y^2n^2 + \dots$$

so that

$$S_{2n,m} = \left\{\left(\frac{d}{dy}\right)^{2m}\left[y^{2n} + n y^{2n+1} + \dots\right]\right\}_{y=0}$$

If $m<n$, then $S_{2n,m}=0$. The smallest m is n:

$$S_{2n,n} = \left(\frac{d}{dy}\right)^{2n}\left[y^{2n}+\dots\right]\Big|_{y=0} = (2n)!$$

(B) <u>n = odd</u>

$$\tilde{M}_{2n-1}(t) = x^{2n-1}\sum_{m=1}^{\infty}\frac{(a^2t)^m}{m!} S_{2n-1,m}$$

$$S_{2n-1,m} = \left(\frac{d}{dy}\right)^{2m}\left(y+\frac{y^2}{2}+\dots\right)^{2n-1}\Big|_{y=0} \simeq \left(\frac{d}{dy}\right)^{2m} y^{2n-1} e^{\frac{y}{2}(2n-1)}$$

$$= \left(\frac{d}{dy}\right)^{2m} y^{2n-1} e^{(n-\frac{1}{2})y} = \left(\frac{d}{dy}\right)^{2m} y^{2n-1}\left[1+\left(n-\frac{1}{2}\right)y+\dots\right]\Big|_{y=0}$$

If $2m < 2n-1$, or $m < n - 1/2$ or $m \lesssim n$, then $S_{2n-1,m}=0$.
The smallest value of m is the next one: $m=n$. Then:

$$S_{2n-1,n} \simeq \left\{\left(\frac{d}{dy}\right)^{2n} y^{2n-1}\left[1+\left(n-\frac{1}{2}\right)y+\dots\right]\right\}_{y=0}$$

$$= \left(\frac{d}{dy}\right)^{2n}\left[y^{2n-1}+\left(n-\frac{1}{2}\right)y^{2n}+O(y^{2n+1})\right]_{y=0} = \left(n-\frac{1}{2}\right)(2n)!$$

Therefore,

$$S_{2n,n} = (2n)! \quad ; \quad S_{2n-1,n} = \left(n-\frac{1}{2}\right)(2n)! \tag{3.82}$$

Therefore,

$$\tilde{M}_{2n}(t) = x^{2n}\frac{(a^2t)^n}{n!}(2n)! + \dots = x^{2n}\frac{(2n)!}{n!}(a^2t)^n + \dots$$

$$\tilde{M}_{2n-1}(t) = x^{2n-1}\underbrace{\left(n-\frac{1}{2}\right)}_{\frac{2n-1}{2}}\frac{(2n)!}{n!}(a^2t)^n + \dots \tag{3.83}$$

• We define Kramers–Moyal coefficients $D^{(n)}(x)$ as:

$$D^{(n)}(x) = \frac{1}{n!} \frac{d}{dt} \tilde{M}_n(t) \Big|_{t=0}$$

Then:

$$D^{(1)}(x) = \frac{d}{dt} \tilde{M}_1(t) \Big|_{t=0} = x \cdot \left(1 - \frac{1}{2}\right) \frac{2}{1} (a^2 t)' = a^2 x$$

$$D^{(2)}(x) = \frac{1}{2} \frac{d}{dt} \tilde{M}_2(t) \Big|_{t=0} = \frac{1}{2} x^2 \frac{2}{1} (a^2 t)' = a^2 x^2$$

$$D^{(3)}(x) = \frac{1}{3!} \frac{d}{dt} \tilde{M}_3(t) \Big|_{t=0} = \frac{1}{3!} x^3 \frac{3}{2} \cdot \frac{4!}{2!} \left[(a^2 t)^2 \right]'_{t=0} = 0$$

$$D^{(4)}(x) \sim \left[\tilde{M}_4(t)' \right]_{t=0}, \quad \tilde{M}_4(t) \sim t^2 \text{ and } (\tilde{M}_4)'_{t=0} = 0$$

$$D^{(n)}(x) = 0 \quad \text{for } \forall n \geq 3. \tag{3.84}$$

• Kramers–Moyal expansion coefficients

$$D^{(n)}(x,t) = \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \left\langle [\xi(t+\tau) - \xi(t)]^n \right\rangle \Big|_{\xi(t)=x} \tag{3.85}$$

