4.5. A Special Case: The Dissipative Langevin Equation

Consider the case where $\boldsymbol{f}$ is a gradient:

$$\boldsymbol{f}(\boldsymbol{q}) = \Omega \nabla_{\boldsymbol{q}} E(\boldsymbol{q}) \qquad f_i(\boldsymbol{q}) = \Omega\, \partial_i E(\boldsymbol{q}) \tag{4.37}$$

Eq(4.1) becomes

$$\dot{q}_i(t) = -\frac{1}{2}\Omega\, \partial_i E(\boldsymbol{q}) + v_i(t) \qquad \left(\partial_i = \frac{\partial}{\partial q_i} \right) \tag{4.38}$$

which is a purely dissipative Langevin eq.

The linear Langevin eq. [see eq(4.9)]

$$\dot{q} = -\omega\, q + v(t)$$

provides the simplest example with

$$\frac{1}{2}\Omega\, \partial_q E = \omega\, q$$

$$\rightarrow \qquad E(q) = \frac{\omega}{\Omega} q^2 \qquad \partial_q E(q) = 2\frac{\omega}{\Omega} q \qquad \partial_q^2 E(q) = 2\frac{\omega}{\Omega}$$

Consider the transformation

$$P(\boldsymbol{q}, t) = e^{-E(\boldsymbol{q})/2} \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle e^{E(\boldsymbol{q}_0)/2} \tag{4.39}$$

$$\rightarrow \qquad \dot{P}(\boldsymbol{q}, t) = e^{-E(\boldsymbol{q})/2} \left(\frac{\partial}{\partial t} \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle \right) e^{E(\boldsymbol{q}_0)/2}$$

$$\partial_i P(\boldsymbol{q}, t) = e^{-E(\boldsymbol{q})/2} \left(-\frac{1}{2}(\partial_i E) + \partial_i \right) \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle e^{E(\boldsymbol{q}_0)/2}$$

$$\nabla_{\boldsymbol{q}} \cdot [\boldsymbol{f}(\boldsymbol{q}) P(\boldsymbol{q}, t)] = e^{-E(\boldsymbol{q})/2}\, \Omega \left(-\frac{1}{2}(\partial_i E) + \partial_i \right) (\partial_i E) \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle e^{E(\boldsymbol{q}_0)/2}$$

$$\nabla_{\boldsymbol{q}}^2 P(\boldsymbol{q}, t) = e^{-E(\boldsymbol{q})/2} \left(-\frac{1}{2}(\partial_i E) + \partial_i \right) \left(-\frac{1}{2}(\partial_i E) + \partial_i \right) \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle e^{E(\boldsymbol{q}_0)/2}$$

where ∂_i in $(\partial_i E)$ operates only on E & nothing else. In other words, $(\partial_i E)$ is to be treated as a function, not an oprator. This point is emphasized by using (∇E), instead of $(\nabla_{\boldsymbol{q}} E)$, to denote the vector form of $(\partial_i E)$.

Eq(4.23) of §4.3

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

thus becomes

$$\frac{\partial}{\partial t} \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle = \frac{1}{2}\Omega \left(-\frac{1}{2}(\partial_i E) + \partial_i \right) \left(\frac{1}{2}(\partial_i E) + \partial_i \right) \langle \boldsymbol{q} \mid U(t, t_0) \mid \boldsymbol{q}_0 \rangle \tag{4.40}$$

$$= \left\langle \boldsymbol{q} \,\middle|\, \frac{1}{2}\Omega \left(-\frac{1}{2}(\partial_i E) + i\hat{p}_i \right) \left(\frac{1}{2}(\partial_i E) + i\hat{p}_i \right) U(t, t_0) \,\middle|\, \boldsymbol{q}_0 \right\rangle$$

