4.7. General Discretized Langevin Equation

In the Langevin eq. on a Euclidean manifold [see eq(4.1)],

$$\dot{\boldsymbol{q}} = -\frac{1}{2}\boldsymbol{f} + \boldsymbol{v}(t)$$

only v_i affects $\dot{q}_i$.

In a Riemannian manifold, every v_a may affect $\dot{q}^j$ so that $\boldsymbol{v}$ enters the eq. in the form $e^i_a v_a$, where $\boldsymbol{e}$ is the coupling tensor.

Note that we use i, j, k ... to denote indices of tensors on the Riemannian manifold, which discriminates contra- & co-variant components.

Indices of tensors with no such discrimination are denoted by a, b, c ....

From §4.3, we have [see eq(4.20)]

$$\int_t^{t+\varepsilon} d\tau\, v_a(\tau) = \sqrt{\varepsilon}\, \overline{v}_a(t)$$

$$\langle \overline{v}_a(t) \rangle = 0 \qquad\qquad \langle \overline{v}_a(t)\, \overline{v}_b(t') \rangle = \Omega\, \delta_{ab}\, \delta_{tt'}$$

Define

$$w_a(t) = \sqrt{\varepsilon}\, \overline{v}_a(t)$$

$$\rightarrow \qquad \langle w_a(t) \rangle = 0 \qquad\qquad \langle w_a(t)\, w_b(t') \rangle = \varepsilon\, \Omega\, \delta_{ab}\, \delta_{tt'}$$

(4.53a)

Hence, each $w_a(t)$ is of order $\sqrt{\varepsilon}$ so that to $O(\varepsilon)$ in the discretized Langevin eq., we need only consider terms up to quadratic in w_a.

The discretized Langevin equation is therefore

$$q^j(t+\varepsilon) = q^j(t) - \frac{1}{2}\varepsilon f^i[\boldsymbol{q}(t)] + e^i_a[\boldsymbol{q}(t)]\, w_a(t) + \frac{1}{2} d^i_{ab}[\boldsymbol{q}(t)]\, w_a(t)\, w_b(t) + O\left(\varepsilon^{3/2}\right)$$

(4.52a)

where $\boldsymbol{e}$ & $\boldsymbol{d}$ are tensors of coupling constants.

Note that we can always assume $d_{ab} = d_{ba}$. For if $d_{ab} \neq d_{ba}$, we can replace d_{ab} with $\frac{1}{2}(d_{ab} + d_{ba})$ without changing eq(4.52a).

Since we do not deal with the generalized Langevin eq. directly, we can, following Zinn-Justin, rename w_a as v_a so that

$$\langle v_a(t) \rangle = 0 \qquad\qquad \langle v_a(t)\, v_b(t') \rangle = \varepsilon\, \Omega\, \delta_{ab}\, \delta_{tt'}$$

(4.53)

$$q^j(t+\varepsilon) = q^j(t) - \frac{1}{2}\varepsilon f^i[\boldsymbol{q}(t)] + e^i_a[\boldsymbol{q}(t)]\, v_a(t) + \frac{1}{2} d^i_{ab}[\boldsymbol{q}(t)]\, v_a(t)\, v_b(t) + O\left(\varepsilon^{3/2}\right) \qquad (4.52)$$

Using eq(4.52), we can derive an equation for the probability distribution [see eq(4.4)]

$$P(\boldsymbol{q}, t+\varepsilon\,; \boldsymbol{q}', t) \equiv \langle \delta[\, \boldsymbol{q}(t+\varepsilon) - \boldsymbol{q}\,] \rangle_v$$