$\xi(t+\tau)$ is a solution of (3.67) with $\xi(t) = x$ exactly. From (3.67):

$$\xi(t+\tau) = \underbrace{\xi(t)}_{x} + \int_t^{t+\tau} [h(\xi(t'),t') + g(\xi(t'),t')\Gamma(t')]\,dt'$$

or

$$\xi(t+\tau) - x = \int_t^{t+\tau} [h(\xi(t'),t') + g(\xi(t'),t')\Gamma(t')]\,dt' \tag{3.86}$$

We expand h and g functions around $\xi(t) = x$:

$$\begin{aligned} h(\xi(t'),t') &= h(x,t') + h'(x,t')(\xi(t') - x) + \ldots \\ g(\xi(t'),t') &= g(x,t') + g'(x,t')(\xi(t') - x) + \ldots \end{aligned} \tag{3.87}$$

giving:

$$\xi(t+\tau)-x = \int_t^{t+\tau} h(x,t')\,dt' + \int_t^{t+\tau} h'(x,t')\,(\xi(t')-x)\,dt' + \dots$$

$$+ \int_t^{t+\tau} g(x,t')\,\Gamma(t')\,dt' + \int_t^{t+\tau} g'(x,t')\,(\xi(t')-x)\,\Gamma(t')\,dt' + \dots \qquad (3.88)$$

Similarly we can write $\xi(t')-x$ since $t'>t$:

$$\xi(t')-x = \int_t^{t'} h(x,t'')\,dt'' + \int_t^{t'} h'(x,t'')\,(\xi(t'')-x)\,dt'' + \dots$$

$$+ \int_t^{t'} g(x,t'')\,\Gamma(t'')\,dt'' + \int_t^{t'} g'(x,t'')\,(\xi(t'')-x)\,\Gamma(t'')\,dt'' + \dots$$

Substitute this into (3.88):

$$\xi(t+\tau)-x = \int_t^{t+\tau} h(x,t')\,dt' + \int_t^{t+\tau} dt'\, h'(x,t') \int_t^{t'} h(x,t'')\,dt'' +$$

$$+ \int_t^{t+\tau} dt'\, h'(x,t') \int_t^{t'} dt''\, g(x,t'')\,\Gamma(t'')\,dt'' +$$

$$+ \int_t^{t+\tau} dt'\, h'(x,t') \int_t^{t'} dt''\, h'(x,t'')\,(\xi(t'')-x)\,dt'' + \dots$$

$$+ \int_t^{t+\tau} dt'\, g(x,t')\,\Gamma(t') + \int_t^{t+\tau} dt'\, g'(x,t')\,\Gamma(t') \int_t^{t'} dt''\, h(x,t'')\,dt''$$

$$+ \int_t^{t+\tau} dt'\, g'(x,t')\,\Gamma(t') \int_t^{t'} dt''\, h'(x,t'')\,(\xi(t'')-x)$$

$$+ \int_t^{t+\tau} dt'\, g'(x,t')\,\Gamma(t') \int_t^{t'} dt''\, g(x,t'')\,\Gamma(t'')$$

$$+ \int_t^{t+\tau} dt'\, g'(x,t')\,\Gamma(t') \int_t^{t'} dt''\, g'(x,t'')\,(\xi(t'')-x)\,\Gamma(t'') + \dots$$

~~Taking average now, recalling that~~ Substitute this repeatly.

$$\xi(t+\tau)-x = \int_t^{t+\tau} h(x,t')dt' + \int_t^{t+\tau} dt' \int_t^{t'} dt'' \Big[h'(x,t')h(x,t'')$$

$$+ h'(x,t')\, g(x,t'')\Gamma(t'') + g'(x,t')\, h(x,t'')\Gamma(t') +$$

$$+ g'(x,t')\, g(x,t'')\, \Gamma(t')\,\Gamma(t'') + \dots \Big] + \int_t^{t+\tau} dt'\, g(x,t')\,\Gamma(t') + \dots$$

