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Non-integrable mappings and fluctuating irreversible processes

M Mehrafarin and M Ghaemi†

Department of Physics, Amir Kabir University of Technology, Tehran, Iran
and
Centre for Theoretical Physics and Mathematics, Atomic Energy Organization of Iran, Tehran, Iran

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Abstract. Employing a widely used model for the dynamics of irreversible processes, we introduce curvature into the Euclidean state space of fluctuating irreversible processes in (quasi-)linear domains via non-integrable coordinate transformations. The Riemannian state space thus obtained pertains to the nonlinear domain of far from equilibrium situations. This technique makes it possible to extend systematically, without the need for adding stochastic assumptions, both the path integral expression for the conditional probability and the Fokker–Planck equation, from (quasi-)linear to nonlinear regimes. Our results agree with those obtained by Grabert and Green which are based on stochastic considerations. The connection with other rigorous results in the literature is also discussed.

1. Introduction

Long ago it was proposed [1] that in presence of fluctuations, irreversible processes can be represented by Markov processes governed by a Fokker–Planck equation. Following this proposition and employing a widely used model (introduced in the next section) for the dynamics of irreversible processes, Onsager and Machlup [2] were able to obtain an expression for the conditional probability relating two macroscopic states as a functional integral. This path integral representation, being perhaps the most seminal expression of the role of fluctuations in non-equilibrium phenomena, was limited to the so-called linear regime of near equilibrium situations in which kinetic coefficients are state independent and the thermodynamic forces are linear in the deviations of the macroscopic (extensive) variables from their equilibrium values.

The path integral concept was later extended (within the context of the same model) to nonlinear irreversible processes by Grabert and Green [3] through making a hypothesis analogous to that of Onsager and Machlup about the short-time conditional probability in nonlinear domains.

Recently, employing the same model, a canonical operator formulation of irreversible processes was proposed by one of us (MM) [4, 5] which, among other features, had a path integral representation that could be obtained just as customarily as done in quantum mechanics. The path integral expression for the conditional probability derived in this manner [4] pertained to the quasi-linear domain which, by definition, is slightly more

† Present address: Department of Chemistry, University of Kashan, Kashan, Iran.

general than the linear domain in that the constraint on the thermodynamic forces is relaxed. This approach for obtaining the functional integral, apart from being more systematic, has the advantage of doing away with explicit stochastic assumptions, in particular about the short-time conditional probability. It is our purpose to pursue that line of approach to obtain the conditional probability in nonlinear regimes. To this end, we transform the flat state space of quasi-linear irreversible processes to a curved state space pertaining to the nonlinear domain, thereby also transforming the corresponding conditional probabilities. We do this by making use of non-integrable coordinate transformations (introduced in section 3), which are a standard means of generating curvature (and torsion) from a Euclidean space, particularly in the study of crystal defects [6]. In the spirit of the operator formulation of non-equilibrium phenomena developed in [4, 5], we mention in passing that our technique is principally a refined version of that employed in quantum mechanics for passage from the path integral representation in flat to curved space [7]. The resulting expression for the nonlinear conditional probability will then be used to derive the Fokker–Planck equation systematically. Our results agree with those obtained by Grabert and Green [3] using a completely different scheme based on stochastic assumptions.

In the literature [8, 9], there exist similar rigorous results by various authors on the derivation of such probability functionals. The work presented here is yet another attempt (via a completely different approach) in this direction. However, our result for the conditional probability functional (equations (5.9*a*, *b*)) differs from that given in references [8, 9] in the last term of (5.9*b*) where they obtain $k^2R/6$. An explanation for this difference, which is also apparent in the work of Grabert and Green, is given by the latter in [3]. Our procedure is therefore to be contrasted with earlier proposals for constructing probability functionals in state spaces with curvature which can be found in the literature, most notably in the work of [8].