$$= \left\langle \boldsymbol{q} \,\middle|\, \frac{1}{2}\Omega \left(-\frac{1}{2}(\nabla E) + i\hat{\boldsymbol{p}} \right) \cdot \left(\frac{1}{2}(\nabla E) + i\hat{\boldsymbol{p}} \right) U(t, t_0) \,\middle|\, \boldsymbol{q}_0 \right\rangle$$

$$= -\left\langle \boldsymbol{q} \,\middle|\, \tilde{H}\, U(t, t_0) \,\middle|\, \boldsymbol{q}_0 \right\rangle$$

$$\rightarrow \qquad \dot{U}(t, t_0) = -\tilde{H}\, U(t, t_0) \tag{4.41}$$

where

$$\tilde{H} = \frac{1}{2}\Omega \left(\frac{1}{2}(\nabla E) - i\hat{\boldsymbol{p}} \right) \cdot \left(\frac{1}{2}(\nabla E) + i\hat{\boldsymbol{p}} \right)$$

$$= \frac{1}{2} \Omega \boldsymbol{A}^{+} \cdot \boldsymbol{A} \qquad (4.41)$$

with

$$\boldsymbol{A} = \frac{1}{2} (\nabla E) + i \hat{\boldsymbol{p}} \qquad \text{(operator form)}$$

$$= \frac{1}{2} (\nabla E) + \nabla_{\boldsymbol{q}} \qquad \text{(} q\text{-representation)} \qquad (4.42)$$

Eq(4.41a) can be expanded to give

$$\tilde{H} = \frac{1}{2} \Omega \left\{ \hat{\boldsymbol{p}}^2 + \frac{1}{4} (\nabla E)^2 - \frac{1}{2} i \left[\hat{p}_k , (\partial_k E) \right] \right\}$$

Using

$$i \left[\hat{p}_k , (\partial_k E) \right] \psi = [\partial_k , (\partial_k E)] \psi$$
$$= \partial_k [(\partial_k E) \psi] - (\partial_k E) \partial_k \psi$$
$$= \left(\partial_k^2 E \right) \psi$$
$$= \left(\nabla^2 E \right) \psi$$

we have

$$\tilde{H} = \frac{1}{2} \Omega \left\{ \hat{\boldsymbol{p}}^2 + \frac{1}{4} (\nabla E)^2 - \frac{1}{2} \left(\nabla^2 E \right) \right\} \qquad (4.41)$$

Eq(4.41a) indicates $\tilde{H}$ is hermitian.

Since $\tilde{H}$ does not dependent of t explicitly, the solution to eq(4.41b) is

$$U(t, t_0) = e^{-\tilde{H} (t - t_0)}$$

(4.41b)

which has the form of a statistical operator.

Consider an eigenvalue λ_i of A_i , then λ_i^* is an eigenvalue of $(A^+)_i$ and $\lambda_i^* \lambda_i \geq 0$ that of $\tilde{H}$.

Since all eigenvalues of $\tilde{H}$ can be constructed in this manner, $\tilde{H}$ is non-negative.

Consider the eigen-equation

$$\boldsymbol{A} \psi = \left[\frac{1}{2} (\nabla E) + \nabla \right] \psi = \lambda \psi$$

The eigen-function for $\lambda = 0$ is simply

$$\psi_0(\boldsymbol{q}) = C e^{-E(\boldsymbol{q})/2} \qquad (C = \text{constant})$$

Furthermore, eq(4.41a) shows that

$$\tilde{H} \psi_0(\boldsymbol{q}) = 0$$

Thus, we have

$$\langle \boldsymbol{q} \mid 0 \rangle = \psi_0(\boldsymbol{q})$$

provided it is normalizable, i.e.,

$$\langle 0 \mid 0 \rangle = \int d\boldsymbol{q} \langle 0 \mid \boldsymbol{q} \rangle \langle \boldsymbol{q} \mid 0 \rangle \qquad (4.41c)$$
$$= | C |^2 \int d\boldsymbol{q}\, e^{-E(\boldsymbol{q})}$$
$$= 1$$