Taking average:

$$\langle \xi(t+\tau)-x \rangle = \int_t^{t+\tau} dt'\, h(x,t') + \int_t^{t+\tau} dt' \int_t^{t'} dt''\, h'(x,t')h(x,t'')$$

$$+ \dots + \int_t^{t+\tau} dt' \int_t^{t'} dt''\, g'(x,t')\, g(x,t'')\, \underbrace{\langle \Gamma(t')\,\Gamma(t'') \rangle}_{2\delta(t'-t'')} + \dots$$

$$= \int_t^{t+\tau} dt'\, h(x,t') + \int_t^{t+\tau} dt' \int_t^{t'} dt''\, h'(x,t')\, h(x,t'') + \int_t^{t+\tau} dt'\, g'(x,t')\, g(x,t') + \dots$$

since $\int_t^{t'} dt''\, \delta(t'-t'')\, g(x,t'') = \frac{1}{2} g(x,t')$.

We are interested in the terms of $O(\tau)$ for (3.85) as $\tau \to 0$ limit will be taken:

$$\int_t^{t+\tau} dt'\, h(x,t') \simeq h(x,t)\,\tau + O(\tau^2) \; ;$$

$$\int_t^{t+\tau} dt' \int_t^{t'} dt''\, h'(x,t')\, h(x,t'') \simeq \int_t^{t+\tau} dt'\, h'(x,t')\, h(x,t')(t'-t)$$

$$\simeq h'(x,t)\, h(x,t) \int_t^{t+\tau} dt'\,(t'-t) = O(\tau^2) \; ;$$

$$\int_t^{t+\tau} dt'\, g'(x,t')\, g(x,t') \simeq g'(x,t)\, g(x,t)\,\tau + O(\tau^2)$$

Therefore, all other terms are at least of $O(\tau^2)$ and can be omitted.

We obtain:

$$D^{(1)}(x,t) = \lim_{\tau\to 0} \frac{1}{\tau} \langle \xi(t+\tau) - x \rangle \Big|_{\xi(t)=x}$$

$$\boxed{D^{(1)} = h(x,t) + g'(x,t)\, g(x,t)} \qquad (3.93)$$

- Now consider $D^{(2)}(x,t) = \frac{1}{2} \lim_{\tau\to 0} \frac{1}{\tau} \langle (\xi(t+\tau) - x)^2 \rangle$.

We can only consider the lowest terms in $\xi(t+\tau)-x$:

$$\xi(t+\tau) - x = \int_t^{t+\tau} h(x,t')\,dt' + \int_t^{t+\tau} g(x,t')\,\Gamma(t')\,dt' + \begin{pmatrix}\text{double integrals} \\ \text{+ triple, etc.}\end{pmatrix}$$

~~$+ \int_t^{t+\tau} dt' \int_t^{t'} dt''\, g'(x,t')$~~ Now square and take average:

$$\langle (\xi(t+\tau)-x)^2 \rangle = \left(\int_t^{t+\tau} dt'\, h(x,t') \right)^2 + \int h(x,t')\,dt' \int g(x,t'') \underbrace{\langle \Gamma(t'') \rangle}_{=0} dt''$$

$$+ \int_t^{t+\tau} dt' \int_t^{t+\tau} dt''\, g(x,t')\, g(x,t'') \underbrace{\langle \Gamma(t')\,\Gamma(t'') \rangle}_{2\delta(t'-t'')} + \begin{pmatrix}\text{other terms} \\ \text{which } O(\tau^2)\end{pmatrix}$$