2. Conditional probability for the flat state space of quasi-linear domains

Consider a system described by a set $\{q^i\}; i = 1, 2, \ldots, r$; of relevant macroscopic extensive variables. This set forms the coordinates for the thermodynamic state (or configuration) space whose origin we take to represent the equilibrium state. The entropy $S(q^i)$ is maximal at equilibrium so that $\chi_i(0) = 0$ where $\chi_i = \partial_i S$ are the so-called thermodynamic forces conjugate to q^i. These forces have a restoring character and drive the system towards equilibrium by causing flows $\dot{q}^i \equiv \mathrm{d}q^i/\mathrm{d}t$. The phenomenological relationship between the forces and the flows (summation convention implied hereafter)

$$\dot{q}^i = \ell^{ij}\chi_j \tag{2.1}$$

defines the dynamical model mentioned in the introduction (and employed by us here), applicable to a variety of irreversible phenomena. In (2.1) the matrix ℓ^{ij}, which is positive semi-definite and symmetric, represents Onsager's kinetic coefficients [10]. In near equilibrium situations (or the linear domain) ℓ^{ij} are constant and χ_i are linear functions of q^i, wherease in far from equilibrium situations (or the nonlinear domain) ℓ^{ij} and χ_i may be arbitrary functions of the state q^i.

The entropy $S(q^i)$, being a function of the state, is clearly a scalar under transformations in the thermodynamic configuration space. For the covariance of the formulation to be manifest under such transformations, it is customary [3, 5] to introduce a Riemannian geometry in the state space by taking the inverse kinetic coefficients ℓ_{ij} (satisfying $\ell_{ik}\ell^{ij} = \delta_k{}^j$) to play the role of the metric components in the coordinate basis representation. We can thus regard q^i (χ_i) as a contravariant (covariant) vector in the usual manner. Of course, in the linear and quasi-linear domains, because ℓ_{ij} are constant, the state space will be Euclidean and, hence, flat.

The functional integral for the conditional probability in the quasi-linear regime derived in [4], when trivially generalized to a multi-dimensional state space reads ($t < t'$):

$$W(q^i, t; q'^i, t') = \int_{q^i(t)=q^i}^{q^i(t')=q'^i} \mathrm{d}[q^i(t)]\ \exp\left\{-\frac{1}{k}\int_t^{t'} \mathrm{d}t\ \left\{\frac{1}{4}\ell_{ij}(\dot{q}^i - \chi^i)(\dot{q}^j - \chi^j) + \frac{k}{2}\chi^i{}_{,i}\right\}\right\} \tag{2.2a}$$

where a prime denotes partial differentiation, $\chi^i = \ell^{ij}\chi_j$ and

$$\int \mathrm{d}[q^i(t)] \equiv \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}} \left\{L(4\pi\epsilon k)^r\right\}^{-N/2} \prod_{n=1}^{N-1} \int \mathrm{d}^r q^i_{(n)}\,. \tag{2.2b}$$

Here $t' - t = \epsilon N$, $L = \det(\ell^{ij})$ and $\mathrm{d}^r q^i_{(n)} = \prod_{i=1}^r \mathrm{d}q^i_{(n)}$. The time integral in (2.2*a*) is sometimes called the thermodynamic action which may be written in discretized form as $\epsilon\sum_{n=1}^N \mathcal{L}^\epsilon_<(q^i_{(n-1)}, q^i_{(n)})$ with $q^i_{(0)} = q^i$ and $q^i_{(N)} = q'^i$ and

$$\mathcal{L}^\epsilon_<(q^i_{(n-1)}, q^i_{(n)}) = \frac{1}{4\epsilon^2}\,\ell_{ij}(q^i_{(n)} - q^i_{(n-1)} - \epsilon\chi^i_{(n-1)})(q^j_{(n)} - q^j_{(n-1)} - \epsilon\chi^j_{(n-1)}) + \frac{k}{2}\,\chi^i{}_{,i(n-1)}\,. \tag{2.3}$$

