4.3. The Fokker–Planck Equation

Eqs(4.1-2) imply a differential equation for $P(\boldsymbol{q}, t)$.

One way to avoid the problems associated with $\left\langle \dot{q}(t)\, q(t) \right\rangle$ [see §4.2] is to deal with $q(t)$ exclusively using $\dot{q}(t) \approx [\, q(t+\varepsilon) - q(t)\,] \,/\, \varepsilon$.

Thus, we integrate the Langevin eq(4.1) over the interval $[\, t,\ t+\varepsilon\,]$ to get

$$q_i(t+\varepsilon) - q_i(t) = \int_t^{t+\varepsilon} d\,\tau \left(-\frac{1}{2} f_i[\boldsymbol{q}(\tau)] + \nu_i(\tau) \right)$$

$$\int_t^{t+\varepsilon} d\,\tau\, f_i[\boldsymbol{q}(\tau)] \approx \int_t^{t+\varepsilon} d\,\tau \left\{ f_i[\boldsymbol{q}(t)] + (\tau - t)\, \dot{\boldsymbol{q}}(t) \cdot \nabla_{\boldsymbol{q}} f_i[\boldsymbol{q}(t)] + \ldots \right\}$$

Using

$$\int_t^{t+\varepsilon} d\,\tau\, (\tau - t) = \frac{1}{2} \left[(t+\varepsilon)^2 - t^2 \right] - \varepsilon\, t \ = \frac{1}{2} \varepsilon^2$$

we have

$$\int_t^{t+\varepsilon} d\,\tau\, f_i[\boldsymbol{q}(\tau)] \approx \varepsilon\, f_i[\boldsymbol{q}(t)] + \frac{1}{2} \varepsilon^2\, \dot{\boldsymbol{q}}(t) \cdot \nabla_{\boldsymbol{q}} f_i[\boldsymbol{q}(t)] + \ldots$$

$$\rightarrow \qquad q_i(t+\varepsilon) - q_i(t) = -\frac{1}{2} \varepsilon\, f_i[\boldsymbol{q}(t)] + \int_t^{t+\varepsilon} d\,\tau\, \nu_i(\tau) + O\left(\varepsilon^2\right) \tag{4.18}$$

From eq(4.4), we have

$$P(\boldsymbol{q},\, t+\varepsilon\,;\ \boldsymbol{q}',\, t) = \left\langle \prod_{i=1}^{d} \delta[\, q_i(t+\varepsilon) - q_i\,] \right\rangle_\nu \qquad \text{with} \qquad \boldsymbol{q}' = \boldsymbol{q}(t)$$

$$\equiv \langle\, \delta[\, \boldsymbol{q}(t+\varepsilon) - \boldsymbol{q}\,] \,\rangle_\nu$$

$$\approx \left\langle \prod_{i=1}^{d} \delta\left[-\frac{1}{2} \varepsilon\, f_i[\boldsymbol{q}(t)] + \int_t^{t+\varepsilon} d\,\tau\, \nu_i(\tau) \right] \right\rangle_\nu$$

Discretized Langevin Equation

Since [see eq(4.11)]

$$\langle\, |\ q_i(t+\varepsilon) - q_i(t)\ |\, \rangle = O\left(\varepsilon^{1/2}\right)$$

eq(4.18) implies

$$\left\langle \left| \int_t^{t+\varepsilon} d\,\tau\ \nu_i(\tau) \right| \right\rangle = O\left(\varepsilon^{1/2}\right)$$

Hence, we define the noise $\overline{\boldsymbol{\nu}}(t)$ by

$$\int_t^{t+\varepsilon} d\,\tau\ \nu_i(\tau) = \sqrt{\varepsilon}\ \overline{\nu}_i(t) \tag{4.20}$$

so that eq(4.18) becomes

$$q_i(t+\varepsilon) - q_i(t) = -\frac{1}{2} \varepsilon\, f_i[\boldsymbol{q}(t)] + \sqrt{\varepsilon}\ \overline{\nu}_i(t) \tag{4.19}$$