Only the term with the δ-function contributes in the $\tau \to 0$ limit:

$$\frac{1}{\tau} \langle (\xi(t+\tau)-x)^2 \rangle = 2 \int_t^{t+\tau} dt'\, g(x,t')\, g(x,t') + O(\tau^2)$$

and hence

$$\boxed{D^{(2)}(x,t) = g(x,t)\, g(x,t) = g^2(x,t)} \qquad (3.94)$$

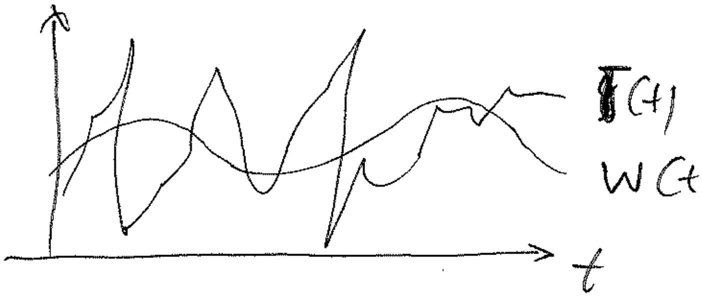
- It is clear that $\boxed{D^{(n)}(x,t) = 0 \text{ for } n \geq 3.}$

~~Another method~~

~~Let us do it in a simpler way:~~

~~$\xi(t+\tau) - \xi(t) =$~~

Itô's + Stratanovich definitions



$$W(t) = \int_0^t \Gamma(t')dt'$$

$\Gamma(t)$ – changes irratically; it is diff. to create such a process with no correlations at all between neighbouring times.

$W(t)$ – behaves better.
↳ $dW = \Gamma(t)dt$

Then: (3.86) takes the form:

$$\xi(t+\tau) = \underbrace{x}_{\xi(t)} + \int_t^{t+\tau} h(\xi, t')dt' + \int_t^{t+\tau} \underbrace{g(\xi, t')\, dW(t')}_{\text{Stieltjes integral}} \qquad (3.97)$$

Here $W(t)$ is a Wiener process.

$$w(\tau) = W(t+\tau) - W(t) = \int_t^{t+\tau} \Gamma(t')dt' \qquad (3.98)$$

Indeed,

$$w(0) = 0$$

$$\langle w(\tau)\rangle = \int_t^{t+\tau} \langle \Gamma(t')\rangle dt' = 0$$

$$\langle w(\tau_2)\, w(\tau_1)\rangle = \int_t^{t+\tau_2} dt' \int_t^{t+\tau_1} dt'' \underbrace{\langle \Gamma(t')\Gamma(t'')\rangle}_{2\delta(t'-t'')}$$

$$= \int_t^{t+\min(\tau_1,\tau_2)} dt'\, 2 = 2\min(\tau_1,\tau_2) = \begin{cases} 2\tau_1, & \text{if } \tau_1 \le \tau_2 \\ 2\tau_2, & \text{if } \tau_1 \ge \tau_2 \end{cases} \qquad (3.99)$$

Hence, $W(\tau)$ is a well defined process which exists at $\varepsilon \to 0$, i.e. it does not require dealing with δ-functions.

We iterate:

$$\xi(t+\tau) = x + \int_t^{t+\tau} h(\xi', t')dt' + \int_t^{t+\tau} g(\xi', t')dW(t') = \left| \begin{matrix} t' = t+\tau' \\ dt' = d\tau' \end{matrix} \right|$$

$$= x + \int_0^\tau h(\xi', t+\tau')d\tau' + \int_0^\tau g(\xi', t+\tau')dW(\tau')$$

$$= x + h(\xi(t+\theta_1\tau), t+\theta_1\tau)\tau + \int_0^\tau g(\xi(t+\tau'), t+\tau')dW(\tau') \quad (*)$$

where $\theta_1 \in (0,1)$. At the 1st iteration ξ is replaced with x:

$$\xi^{(1)}(t+\tau) = x + h(x, t+\theta_1\tau)\tau + g(x, t+\theta_1\tau)W(\tau) = x + \Delta\xi_1 \quad (*')$$