$\mathcal{L}^\epsilon_<$ is the so-called (discretized) thermodynamic Lagrangian, evaluated at the prepoint $q^i_{(n-1)}$ of the interval $\Delta q^i_{(n)} = q^i_{(n)} - q^i_{(n-1)}$. The suffix '<' is used to emphasize prepoint evaluation and we use the shorthand notation $\chi_{i(n-1)} \equiv \chi_i(q^j_{(n-1)})$, etc. We have deliberately chosen a prepoint expansion for the action to make direct contact with the result of Grabert and Green [3] for the conditional probability. The prepoint action gives ready access to the evolution of the system backward in time as is evident from the normalization condition for the short-time conditional probability $W^\epsilon_<$

$$\lim_{\epsilon\to 0}\int W^\epsilon_<(q^i_{(n-1)}, t_{(n-1)}; q^i_{(n)}, t_{(n)})\,\mathrm{d}^r q^i_{(n-1)} = \lim_{\epsilon\to 0}\left\{L(4\pi\epsilon k)^r\right\}^{-1/2}\int \exp\left\{-\frac{\epsilon}{k}\mathcal{L}^\epsilon_<(q^i_{(n)} - \Delta q^i_{(n)}, q^i_{(n)})\right\}\,\mathrm{d}^r\Delta q^i_{(n)} = 1\,. \tag{2.4}$$

This is readily proved using (2.3) and the well known properties of Gaussian integrals listed in the appendix. The finite-time conditional probability, thus, satisfies the normalization condition

$$\int W_<(q^i, t; q'^i, t')\,\mathrm{d}^r q^i = 1 = \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}} \left\{L(4\pi\epsilon k)^r\right\}^{-N/2}\left\{\prod_{n=0}^{N-1}\int \mathrm{d}^r q^i_{(n)}\right\}\exp\left\{-\frac{\epsilon}{k}\sum_{n=1}^N \mathcal{L}^\epsilon_<(q^i_{(n-1)}, q^i_{(n)})\right\} \tag{2.5}$$

with $q^i_{(0)} = q^i$ and $q^i_{(N)} = q'^i$, of course. As mentioned in the introduction, the result (2.2*a*) for the conditional probability does not rest on explicit stochastic assumptions. We shall demonstrate, in the following sections, that it is possible to extend it directly to the nonlinear domain (where ℓ^{ij} are no longer constant) by transforming the invariant property of normalization (2.5), from flat to curved configuration space via non-integrable coordinate transformations.

3. Non-integrable coordinate transformations

We shall work in the coordinate basis representation throughout this paper. In the coordinate basis induced by the 'Cartesian-like' coordinates q^i of the flat state space of quasi-linear domains, the metric components ℓ_{ij} are constant. Now consider the coordinate transformation $q^i \to q^a$ where

$$dq^i = \frac{\partial q^i(q^a)}{\partial q^a}\, dq^a \equiv e^i{}_a(q^a)\, dq^a\,. \tag{3.1}$$

We have deliberately used indices from the beginning of the alphabet, reserving the middle alphabet letters for the Cartesian-like coordinate representation. The coefficients $e^i{}_a(q^a)$ are called basis tetrads and are state dependent. The metric in the new coordinate basis induced by q^a thus becomes

$$\ell_{ab} = \ell_{ij}\; e^i{}_a e^j{}_b \equiv e^i{}_a e_{ib}\,. \tag{3.2}$$

As is obvious, indices $a, b, c, \ldots$ $(i, j, k, \ldots)$ are raised and lowered by ℓ_{ab} (ℓ_{ij}). The mapping in (3.1) is invertible and the reciprocal tetrads satisfy

$$e_i{}^a e^j{}_a = \delta_i{}^j \qquad e^i{}_a e_i{}^b = \delta_a{}^b\,. \tag{3.3}$$

The connection coefficients (which obviously vanish in the Cartesian-like coordinates) are defined for the new coordinate system in the usual manner by

$$\Gamma_{ab}{}^c = e_i{}^c e^i{}_{b,a} = -\; e^i{}_b e_i{}^c{}_{,a} \tag{3.4}$$

where the last equality follows from (3.3). Clearly, a trivial coordinate transformation, i.e. a transformation for which $q^i(q^a)$ together with its derivatives are smooth and single-valued, cannot change the intrinsic properties of the state space. In particular, it cannot generate curvature nor torsion. For instance, if the mapping $q^i(q^a)$ is smooth and single-valued, it is integrable in the sense that the Schwarz's integribility condition is satisfied, namely

$$(\partial_a\partial_b - \partial_b\partial_a)\; q^i(q^a) = 0\,. \tag{3.5a}$$

This implies that the connection (3.4) is symmetric, i.e. $\Gamma_{ab}{}^c = \Gamma_{ba}{}^c$ and the mapping carries no torsion. We shall impose (3.5a) on our mapping because we do not want torsion. However, we demand that our transformation be non-integrable in the sense that