Since $\overline{\boldsymbol{\nu}}(t)$ is linearly related to $\boldsymbol{\nu}(t)$, it also has a gaussian distribution characterized by [c.f. eq(4.3)]

$$\langle \bar{v}_i(t) \rangle = \frac{1}{\sqrt{\varepsilon}} \int_t^{t+\varepsilon} d\tau \langle v_i(\tau) \rangle = 0$$

$$\langle \bar{v}_i(t)\, \bar{v}_j(t') \rangle = \frac{1}{\varepsilon} \int_t^{t+\varepsilon} d\tau \int_{t'}^{t'+\varepsilon} d\tau' \langle v_i(\tau)\, v_j(\tau') \rangle$$

$$= \frac{\Omega}{\varepsilon} \int_t^{t+\varepsilon} d\tau \int_{t'}^{t'+\varepsilon} d\tau'\, \delta_{ij}\, \delta(\tau - \tau') \qquad \text{[eq(4.3) used]}$$

Note that $\delta(\tau - \tau') \neq 0$ only in the interval where the domains of the two integrals overlap, i.e., where

$$[a, b] = [t, t+\varepsilon] \cap [t', t'+\varepsilon] \neq \Phi \qquad \Phi = \text{empty set}$$

With

$$[a, b] = \begin{cases} [t, t'+\varepsilon] & \text{if } 0 \le t - t' \le \varepsilon \\ [t', t+\varepsilon] & \text{if } 0 \le t' - t \le \varepsilon \\ \text{null} & \text{otherwise} \end{cases}$$

we have

$$\langle \bar{v}_i(t)\, \bar{v}_j(t') \rangle = \delta_{ij} \frac{\Omega}{\varepsilon} \int_a^b d\tau \int_a^b d\tau'\; \delta(\tau - \tau')$$

$$= \begin{cases} \delta_{ij} \dfrac{\Omega}{\varepsilon} (b - a) & \text{if } |\, t - t' \,| \le \varepsilon \\ 0 & \text{otherwise} \end{cases}$$

If we discretize the time interval so that $\dfrac{t - t'}{\varepsilon} = n \in \mathbb{Z}$, then $b - a \neq 0$ if and only if $t = t'$. In which case, $b - a = \varepsilon$ so that

$$\langle \bar{v}_i(t)\, \bar{v}_j(t') \rangle = \Omega\, \delta_{ij}\, \delta_{t t'}$$

Fokker–Planck Equation

The Fourier transform $\tilde{P}$ of P with repect to $\boldsymbol{q}$ is

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

Using eq(4.4), we have

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

$$= \left\langle e^{-i\boldsymbol{p}\cdot\boldsymbol{q}(t+\varepsilon)} \right\rangle_v$$

$$= \left\langle \exp\left\{ -i\boldsymbol{p}\cdot \left[\boldsymbol{q}(t) - \frac{1}{2}\varepsilon \boldsymbol{f}[\boldsymbol{q}(t)] + \sqrt{\varepsilon}\, \bar{\boldsymbol{v}}(t) \right] \right\} \right\rangle_v \qquad \text{[Eq(4.19) used]}$$

$$= \exp\left\{ -i\boldsymbol{p}\cdot \left[\boldsymbol{q}' - \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}') \right] \right\} \left\langle \exp\left[-i\sqrt{\varepsilon}\, \boldsymbol{p}\cdot \bar{\boldsymbol{v}}(t) \right] \right\rangle_v$$

$$= \exp\left\{ -i\boldsymbol{p}\cdot \left[\boldsymbol{q}' - \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}') \right] \right\} \left\langle \exp\left[-i\boldsymbol{p}\cdot \int_t^{t+\varepsilon} d\tau\; \boldsymbol{v}(\tau) \right] \right\rangle_v \qquad \text{[Eq(4.20) used]}$$