Next, we replace ξ in (*) by (*'):

$$\xi^{(2)}(t+\tau) = x + h(x+\Delta\xi_1, t+\theta_1\tau)\tau + \int_0^\tau g(x+\Delta\xi_1, t+\tau')dW(\tau')$$

$$= x + h(x, t+\theta_1\tau)\tau + h'(x, t+\theta_1\tau)\tau\Delta\xi_1 + \underbrace{\int_0^\tau g(x, t+\tau')dW(\tau')}_{g(x, t+\theta_1\tau)W(\tau)}$$

$$+ \int_0^\tau g'(x, t+\tau')\Delta\xi_1 dW(\tau') + \ldots$$

$$= x + h(x, t+\theta_1\tau)\tau + h'(x, t+\theta_1\tau)\left[h(x, t+\theta_1\tau)\tau^2 + \tau g(x, t+\theta_1\tau)W(\tau) + \ldots\right] + g(x, t+\theta_1\tau)W(\tau) + \int_0^\tau g'(x, t+\tau')\left[h(x, t+\theta_1\tau')\tau'\right.$$

$$\left. + g(x, t+\theta_1\tau')W(\tau') + \ldots\right]dW(\tau')$$

When we take $\langle \ldots \rangle$, linear terms in W disappear:

$$\left\langle \xi^{(2)}(t+\tau) - x \right\rangle = h(x, t+\theta_1\tau)\tau + O(\tau^2)$$

$$+ \underbrace{\int_0^\tau g'(x, t+\tau')g(x, t+\theta_1\tau')W(\tau')dW(\tau')}_{g'(x, t+\theta_2\tau)g(x, t+\theta_1\theta_2\tau)\left\langle \int_0^\tau W(\tau')dW(\tau') \right\rangle}$$

$$\hookrightarrow \frac{1}{\tau}\left\langle \xi^{(2)}(t+\tau) - x \right\rangle_{\tau\to 0} = h(x,t) + g'(x,t)g(x,t)\lim_{\tau\to 0}\frac{1}{\tau}\left\langle \int_0^\tau W(\tau')dW(\tau') \right\rangle$$

To calculate $\mathcal{D}^{(2)}$, we need $\langle (\xi(t+\tau)-x)^2 \rangle$. For this the 1st approximation suffices:

$$\frac{1}{\tau}\langle(\xi(t+\tau)-x)^2\rangle = \frac{1}{\tau}\langle \left[h(x,t')^2\tau^2 + 2h(x,t')\tau\, g(x,t')\, W(\tau) + \right.$$

$$\left. + g(x,t+\theta_1\tau)\, g(x,t+\theta_1\tau)\, W(\tau)^2 \right]\rangle \to g^2(x,t)\frac{1}{\tau}\langle W(\tau)^2\rangle =$$

$$= g^2(x,t)\, 2\tau$$

for either (I) or (S), and hence

$$\mathcal{D}^{(2)}(x,t) = \frac{1}{2!}\lim_{\tau\to 0}\frac{1}{\tau}\langle(\xi(t+\tau)-x)^2\rangle = g^2(x,t) \qquad (3.108)$$

3.4. Several variables

$$\dot{\xi}_i = h_i(\{\xi_j\},t) + g_{ij}(\{\xi_k\},t)\,\Gamma_j(t) \qquad (3.110)$$

$$\langle\Gamma_i(t)\rangle = 0, \qquad \langle\Gamma_i(t)\Gamma_j(t')\rangle = 2\,\delta_{ij}\,\delta(t-t') \qquad (3.111)$$

Drift coefficients:

$$\mathcal{D}_i(\{x\},t) = \lim_{\tau\to 0}\frac{1}{\tau}\langle \xi_i(t+\tau)-x_i\rangle\Big|_{\xi_k(t)=x_k} \qquad (3.112)$$

Diffusion coefficients:

$$\mathcal{D}_{ij}(\{x\},t) = \frac{1}{2}\lim_{\tau\to 0}\frac{1}{\tau}\langle(\xi_i(t+\tau)-x_i)(\xi_j(t+\tau)-x_j)\rangle_{\xi_k(t)=x_k} \qquad (3.113)$$

