4.6. Path Integral Representation

Using [see §4.3, eq(4.24)]

$$P(\boldsymbol{q},\, t+\varepsilon\,;\, \boldsymbol{q}'\, t) = \left(\frac{1}{2\,\pi\,\varepsilon\,\Omega}\right)^{d/2} \exp\!\left[-\frac{1}{2\,\varepsilon\,\Omega}\left(\boldsymbol{q}-\boldsymbol{q}' + \frac{1}{2}\,\varepsilon\,\boldsymbol{f}\,(\boldsymbol{q}')\right)^2\right]$$

and the semi-group property [see §4.1, eq(4.6)]

$$P(\boldsymbol{q}_3,\, t_3;\, \boldsymbol{q}_1,\, t_1) = \int d\,\boldsymbol{q}_2\, P(\boldsymbol{q}_3,\, t_3;\, \boldsymbol{q}_2,\, t_2)\, P(\boldsymbol{q}_2,\, t_2;\, \boldsymbol{q}_1,\, t_1) \qquad (t_3 \geq t_2 \geq t_1)$$

we can construct the finite time evolution as a path integral:

$$P(\boldsymbol{q},\, t\,;\, \boldsymbol{q}_0,\, t_0) = \int_{\boldsymbol{q}(t_0)=\boldsymbol{q}_0}^{\boldsymbol{q}(t)=\boldsymbol{q}} [d\,\boldsymbol{q}(\tau)]\, e^{-S(\boldsymbol{q})/\Omega}$$

(4.48)

with

$$t - t_0 = N\,\varepsilon \qquad \boldsymbol{q}_k = \boldsymbol{q}(t_k)$$

$$[d\,\boldsymbol{q}(\tau)] = \left(\frac{1}{2\,\pi\,\varepsilon\,\Omega}\right)^{N\,d/2} \prod_{k=1}^{N-1} d\,\boldsymbol{q}_k$$

$$S(\boldsymbol{q}) = \sum_{k=1}^{N} \frac{1}{2\,\varepsilon}\left(\boldsymbol{q}_k - \boldsymbol{q}_{k-1} + \frac{1}{2}\,\varepsilon\,\boldsymbol{f}\,(\boldsymbol{q}_{k-1})\right)^2$$

(4.48a)

In order to turn eq(4.48a) into an integral, we need to expand each $(\ldots)^2$ term to $O[\varepsilon]$. As in §3.1, we symmetrize the argument of $\boldsymbol{f}$ by Taylor expanding it at mid-point:

$$\boldsymbol{q}_k - \boldsymbol{q}_{k-1} + \frac{1}{2}\,\varepsilon\,\boldsymbol{f}\,(\boldsymbol{q}_{k-1}) = \boldsymbol{q}_k - \boldsymbol{q}_{k-1} + \frac{1}{2}\,\varepsilon\left[\boldsymbol{f}\left(\frac{\boldsymbol{q}_{k-1}+\boldsymbol{q}_k}{2}\right) + \left(\frac{\boldsymbol{q}_{k-1}-\boldsymbol{q}_k}{2}\cdot\nabla_{\boldsymbol{q}}\right)\boldsymbol{f}\,(\boldsymbol{q})\Big|_{\boldsymbol{q}=\frac{\boldsymbol{q}_{k-1}+\boldsymbol{q}_k}{2}} + \ldots\right]$$

(1)

From eq(4.11), we have

$$|\; \boldsymbol{q}_{k-1} - \boldsymbol{q}_k \;| = O\left(\varepsilon^{1/2}\right)$$

Since the next neglected term in eq(1) is proportional to $\varepsilon\left(\frac{\boldsymbol{q}_{k-1}-\boldsymbol{q}_k}{2}\cdot\nabla_{\boldsymbol{q}}\right)^2 \boldsymbol{f}\,(\boldsymbol{q})$, it is $O\left(\varepsilon^2\right)$.