From eqs(4.39 & 4.41b), we have

$$\lim_{t \to \infty} P(\boldsymbol{q}, t) = \lim_{t \to \infty} e^{-E(\boldsymbol{q})/2} \left\langle \boldsymbol{q} \middle| e^{-\tilde{H} (t - t_0)} \middle| \boldsymbol{q}_0 \right\rangle e^{E(\boldsymbol{q}_0)/2}$$

$$= \lim_{t\to\infty} e^{-E(\boldsymbol{q})/2} \sum_E \langle \boldsymbol{q} \mid E\rangle \left\langle E \left| e^{-\tilde{H}(t-t_0)} \right| \boldsymbol{q}_0 \right\rangle e^{E(\boldsymbol{q}_0)/2}$$
$$= e^{-E(\boldsymbol{q})/2} \langle \boldsymbol{q} \mid 0\rangle\langle 0 \mid \boldsymbol{q}_0 \rangle e^{E(\boldsymbol{q}_0)/2}$$
$$= |C|^2 e^{-E(\boldsymbol{q})/2} e^{-E(\boldsymbol{q})/2} e^{-E(\boldsymbol{q}_0)/2} e^{E(\boldsymbol{q}_0)/2}$$
$$= |C|^2 e^{-E(\boldsymbol{q})} \tag{4.41d}$$

so that the equilibrium distribution is proportional to $e^{-E(\boldsymbol{q})}$ with

$$\int d\,\boldsymbol{q} \lim_{t\to\infty} P(\boldsymbol{q}, t) = |C|^2 \int d\,\boldsymbol{q}\; e^{-E(\boldsymbol{q})} = 1 \qquad [\text{ If } \psi_0(\boldsymbol{q}) \text{ is normalizable }]$$

If $\psi_0(\boldsymbol{q})$ is not normalizable, then

$$\int d\,\boldsymbol{q} \lim_{t\to\infty} P(\boldsymbol{q}, t) = \infty$$

so that $P(\boldsymbol{q}, t)$ cannot be interpreted as a probability distribution.

Remark

The case of the purely dissipative Langevin eq(4.38) corresponds to detailed balance for discrete processes (see Appendix A4.2). The driving term f_i is then said to be conservative. In the absence of noise, the Langevin eq(4.38) reduces to a gradient flow:

$$\dot{q}_i(t) = -\frac{1}{2}\Omega\,\partial_i E(\boldsymbol{q}) \tag{4.43}$$

or $$\dot{\boldsymbol{q}}(t) = -\frac{1}{2}\Omega\,\nabla E(\boldsymbol{q})$$

→ $$\dot{\boldsymbol{q}}(t)^2 = -\frac{1}{2}\Omega\,\dot{\boldsymbol{q}}(t)\cdot\nabla E$$

$$\int_{t_0}^{t} d\,\tau\,\dot{\boldsymbol{q}}(\tau)^2 = -\frac{1}{2}\Omega \int_{t_0}^{t} d\,\tau\,\dot{\boldsymbol{q}}(\tau)\cdot\nabla E$$
$$= -\frac{1}{2}\Omega \int_{\boldsymbol{q}(t_0)}^{\boldsymbol{q}(t)} d\,\boldsymbol{q}\cdot\nabla E$$
$$= -\frac{1}{2}\Omega \int_{E[\boldsymbol{q}(t_0)]}^{E[\boldsymbol{q}(t)]} d\,E$$
$$= -\frac{1}{2}\Omega\left\{E[\boldsymbol{q}(t)] - E[\boldsymbol{q}(t_0)]\right] \tag{4.44}$$

The Linear Langevin Equation

As mentioned before, the linear Langevin eq. [see eq(4.9)]

$$\dot{q} = -\omega\,q + v(t)$$

provides the simplest example with

$$\frac{1}{2}\Omega\,\partial_q E = \omega\,q$$

→ $$E(q) = \frac{\omega}{\Omega} q^2 \qquad \partial_q E(q) = 2\frac{\omega}{\Omega} q \qquad \partial_q^2 E(q) = 2\frac{\omega}{\Omega}$$