As in §4.3, we first calculate the Fourier transform $\tilde{P}$ of P [see derivation of eq(4.21)]

$$\tilde{P}(\boldsymbol{p}, t+\varepsilon\,; \boldsymbol{q}', t) = \int d\boldsymbol{q}\, e^{-i\boldsymbol{p}\cdot\boldsymbol{q}} \langle \delta[\, \boldsymbol{q}(t+\varepsilon) - \boldsymbol{q}\,] \rangle_v$$

$$= \left\langle e^{-i\boldsymbol{p}\cdot\boldsymbol{q}(t+\varepsilon)} \right\rangle_v \qquad\qquad [\, \boldsymbol{q}(t) = \boldsymbol{q}'\,]$$

$$= e^{-i\boldsymbol{p}\cdot\left[\boldsymbol{q}' - \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}')\right]} \left\langle \exp\left[-i p_i \left\{ e^i_a(\boldsymbol{q}')\, v_a(t) + \frac{1}{2} d^i_{ab}(\boldsymbol{q}')\, v_a(t)\, v_b(t) \right\} \right] \right\rangle_v$$

$$= e^{-i\,\boldsymbol{p}\cdot\left[\boldsymbol{q}' - \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}')\right]} \left(\frac{1}{2\pi\Omega\varepsilon}\right)^{d/2} \int_{-\infty}^{\infty} d^d\, \nu(t)$$

$$\times \exp\left[-\frac{1}{2\Omega\varepsilon} \nu_a(t)\,\nu_a(t) - i\,p_i \left\{ e_a^i(\boldsymbol{q}')\ \nu_a(t) + \frac{1}{2} d_{ab}^i(\boldsymbol{q}')\ \nu_a(t)\,\nu_b(t) \right\}\right]$$

where the gaussian distribution

$$\left(\frac{1}{2\pi\Omega\varepsilon}\right)^{d/2} \exp\left[-\frac{1}{2\Omega\varepsilon} \nu_a(t)\,\nu_a(t)\right]$$

was chosen to satisfy eq(4.53).

The gaussian integral can be evaluated using [see eq(1.8)]

$$\int d^n x \exp\left(-\frac{1}{2}\boldsymbol{x}^T \boldsymbol{A}\,\boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x}\right) = \frac{(2\pi)^{n/2}}{\sqrt{\det \boldsymbol{A}}} \exp\left(\frac{1}{2}\boldsymbol{b}^T \boldsymbol{A}^{-1}\boldsymbol{b}\right) \qquad (\ \boldsymbol{A} = \boldsymbol{A}^T\ )$$

by setting

$$A_{ab} = \frac{1}{\Omega\varepsilon}\delta_{ab} + \frac{i}{2} p_i\, d_{ab}^i \qquad\qquad b_a = i\,p_i\, e_a^i$$

To satisfy $\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{1}$ to $O(\varepsilon)$, we have

$$A_{ab}^{-1} = \Omega\,\varepsilon\,\delta_{ab} - \frac{i}{2}\varepsilon^2\,\Omega^2\, p_i\, d_{ab}^i$$

so that

$$A_{ab}^{-1} A_{bc} = \left(\Omega\,\varepsilon\,\delta_{ab} - \frac{i}{2}\varepsilon^2\,\Omega^2\, p_i\, d_{ab}^i\right)\left(\frac{1}{\Omega\varepsilon}\delta_{bc} + \frac{i}{2} p_i\, d_{bc}^i\right)$$

$$= \delta_{ac} + O(\varepsilon^2)$$

$$\to \qquad \frac{1}{2}\boldsymbol{b}^T \boldsymbol{A}^{-1}\boldsymbol{b} = -\frac{1}{2}\Omega\,\varepsilon\, p_i\, e_a^i\, p_j\, e_a^j + O(\varepsilon^2)$$

To lowest order of ε,

$$\frac{1}{\det \boldsymbol{A}} = \det \boldsymbol{A}^{-1} \approx \prod_{a=1}^{d} A_{aa}^{-1} \qquad (\text{ no summation over } a \text{ })$$

$$= (\Omega\,\varepsilon)^d \left(1 - \frac{i}{2}\varepsilon\,\Omega\, p_i\, d_{aa}^i\right) \qquad (\text{ implicit summation over repeated } a \text{ })$$

$$\approx (\Omega\,\varepsilon)^d \exp\left(-\frac{i}{2}\varepsilon\,\Omega\, p_i\, d_{aa}^i\right)$$