Setting

$$\tilde{q}_k = \boldsymbol{q}_k - \frac{1}{2}\,\varepsilon\left(\frac{\boldsymbol{q}_k-\boldsymbol{q}_{k-1}}{2}\cdot\nabla_{\boldsymbol{q}}\right)\boldsymbol{f}\,(\boldsymbol{q})\Big|_{\boldsymbol{q}=\frac{\boldsymbol{q}_{k-1}+\boldsymbol{q}_k}{2}}$$

(2)

eq(1) becomes

$$\boldsymbol{q}_k - \boldsymbol{q}_{k-1} + \frac{1}{2}\,\varepsilon\,\boldsymbol{f}\,(\boldsymbol{q}_{k-1}) = \tilde{\boldsymbol{q}}_k - \boldsymbol{q}_{k-1} + \frac{1}{2}\,\varepsilon\,\boldsymbol{f}\left(\frac{\boldsymbol{q}_{k-1}+\boldsymbol{q}_k}{2}\right) + O\left(\varepsilon^2\right)$$

$$= \varepsilon\left[\dot{\tilde{\boldsymbol{q}}}_k + \frac{1}{2}\,\boldsymbol{f}\,(\tilde{\boldsymbol{q}}_k)\right] + O\left(\varepsilon^2\right)$$

(3)

Eq(4.48a) becomes

$$S(\boldsymbol{q}) = \lim_{N\to\infty} \sum_{k=1}^{N} \frac{1}{2}\,\varepsilon\left(\dot{\tilde{\boldsymbol{q}}}_k + \frac{1}{2}\,\boldsymbol{f}\,(\tilde{\boldsymbol{q}}_k)\right)^2$$

$$= \int_{t_0}^{t} d\tau \, \frac{1}{2} \left(\dot{\tilde{\boldsymbol{q}}} + \frac{1}{2} \boldsymbol{f}(\tilde{\boldsymbol{q}}) \right)^2$$

(4)

The transformation eq(2) has a jacobian matrix $\boldsymbol{J}$ at $\boldsymbol{q} = \boldsymbol{q}_k$ given by

$$(\boldsymbol{J}^{-1})_{ij} = \frac{\partial \tilde{q}_i}{\partial q_j} = \delta_{ij} - \frac{1}{4} \varepsilon \, \partial_j f_i + O(\varepsilon^{3/2})$$

$$\rightarrow \qquad \det(\boldsymbol{J}^{-1}) = \prod_{i=1}^{d} (\boldsymbol{J}^{-1})_{ii} + O(\varepsilon^{3/2})$$

$$= \prod_{i=1}^{d} \left(1 - \frac{1}{4} \varepsilon \, \partial_i f_i \right) + O(\varepsilon^{3/2}) \qquad \text{(no summation over } i \text{ in } \partial_i f_i \text{)}$$

$$= 1 - \frac{1}{4} \varepsilon \, \partial_i f_i + O(\varepsilon^{3/2}) \qquad \text{(summation over } i \text{ in } \partial_i f_i \text{)}$$

Therefore, the jacobian of eq(2) is

$$J(\tilde{\boldsymbol{q}}_k) = \frac{1}{\det(\boldsymbol{J}^{-1})} = 1 + \frac{1}{4} \varepsilon \, \partial_i f_i(\tilde{\boldsymbol{q}}_k) + O(\varepsilon^{3/2})$$

Hence, to lowest order in ε,

$$[d\,\boldsymbol{q}(\tau)] = [d\,\tilde{\boldsymbol{q}}(\tau)] \prod_{k=1}^{N-1} \left[1 + \frac{1}{4} \varepsilon \, \partial_i f_i(\tilde{\boldsymbol{q}}_k) \right]$$

$$= [d\,\tilde{\boldsymbol{q}}(\tau)] \exp\left[\frac{1}{4} \varepsilon \sum_k \partial_i f_i(\tilde{\boldsymbol{q}}_k) \right]$$

$$= [d\,\tilde{\boldsymbol{q}}(\tau)] \exp\left[\frac{1}{4} \int_{t_0}^{t} d\tau \, \partial_i f_i(\tilde{\boldsymbol{q}}) \right]$$

Eq(4.48) thus becomes,

$$P(\boldsymbol{q}, t\,;\, \boldsymbol{q}_0, t_0) = \int_{\tilde{\boldsymbol{q}}(t_0) = \boldsymbol{q}_0}^{\tilde{\boldsymbol{q}}(t) = \boldsymbol{q}} [d\,\tilde{\boldsymbol{q}}(\tau)] \, e^{-S(\tilde{\boldsymbol{q}})/\Omega} \exp\left[\frac{1}{4} \int_{t_0}^{t} d\tau \, \partial_i f_i(\tilde{\boldsymbol{q}}) \right]$$

$$= \int_{\boldsymbol{q}(t_0) = \boldsymbol{q}_0}^{\boldsymbol{q}(t) = \boldsymbol{q}} [d\,\boldsymbol{q}(\tau)] \, e^{-\tilde{S}(\boldsymbol{q})/\Omega}$$