Following the procedure used in the derivation of eq(4.14), we have

$$\left\langle \exp\left[-i\boldsymbol{p}\cdot \int_t^{t+\varepsilon} d\tau\; \boldsymbol{v}(\tau) \right] \right\rangle_v = \int [d\boldsymbol{v}(s)]\, \exp\left[-i\boldsymbol{p}\cdot \int_t^{t+\varepsilon} d\tau\; \boldsymbol{v}(\tau) - \frac{1}{2\Omega} \int_{-\infty}^{\infty} ds\; \boldsymbol{v}(s)^2 \right]$$

$$= \int [d\,\boldsymbol{\nu}(\tau)]\ \exp\left(-\int_t^{t+\varepsilon} d\,\tau\left[\,i\,\boldsymbol{p}\cdot\boldsymbol{\nu}(\tau) + \frac{1}{2\,\Omega}\,\boldsymbol{\nu}(\tau)^2\right]\right)$$
$$= \left(\frac{\varepsilon}{2\,\pi\,\Omega}\right)^{d/2} \int_{-\infty}^{\infty} d^d\,\nu\ \exp\left(-\varepsilon\left[\,i\,\boldsymbol{p}\cdot\boldsymbol{\nu} + \frac{1}{2\,\Omega}\,\boldsymbol{\nu}^2\right]\right)$$
$$= \left(\frac{\varepsilon}{2\,\pi\,\Omega}\right)^{d/2} \int_{-\infty}^{\infty} d^d\,\nu\ \exp\left[-\frac{\varepsilon}{2\,\Omega}\left(2\,i\,\Omega\,\boldsymbol{p}\cdot\boldsymbol{\nu} + \boldsymbol{\nu}^2\right)\right]$$
$$= \exp\left(-\frac{\varepsilon\,\Omega}{2}\,\boldsymbol{p}^2\right)$$

$$\rightarrow \qquad \tilde{P}(\boldsymbol{p}, t+\varepsilon\,;\ \boldsymbol{q}', t) = \exp\left[-\frac{\varepsilon\,\Omega}{2}\,\boldsymbol{p}^2 + \frac{1}{2}\,i\,\varepsilon\,\boldsymbol{p}\cdot\boldsymbol{f}(\boldsymbol{q}') - i\,\boldsymbol{p}\cdot\boldsymbol{q}'\right]$$
$$= e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'}\left\{1 - \frac{\varepsilon}{2}\left[\Omega\,\boldsymbol{p}^2 - i\,\boldsymbol{p}\cdot\boldsymbol{f}(\boldsymbol{q}')\right] + O\left(\varepsilon^2\right)\right\} \qquad (4.21)$$

From eqs(4.7-8), we have

$$P(\boldsymbol{q}, t+\varepsilon\,;\ \boldsymbol{q}', t) = \left\langle \boldsymbol{q}\ \middle|\ e^{-\varepsilon H}\ \middle|\ \boldsymbol{q}'\right\rangle$$
$$= \left\langle \boldsymbol{q}\ \middle|\ \left(1 - \varepsilon\,H + O\left(\varepsilon^2\right)\right)\ \middle|\ \boldsymbol{q}'\right\rangle$$
$$= \delta(\boldsymbol{q}-\boldsymbol{q}') - \varepsilon\,H(\boldsymbol{q}, \boldsymbol{q}') + O\left(\varepsilon^2\right)$$

where we’ve used

$$\langle\,\boldsymbol{q}\mid\boldsymbol{q}'\,\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}') \qquad\qquad H(\boldsymbol{q}, \boldsymbol{q}') = \langle\,\boldsymbol{q}\mid H\mid\boldsymbol{q}'\,\rangle$$

Hence,

$$\tilde{P}(\boldsymbol{p}, t+\varepsilon\,;\ \boldsymbol{q}', t) = \int d\,\boldsymbol{q}\,e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}}\,P(\boldsymbol{q}, t+\varepsilon\,;\ \boldsymbol{q}', t)$$
$$= \int d\,\boldsymbol{q}\,e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}}\left[\,\delta(\boldsymbol{q}-\boldsymbol{q}') - \varepsilon\,H(\boldsymbol{q}, \boldsymbol{q}') + O\left(\varepsilon^2\right)\right]$$
$$= e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'} - \varepsilon\int d\,\boldsymbol{q}\,e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}}\,H(\boldsymbol{q}, \boldsymbol{q}') + O\left(\varepsilon^2\right) \qquad (4.21a)$$