Putting everything together, we have

$$\tilde{P}(\boldsymbol{p},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) = \exp\left[-i\,p_i\left(q'^{\,i} - \frac{1}{2}\varepsilon\, f^i(\boldsymbol{q}')\right) - \frac{i}{2}\varepsilon\,\Omega\, p_i\, d_{aa}^i(\boldsymbol{q}') - \frac{1}{2}\Omega\,\varepsilon\, p_i\, e_a^i(\boldsymbol{q}')\, p_j\, e_a^j(\boldsymbol{q}')\right] \qquad (4.54)$$

Let

$$g^{ij}(\boldsymbol{q}) = e_a^i(\boldsymbol{q})\, e_a^j(\boldsymbol{q}) = g^{ji}(\boldsymbol{q}) \qquad (4.55a)$$

$$g_{ij}\, g^{jk} = \delta_i^k$$

$$g = \det g_{ij} = \frac{1}{\det g^{ij}} \qquad (4.55b)$$

&

$$h^i(\boldsymbol{q}) = f^i(\boldsymbol{q}) - \Omega\, d^i_{a\,a}(\boldsymbol{q}) \tag{4.56}$$

then eq(4.54) becomes

$$\tilde{P}(\boldsymbol{p},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) = \exp\left\{ -i\, p_i \left[q'^{\,i} - \frac{1}{2}\,\varepsilon\, h^i(\boldsymbol{q}') \right] - \frac{1}{2}\,\Omega\,\varepsilon\, p_i\, p_j\, g^{i\,j}(\boldsymbol{q}') \right\} \tag{4.56a}$$

$$\begin{aligned} P(\boldsymbol{q},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) &= \int_{-\infty}^{\infty} \frac{d^d p}{(2\,\pi)^d}\, e^{i\,\boldsymbol{p}\cdot\boldsymbol{q}}\, \tilde{P}(\boldsymbol{p},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) \\ &= \int_{-\infty}^{\infty} \frac{d^d p}{(2\,\pi)^d} \exp\left[i\, p_i \left(q^i - q'^{\,i} + \frac{1}{2}\,\varepsilon\, h^i(\boldsymbol{q}') \right) - \frac{1}{2}\,\Omega\,\varepsilon\, p_i\, p_j\, g^{i\,j}(\boldsymbol{q}') \right] \end{aligned}$$

Once again, using eq(1.8) with

$$A_{i\,j} = \Omega\,\varepsilon\, g^{i\,j}(\boldsymbol{q}') \qquad\qquad b_i = i\left(q^i - q'^{\,i} + \frac{1}{2}\,\varepsilon\, h^i(\boldsymbol{q}') \right)$$

$$\to \qquad A^{-1}_{i\,j} = \frac{1}{\Omega\,\varepsilon}\, g_{i\,j}(\boldsymbol{q}') \qquad \text{where} \qquad g_{i\,j}\, g^{j\,k} = \delta_i^k$$

$$\det \boldsymbol{A} = \frac{(\Omega\,\varepsilon)^d}{g(\boldsymbol{q}')}$$

$$\frac{1}{2}\,\boldsymbol{b}^T\, \boldsymbol{A}^{-1}\, \boldsymbol{b} = -\frac{1}{2\,\Omega\,\varepsilon}\, d^{\,i}\, g_{i\,j}(\boldsymbol{q}')\, d^j$$

where

$$\boldsymbol{d} = \boldsymbol{q} - \boldsymbol{q}' + \frac{1}{2}\,\varepsilon\, \boldsymbol{h}(\boldsymbol{q}') \tag{4.58}$$

we have

$$P(\boldsymbol{q},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) = \frac{\sqrt{g(\boldsymbol{q}')}}{(2\,\pi\,\Omega\,\varepsilon)^{d/2}} \exp\left[-\frac{1}{2\,\Omega\,\varepsilon}\, g_{i\,j}(\boldsymbol{q}')\, d^{\,i}\, d^j \right] \tag{4.57}$$

which is a generalization of eq(4.24) with $g_{i\,j}$ playing the role of a metric tensor.