(4.49a)

where

$$\tilde{S}(\boldsymbol{q}) = \int_{t_0}^{t} d\tau \left[\frac{1}{2} \left(\dot{\boldsymbol{q}} + \frac{1}{2} \boldsymbol{f}(\boldsymbol{q}) \right)^2 - \frac{1}{4} \Omega \, \partial_i f_i(\boldsymbol{q}) \right]$$

(4.49)

$$= \int_{t_0}^{t} d\tau \left[\frac{1}{2} \left(\dot{\boldsymbol{q}} + \frac{1}{2} \boldsymbol{f} \right)^2 - \frac{1}{4} \Omega \, \nabla_{\boldsymbol{q}} \cdot \boldsymbol{f} \right]$$

Remarks

(i) Since $\tilde{S}$ contains a term $\dot{\boldsymbol{q}} \cdot \boldsymbol{f}$ in the integrand, perturbative calculations will involve the ill-defined quantity $\varepsilon(0)$.

Consistency with the choice of symmetrizing the argument of f requires $\varepsilon(0) = 0$. [See §4.2]

(ii) In the case of the dissipative Langevin equation [see §4.5, eq(4.37)]

$$\boldsymbol{f}(\boldsymbol{q}) = \Omega \, \nabla_{\boldsymbol{q}} E(\boldsymbol{q})$$

so that

$$\left(\dot{\boldsymbol{q}} + \frac{1}{2}\boldsymbol{f}\right)^2 = \left(\dot{\boldsymbol{q}} + \frac{1}{2}\Omega\nabla_{\boldsymbol{q}}E\right)^2$$

$$= \dot{\boldsymbol{q}}^2 + \Omega\,\dot{\boldsymbol{q}}\cdot\nabla_{\boldsymbol{q}}E + \frac{1}{4}\Omega^2(\nabla_{\boldsymbol{q}}E)^2$$

Using

$$\int_{t_0}^{t} d\tau\,\dot{\boldsymbol{q}}\cdot\nabla_{\boldsymbol{q}}E = \int_{\boldsymbol{q}(t_0)}^{\boldsymbol{q}(t)} d\boldsymbol{q}\cdot\nabla_{\boldsymbol{q}}E = \int_{E[\boldsymbol{q}(t_0)]}^{E[\boldsymbol{q}(t)]} dE = E[\boldsymbol{q}(t)] - E[\boldsymbol{q}(t_0)]$$

we have

$$\frac{1}{2}\int_{t_0}^{t} d\tau\left(\dot{\boldsymbol{q}} + \frac{1}{2}\boldsymbol{f}\right)^2 = \frac{1}{2}\int_{t_0}^{t} d\tau\left[\dot{\boldsymbol{q}}^2 + \frac{1}{4}\Omega^2(\nabla_{\boldsymbol{q}}E)^2\right] + \frac{1}{2}\Omega\,\{E[\boldsymbol{q}(t)] - E[\boldsymbol{q}(t_0)]\}$$

This result is consistent with the eqs(4.39 & 4.41).

It again requires $\varepsilon(0) = 0$, in order that the derivative and the average commute.

(iii) Using eq(4.5)

$$\langle O[\boldsymbol{q}(t)]\rangle_\nu = \int d\boldsymbol{q}\,P(\boldsymbol{q}, t;\, \boldsymbol{q}_0, t_0)\,O(\boldsymbol{q})$$

we obtain a path integral representation of correlation functions:

$$Z^{(n)}_{i_1 \dots i_n}(t_1, \dots, t_n) = \langle q_{i_1}(t_1)\dots q_{i_n}(t_n)\rangle_\nu$$

$$= \int [d\boldsymbol{q}(\tau)]\, q_{i_1}(t_1)\dots q_{i_n}(t_n)\, e^{-\tilde{S}(\boldsymbol{q})/\Omega}$$

(4.50)

where $\boldsymbol{q}(t_0) = \boldsymbol{q}_0$.

Perturbative Expansion

See Zinn-Justin’s text.