$$(\partial_a\partial_b - \partial_b\partial_a)\; e^i{}_c(q^a) \neq 0 \tag{3.5b}$$

i.e. we demand that the first derivatives of the coordinate transformation $q^i(q^a)$ should violate the integrability condition for smoothness and single-valuedness. In this manner we generate curvature, because according to its usual definition in terms of the basis tetrads, the curvature tensor will be given by

$$R_{abc}{}^d = e_i{}^d\; (\partial_a\partial_b - \partial_b\partial_a)\; e^i{}_c(q^a) \neq 0 \tag{3.6}$$

Having avoided introducing torsion into the state space, the connections (3.4) and the curvature tensor (3.6) are just the Riemannian connections (Christoffel's symbols) and the Riemannian curvature, respectively. Working out the derivatives in (3.6), one can re-write the curvature tensor (3.6) in the equivalent form involving connections (3.4)

$$R_{abc}{}^d = \Gamma_{bc}{}^d{}_{,a} - \Gamma_{ac}{}^d{}_{,b} - \Gamma_{ac}{}^e\Gamma_{eb}{}^d + \Gamma_{bc}{}^e\Gamma_{ea}{}^d \tag{3.7}$$

Let us also define here the Ricci tensor R_{ac} and the scalar curvature R according to

$$R_{ac} = R_{abc}{}^b \qquad R = \ell^{ac} R_{ac} = R_a{}^a \tag{3.8}$$

which we shall need later.

The non-integrable transformation (for which $q^i(q^a)$ is integrable while its first derivatives $e^i{}_a(q^a)$ are not) envisaged in this section, carries a flat state space region into a curved one. We shall use it to transform both the thermodynamic Lagrangian and the measure of the Cartesian-like path integral in (2.5) to the curved configuration space of nonlinear regimes.

4. Transformation of the flat configuration space Lagrangian

The normalization condition (2.5), being an invariant property, must remain valid when properly transformed to a state space with curvature. Let us focus first on the transformation of the thermodynamic Lagrangian in (2.3). It must be transformed in such a manner that the new Lagrangian remains a prepoint Lagrangian, evaluated at the prepoint of the transformed interval $\Delta q^a_{(n)}$. Thus we write, under our non-integrable mapping

$$q^i_{(n)} \equiv q^i(q^a_{(n)}) = q^i(q^a_{(n-1)} + \Delta q^a_{(n)}) = q^i_{(n-1)} + \Delta q^a_{(n)} e^i{}_{a(n-1)} + \frac{1}{2!}\Delta q^a_{(n)}\Delta q^b_{(n)} e^i{}_{a,b(n-1)} + \frac{1}{3!}\Delta q^a_{(n)}\Delta q^b_{(n)}\Delta q^c_{(n)} e^i{}_{a,bc(n-1)} + \cdots$$

that is

$$\Delta q^i_{(n)} = e^i{}_{a(n-1)}\left[\Delta q^a_{(n)} + \frac{1}{2!}\Gamma_{bc}{}^a \Delta q^b_{(n)}\Delta q^c_{(n)} + \frac{1}{3!}(\Gamma_{bd}{}^a{}_{,c} + \Gamma_{bd}{}^f\Gamma_{fc}{}^a)\Delta q^b_{(n)}\Delta q^c_{(n)}\Delta q^d_{(n)} + \cdots\right]_{(n-1)} \tag{4.1}$$

having used (3.4). (Had we started from $q^i_{(n-1)} = q^i(q^a_{(n)} - \Delta q^a_{(n)})$, we would have obtained a postpoint expansion for $\Delta q^i_{(n)}$ evaluated at $q^a_{(n)}$, suitable for a postpoint Lagrangian). Also

$$\chi_i = e_i{}^a \chi_a \tag{4.2}$$

where, of course, $\chi_a = \partial_a S(q^a)$ is the thermodynamic force in the curved state space. Hence

$$\chi^i{}_{,i} = e^{ib}\partial_b(e_i{}^a\chi_a) = \ell^{ab}(\chi_{a,b} - \Gamma_{ab}{}^c\chi_c)\,.$$