As in eq(4.21a) of §4.3, we expand eq(4.56a) to $O(\varepsilon)$ so that

$$\begin{aligned} \tilde{P}(\boldsymbol{p},\, t+\varepsilon\,;\, \boldsymbol{q}',\, t) &= e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'} \left\{ 1 + \frac{1}{2}\, i\,\varepsilon\, p_i\, h^i(\boldsymbol{q}') - \frac{1}{2}\,\Omega\,\varepsilon\, p_i\, p_j\, g^{i\,j}(\boldsymbol{q}') \right\} + O\left(\varepsilon^2\right) \\ &= e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'} - \varepsilon\, H(\boldsymbol{p},\, \boldsymbol{q}') + O\left(\varepsilon^2\right) \end{aligned}$$

$$\to \qquad H(\boldsymbol{p},\, \boldsymbol{q}') = \frac{1}{2}\, e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'} \left\{ -i\, p_i\, h^i(\boldsymbol{q}') + \Omega\, p_i\, p_j\, g^{i\,j}(\boldsymbol{q}') \right\} \tag{4.59}$$

$$\begin{aligned} H(\boldsymbol{q},\, \boldsymbol{q}') &= \frac{1}{2} \int \frac{d\,\boldsymbol{p}}{(2\,\pi)^d}\, e^{i\,\boldsymbol{p}\cdot(\boldsymbol{q}-\boldsymbol{q}')} \left\{ -i\, p_i\, h^i(\boldsymbol{q}') + \Omega\, p_i\, p_j\, g^{i\,j}(\boldsymbol{q}') \right\} \\ &= \frac{1}{2} \left\{ -h^i(\boldsymbol{q}')\,\partial_i - \Omega\, g^{i\,j}(\boldsymbol{q}')\,\partial_i \partial_j \right\} \int \frac{d\,\boldsymbol{p}}{(2\,\pi)^d}\, e^{i\,\boldsymbol{p}\cdot(\boldsymbol{q}-\boldsymbol{q}')} \\ &= \frac{1}{2} \left\{ -h^i(\boldsymbol{q}')\,\partial_i - \Omega\, g^{i\,j}(\boldsymbol{q}')\,\partial_i \partial_j \right\} \langle\, \boldsymbol{q} \mid \boldsymbol{q}' \,\rangle \\ &= \left\langle \boldsymbol{q} \;\middle|\; \frac{1}{2} \left\{ -i\, \hat{p}_i\, h^i(\hat{\boldsymbol{q}}) + \Omega\, \hat{p}_i\, \hat{p}_j\, g^{i\,j}(\hat{\boldsymbol{q}}) \right\} \;\middle|\; \boldsymbol{q}' \right\rangle \end{aligned}$$

$$\begin{aligned} \to \qquad H &= \frac{1}{2} \left\{ -i\, \hat{p}_i\, h^i(\hat{\boldsymbol{q}}) + \Omega\, \hat{p}_i\, \hat{p}_j\, g^{i\,j}\, (\hat{\boldsymbol{q}}) \right\} \\ &= \frac{1}{2}\, \hat{p}_i \left\{ \Omega\, \hat{p}_j\, g^{i\,j}(\hat{\boldsymbol{q}}) - i\, h^i(\hat{\boldsymbol{q}}) \right\} \end{aligned} \tag{4.60}$$

The corresponding FP eq is [see eq(4.23)]

$$
\begin{aligned}
\frac{\partial}{\partial t} P(\boldsymbol{q}, t) &= -H P(\boldsymbol{q}, t) \\
&= \frac{1}{2} i \partial_i \left\{ -i \Omega \partial_j g^{ij} - i h^i \right\} P \\
&= \frac{1}{2} \partial_i \left[\Omega \partial_j \left(g^{ij} P \right) + i h^i P \right]
\end{aligned}
\tag{4.61}
$$

Since d^i_{ab} always appears via [see eq(4.56)] $h^i = f^i - \Omega d^i_{aa}$, it can be absolved into f^i so that without loss of generality, we can re-write eq(4.52) as

$$
q^j(t+\varepsilon) = q^j(t) - \frac{1}{2} \varepsilon f^i[\boldsymbol{q}(t)] + e^i_a[\boldsymbol{q}(t)] \nu_a(t) \tag{4.62}
$$