Comparing eqs(4.21 & 21a), we have

$$\frac{1}{2}\,e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}'}\left[\,\Omega\,\boldsymbol{p}^2 - i\,\boldsymbol{p}\cdot\boldsymbol{f}(\boldsymbol{q}')\right] = \int d\,\boldsymbol{q}\,e^{-i\,\boldsymbol{p}\cdot\boldsymbol{q}}\,H(\boldsymbol{q}, \boldsymbol{q}')$$
$$= H(\boldsymbol{p}, \boldsymbol{q}')$$

$$\therefore \qquad H(\boldsymbol{q}, \boldsymbol{q}') = \int \frac{d\,\boldsymbol{p}}{(2\,\pi)^d}\,e^{i\,\boldsymbol{p}\cdot\boldsymbol{q}}\,H(\boldsymbol{p}, \boldsymbol{q}')$$
$$= \frac{1}{2}\int \frac{d\,\boldsymbol{p}}{(2\,\pi)^d}\,e^{i\,\boldsymbol{p}\cdot(\boldsymbol{q}-\boldsymbol{q}')}\left[\,\Omega\,\boldsymbol{p}^2 - i\,\boldsymbol{p}\cdot\boldsymbol{f}(\boldsymbol{q}')\right]$$
$$= \frac{1}{2}\left[-\Omega\,\nabla_{\boldsymbol{q}}^2 - \boldsymbol{f}(\boldsymbol{q}')\cdot\nabla_{\boldsymbol{q}}\right]\int \frac{d\,\boldsymbol{p}}{(2\,\pi)^d}\,e^{i\,\boldsymbol{p}\cdot(\boldsymbol{q}-\boldsymbol{q}')}$$
$$= \frac{1}{2}\left[-\Omega\,\nabla_{\boldsymbol{q}}^2 - \boldsymbol{f}(\boldsymbol{q}')\cdot\nabla_{\boldsymbol{q}}\right]\delta(\boldsymbol{q}-\boldsymbol{q}')$$
$$= \frac{1}{2}\left[-\Omega\,\nabla_{\boldsymbol{q}}^2 - \boldsymbol{f}(\boldsymbol{q}')\cdot\nabla_{\boldsymbol{q}}\right]\langle\,\boldsymbol{q}\mid\boldsymbol{q}'\,\rangle$$

(4.21b)

The quantum momentum operator in the $\boldsymbol{q}$-representation is defined by

$$\left\langle \boldsymbol{q} \mid \hat{\boldsymbol{p}} \mid \psi \right\rangle = \frac{\hbar}{i} \nabla_{\boldsymbol{q}} \langle \boldsymbol{q} \mid \psi \rangle = \frac{\hbar}{i} \nabla_{\boldsymbol{q}} \psi(\boldsymbol{q})$$

Eq(4.21b) thus becomes

$$H(\boldsymbol{q}, \boldsymbol{q}') = \left\langle \boldsymbol{q} \,\middle|\, \frac{1}{2}\left[\Omega\, \hat{\boldsymbol{p}}^2 - i\, \hat{\boldsymbol{p}} \cdot \boldsymbol{f}(\hat{\boldsymbol{q}})\right] \middle|\, \boldsymbol{q}' \right\rangle$$

$$= \langle \boldsymbol{q} \mid H \mid \boldsymbol{q}' \rangle$$

$$\rightarrow \qquad H = \frac{1}{2}\left[\Omega\, \hat{\boldsymbol{p}}^2 - i\, \hat{\boldsymbol{p}} \cdot \boldsymbol{f}(\hat{\boldsymbol{q}})\right]$$

$$= \frac{1}{2} \hat{\boldsymbol{p}} \cdot \left[\Omega\, \hat{\boldsymbol{p}} - i\, \boldsymbol{f}(\hat{\boldsymbol{q}})\right] \tag{4.22}$$