However, the last expression is just the usual definition of the covariant derivative which we denote by a semicolon (;), so that

$$\chi^i{}_{,i} = \chi^a{}_{;a}\,. \tag{4.3}$$

Substituting results (4.1)–(4.3) in (2.3) yields via (3.2) for the transformed (discretized) Lagrangian

$$\mathcal{L}^\epsilon_<(q^i_{(n-1)}, q^i_{(n)}) \to \mathcal{L}^\epsilon_<(q^a_{(n-1)}, q^a_{(n)}) = \frac{1}{4\epsilon^2}\ell_{ab(n-1)}(\Delta q^a_{(n)} - \epsilon\chi^a_{(n-1)})(\Delta q^b_{(n)} - \epsilon\chi^b_{(n-1)}) + \frac{k}{2}\chi^a{}_{;a(n-1)} + H^\epsilon(\Delta q^a_{(n)}) \tag{4.4a}$$

where

$$H^\epsilon(\Delta q^a_{(n)}) = -\frac{1}{4\epsilon}(\Gamma_{bc}{}^a\chi_a)_{(n-1)}\Delta q^b_{(n)}\Delta q^c_{(n)} + \frac{1}{4\epsilon^2}\Gamma_{abc(n-1)}\Delta q^a_{(n)}\Delta q^b_{(n)}\Delta q^c_{(n)} + \frac{1}{4\epsilon^2}\left\{\frac{1}{3}\ell_{ab}(\Gamma_{ed}{}^b{}_{,c} + \Gamma_{ed}{}^f\Gamma_{fc}{}^b) + \frac{1}{4}\Gamma_{cd}{}^b\Gamma_{eab}\right\}_{(n-1)} \times\Delta q^a_{(n)}\Delta q^c_{(n)}\Delta q^d_{(n)}\Delta q^e_{(n)} + \cdots \tag{4.4b}$$

which clearly has the prepoint form. In the above $\Gamma_{abc} = \ell_{cd}\Gamma_{ab}{}^{d}$ is the Christoffel's symbol of the first kind. Equation (4.4a) gives, in fact, only a part of the desired Lagrangian in the curved thermodynamic configuration space of far from equilibrium situations. As we shall show in the next section, proper transformation of the integration measure in the normalization condition (2.5) will yield another contribution to the thermodynamic Lagrangian which depends on the scalar curvature.

5. Path integration measure in the curved state space of nonlinear domains

A crucial step in our derivation of the nonlinear conditional probability is the systematic transformation of the integration measure in (2.5). To this end, we first replace the integration volume in (2.5) by $\mathrm{d}^r\Delta q^i_{(n)}$ as in (2.4), so that the normalization condition becomes

$$1 = \int W_<(q^i, t; q'^i, t')\,\mathrm{d}^r q^i$$

$$= \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}} \{L(4\pi\epsilon k)^r\}^{-N/2} \left\{\prod_{n=1}^{N} \int \mathrm{d}^r\,\Delta q^i_{(n)}\right\}$$

$$\times \exp\left\{-\frac{\epsilon}{k}\sum_{n=1}^{N} \mathcal{L}^\epsilon_<(q^i_{(n)} - \Delta q^i_{(n)}, q^i_{(n)})\right\}. \tag{5.1}$$

These integrals are obviously to be performed successively over $\Delta q^i_{(n)} = q^i_{(n)} - q^i_{(n-1)}$ with fixed $q^i_{(n)}$ (a consequence of backward time developement, just as in (2.4)). Using (4.1) one can now transform the integration volume $\mathrm{d}^r\Delta q^i_{(n)}$ to curved state space according to

$$\mathrm{d}^r\Delta q^i_{(n)} = J_{n,n-1}\,\mathrm{d}^r\Delta q^a_{(n)} \tag{5.2}$$

with the Jacobian $J_{n,n-1} = \partial(\Delta q^i_{(n)})/\partial(\Delta q^a_{(n)})$ given by

$$J_{n,n-1} = \det(e^i{}_{b(n-1)})\det\left\{\delta_a{}^b + \Gamma_{ac}{}^b\Delta q^c_{(n)} + \tfrac{1}{2}[\Gamma_{(ad}{}^b{}_{,c)} + \Gamma_{f(c}{}^b\Gamma_{ad)}{}^f]\Delta q^c_{(n)}\Delta q^d_{(n)} + \cdots\right\}_{(n-1)}.$$