Eq(4.41) becomes

$$\tilde{H} = \frac{1}{2}\Omega\left[\hat{p}^2 + \left(\frac{\omega}{\Omega} q\right)^2 - \frac{\omega}{\Omega}\right]$$

Setting $\Omega = 1$, we have

$$\tilde{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2 q^2 - \frac{1}{2}\omega \tag{4.45}$$

As a quantum oscillator, the spectrum of $\tilde{H}$ is

$$\varepsilon_n = \left(n + \frac{1}{2}\right)|\omega| - \frac{1}{2}\omega \qquad n = 0, 1, 2, \ldots \tag{4.46}$$

$$= \begin{cases} n\,\omega & \text{for } \omega \geq 0 \\ (n+1)\,|\omega| & \text{for } \omega \leq 0 \end{cases}$$

$$\therefore \qquad \varepsilon_0 = \begin{cases} 0 & \text{for } \omega \geq 0 \\ |\omega| & \text{for } \omega \leq 0 \end{cases}$$

With

$$e^{-E(q)} = e^{-\omega q^2}$$

eq(4.41c) becomes

$$\langle 0 \mid 0 \rangle = |C|^2 \int_{-\infty}^{\infty} dq\, e^{-\omega q^2}$$

$$= \begin{cases} |C|^2 \sqrt{\dfrac{\pi}{\omega}} & \text{if } \omega > 0 \\ \infty & \text{if } \omega \leq 0 \end{cases}$$

Hence, for $\omega > 0$, we have $\varepsilon_0 = 0$ & $\langle 0 \mid 0 \rangle = \text{finite}$ so that the equilibrium distribution exists & equal to $\sqrt{\dfrac{\omega}{\pi}}\, e^{-\omega q^2}$.

For $\omega < 0$, the eigenstates $\langle q \mid n \rangle$ are the same as $\omega > 0$ but the eigenvalues are shifted as given by eq(4.46). Thus, $\varepsilon_0 = |\omega| \neq 0$ & $\langle 0 \mid 0 \rangle = \infty$ so that the equilibrium distribution does not exist.

With $\varepsilon_0 = |\omega|$, eq(4.41d) becomes

$$\lim_{t\to\infty} P(q, t) \approx e^{-E(q)/2} \langle q \mid 0 \rangle \left\langle 0 \,\middle|\, e^{-|\omega|(t-t_0)} \,\middle|\, q_0 \right\rangle e^{E(q_0)/2}$$

$$= \sqrt{\frac{\omega}{\pi}}\, e^{|\omega| q^2/2}\, e^{-|\omega| q^2/2}\, e^{-|\omega|(t-t_0)}\, e^{-|\omega| q_0^2/2}\, e^{-|\omega| q_0^2/2}$$

$$= \sqrt{\frac{\omega}{\pi}}\, e^{-|\omega|(t-t_0)}\, e^{-|\omega| q_0^2} \tag{4.47}$$

with the next correction term being

$$e^{|\omega| q^2/2} \langle q \mid 1 \rangle \langle 1 \mid q_0 \rangle e^{-2|\omega|(t-t_0)}\, e^{-|\omega| q_0^2/2} \propto e^{-2|\omega|(t-t_0)}$$

Eq(4.47) shows an exponential decay of $P(q, t)$ with relaxation time $\tau = \dfrac{1}{|\omega|}$.

For special case $\omega = 0$, eq(4.45) becomes

$$\tilde{H} = \frac{1}{2}\hat{p}^2$$

which gives a Brownian motion [see §4.2] with

$$\lim_{t\to\infty} P(q, t) \propto \frac{1}{\sqrt{t}} \qquad \text{[see eq(4.10b)]}$$