We can write:

$$\xi_i(t+\tau)-x_i = \int_t^{t+\tau} h_i(\{\xi(t')\},t')\,dt' + \int_t^{t+\tau} g_{ij}(\{\xi(t')\},t')\,\Gamma_j(t')\,dt' \qquad (3.114)$$

$$\begin{cases} h_i(\{\xi(t')\},t') = h_i(\{\xi(t)\},t') + \left[\dfrac{\partial h_i(\{\xi(t)\},t')}{\partial x_k}\right]\cdot(\xi_k(t')-x_k)+\dots \\ g_{ij}(\{\xi(t')\},t') = g_{ij}(\{\xi(t)\},t') + \left[\dfrac{\partial}{\partial x_k} g_{ij}(\{\xi(t)\},t')\right](\xi_k(t')-x_k)+\dots \end{cases} \qquad (3.115)$$

We obtain:

$$\xi_i(t+\tau)-x_i = \Big[h_i(\{x\}, t+\theta_i\tau)\,\tau + \int_t^{t+\tau} dt' \frac{\partial h_i}{\partial x_k}\Big[\int_t^{t'} h_k\, dt'' + \int_t^{t'} g_{kk'}\Gamma_{k'}\, dt''\Big] + \dots\Big] + \Big[\int_t^{t+\tau} dt'\, g_{ij}\Gamma_j +$$

$$+ \int_t^{t+\tau} dt' \frac{\partial g_{ij}}{\partial x_k}\Big[\int_t^{t'} h_i\, dt'' + \int_t^{t'} g_{kk'}\Gamma_{k'}\, dt''\Big]\Gamma_j(t') + \dots\Big]$$

After taking averaging:

$$\langle \xi_i(t+\tau)-x_i\rangle = h_i\tau + \int_t^{t+\tau} dt' \int_t^{t'} dt'' \frac{\partial g_{ij}(t')}{\partial x_k} g_{kk'}(t'') \underbrace{\langle \Gamma_j(t')\Gamma_{k'}(t'')\rangle}_{2\delta_{jk'}\delta(t'-t'')}$$

$$+ O(\tau^2) = h_i\tau + \int_t^{t+\tau} dt' \frac{\partial g_{ij}(t')}{\partial x_k}\int_t^{t'} g_{kj}(t'')\, 2\delta(t'-t'')\, dt'' + O(\tau^2)$$

Here,

$$\int_t^{t'} \delta(t'-t'')\, dt'' = \frac{1}{2} \quad \text{(one of the limits is in the } \delta\text{-function)}$$

$$\hookrightarrow \int_t^{t'} g_{kj}(t'')\, 2\delta(t'-t'')\, dt'' = g_{kj}(t')$$

Then

$$\int_t^{t+\tau} dt' \frac{\partial g_{ij}(t')}{\partial x_k} g_{kj}(t') = \frac{\partial g_{ij}(t+\theta_1\tau)}{\partial x_k} g_{kj}(t+\theta_1\tau)\,\tau$$

and in the $\tau\to 0$ limit we obtain

$$D_i^{(1)}(x,t) = \lim_{\tau\to 0}\frac{1}{\tau}\langle \xi_i(t+\tau)-x_i\rangle = h_i(\{x\},t) + \frac{\partial g_{ij}(x,t)}{\partial x_k} g_{kj}(x,t) \qquad (3.118)$$

The diffusion coefficient [we use directly (3.114)]:

$$\langle(\xi_i(t+\tau)-x_i)(\xi_j(t+\tau)-x_j)\rangle = h_i h_j \tau^2 + h_i g_{jk}\tau\langle\Gamma_k\rangle + h_j g_{ik}\tau\langle\Gamma_k\rangle$$

$$+ g_{ik} g_{jk'} \int_t^{t+\tau} dt' \int_t^{t+\tau} dt'' \underbrace{\langle \Gamma_k(t') \Gamma_{k'}(t'') \rangle}_{2\delta_{kk'}\delta(t'-t'')}$$

$$= O(\tau^2) + g_{ik} g_{jk} \int_t^{t+\tau} dt' \, 2 = 2 g_{ik} g_{jk} \tau$$

and

$$D^{(2)}_{ij} = \frac{1}{2} \lim_{\tau \to 0} \langle (\xi_i - x)(\xi_j - x) \rangle = g_{ik}(x,t)\, g_{jk}(x,t) \qquad (3.119)$$