From eq(4.8), we have

$$\dot{P}(t) = \lim_{\varepsilon \to 0} \frac{P(\boldsymbol{q}, t + \varepsilon;\, \boldsymbol{q}', t) - P(\boldsymbol{q}, t;\, \boldsymbol{q}', t)}{\varepsilon} \tag{4.22b}$$

$$= \lim_{\varepsilon \to 0} \frac{\left\langle \boldsymbol{q} \,\middle|\, e^{-\varepsilon H} - 1 \,\middle|\, \boldsymbol{q}' \right\rangle}{\varepsilon}$$

$$= -\langle \boldsymbol{q} \mid H \mid \boldsymbol{q}' \rangle$$

$$= -\hat{H}(\boldsymbol{q}) \langle \boldsymbol{q} \mid \boldsymbol{q}' \rangle$$

where $\hat{H}(\boldsymbol{q})$ is the $\boldsymbol{q}$-representation of the H operator, e.g.,

$$\hat{H}(\boldsymbol{q}) = \frac{1}{2}\left[-\Omega\, \nabla_{\boldsymbol{q}}^2 - \nabla_{\boldsymbol{q}} \cdot \boldsymbol{f}(\boldsymbol{q})\right]$$

Reminder: Operator relations are meaningful only when applied to a function:

$$\hat{H}(\boldsymbol{q})\, \psi = \frac{1}{2}\left[-\Omega\, \nabla_{\boldsymbol{q}}^2 \psi - \nabla_{\boldsymbol{q}} \cdot (\boldsymbol{f}\, \psi)\right]$$

Since

$$P(t) = P(\boldsymbol{q}, t;\, \boldsymbol{q}', t) = \langle \boldsymbol{q} \mid \boldsymbol{q}' \rangle$$

we have

$$\dot{P}(t) = -\hat{H}\, P(t)$$

(4.23a)

More explicitly,

$$\dot{P}(\boldsymbol{q}, t) = -\hat{H}(\boldsymbol{q})\, P(\boldsymbol{q}, t)$$

$$= \frac{1}{2}\left[\Omega\, \nabla_{\boldsymbol{q}}^2 + \nabla_{\boldsymbol{q}} \cdot \boldsymbol{f}\,(\boldsymbol{q})\right] P(\boldsymbol{q}, t) \tag{4.23}$$

Eq(4.23b) can be written as

$$\dot{P} = \frac{1}{2} \nabla_{\boldsymbol{q}} \cdot \left(\Omega\, \nabla_{\boldsymbol{q}} P + \boldsymbol{f}\, P\right)$$

$$\int d\, \boldsymbol{q}\, \dot{P} = 0 = \frac{\partial}{\partial t} \int d\, \boldsymbol{q}\, P$$

(4.23c)

which shows that the probability $\int d\, \boldsymbol{q}\, P$ is conserved.

Finally, taking the inverse Fourier transform of eq(4.21) gives

$$\begin{aligned} P(\boldsymbol{q}, t+\varepsilon;\ \boldsymbol{q}'\,t) &= \int \frac{d\boldsymbol{p}}{(2\pi)^d}\, e^{i\boldsymbol{p}\cdot\boldsymbol{q}}\, \tilde{P}(\boldsymbol{p}, t+\varepsilon;\ \boldsymbol{q}', t) \\ &\approx \int \frac{d\boldsymbol{p}}{(2\pi)^d} \exp\left[i\boldsymbol{p}\cdot \left(\boldsymbol{q}-\boldsymbol{q}' + \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}') \right) - \frac{\varepsilon\Omega}{2}\boldsymbol{p}^2 \right] \\ &= \left(\frac{1}{2\pi\varepsilon\Omega} \right)^{d/2} \exp\left[-\frac{1}{2\varepsilon\Omega} \left(\boldsymbol{q}-\boldsymbol{q}' + \frac{1}{2}\varepsilon \boldsymbol{f}(\boldsymbol{q}') \right)^2 \right] \end{aligned} \tag{4.24}$$

Note that Zinn-Justin’s eq(4.24) is off by a pre-factor of $\varepsilon^{-d/2}$.