Here parentheses around indices denotes their symmetrization, e.g.

$$\Gamma_{(ad}{}^b{}_{,c)} = \tfrac{1}{3}(\Gamma_{ad}{}^b{}_{,c} + \Gamma_{dc}{}^b{}_{,a} + \Gamma_{ca}{}^b{}_{,d}).$$

Using the well known identity

$$\det(1+B) = \exp\{\mathrm{tr}[\ln(1+B)]\} = \exp\left\{\mathrm{tr}\left(B - \frac{B^2}{2} + \frac{B^3}{3} - \cdots\right)\right\} \tag{5.3}$$

the above Jacobian reduces to

$$J_{n,n-1} = \det(e^i{}_{a(n-1)})\mathrm{e}^{A^\epsilon_{n,n-1}} = \sqrt{\frac{L}{L'(q^a_{(n-1)})}}\,\mathrm{e}^{A^\epsilon_{n,n-1}} \tag{5.4a}$$

where the final equality follows from (3.2) with $L' = \det(\ell^{ab})$, and

$$A^\epsilon_{n,n-1} = \Gamma_{ab(n-1)}^{a}\Delta q^b_{(n)} + \tfrac{1}{2}\left\{\Gamma_{(ab}{}^a{}_{,c)} + \Gamma_{d(c}{}^a\Gamma_{ab)}{}^d - \Gamma_{db}{}^a\Gamma_{ac}{}^d\right\}_{(n-1)}\Delta q^b_{(n)}\Delta q^c_{(n)} + \cdots. \tag{5.4b}$$

$A^\epsilon_{n,n-1}$ clearly contributes to the thermodynamic action. Now since $q^a_{(n)}$ is fixed in successive integrations over $\Delta q^a_{(n)}$ (refer to the remark made after equation (5.1)), we write the contribution of $L'(q^a_{(n-1)})$ in (5.4a) in terms of $L'(q^a_{(n)})$ keeping in mind that we want all the coefficients to be evaluated at the prepoint. These terms will then also contribute, as we shall see shortly, to the prepoint action. Thus we write, under our non-integrable coordinate transformation

$$\begin{aligned} e^i{}_{a(n)} &= e^i{}_a(q^a_{(n-1)} + \Delta q^a_{(n)}) \\ &= \left\{ e^i{}_a + \Delta q^b_{(n)} e^i{}_{a,b} + \frac{1}{2!}\Delta q^b_{(n)} \Delta q^c_{(n)} e^i{}_{a,bc} + \cdots \right\}_{(n-1)} \\ &= e^i{}_{d(n-1)} \left\{ \delta_a{}^d + \Gamma_{ab}{}^d \Delta q^b_{(n)} + \tfrac{1}{2}(\Gamma_{ab}{}^d{}_{,c} + \Gamma_{fc}{}^d \Gamma_{ab}{}^f) \Delta q^b_{(n)} \Delta q^c_{(n)} + \cdots \right\}_{(n-1)} . \end{aligned}$$

Using the identity (5.3), as before, yields

$$\sqrt{\frac{L}{L'(q^a_{(n-1)})}} = \sqrt{\frac{L}{L'(q^a_{(n)})}} \mathrm{e}^{-\bar{A}^\epsilon_{n,n-1}} \tag{5.5a}$$

where

$$\bar{A}^\epsilon_{n,n-1} = \Gamma_{ab(n-1)}{}^a \Delta q^b_{(n)} + \tfrac{1}{2}\Gamma_{ab}{}^a{}_{,c(n-1)} \Delta q^b_{(n)} \Delta q^c_{(n)} + \cdots . \tag{5.5b}$$

Substitution of (5.5a) in (5.4a) leads via (5.2) to

$$\mathrm{d}^r \Delta q^i_{(n)} = \sqrt{\frac{L}{L'(q^a_{(n)})}} \mathrm{e}^{A^\epsilon_{n,n-1} - \bar{A}^\epsilon_{n,n-1}} \mathrm{d}^r \Delta q^a_{(n)} . \tag{5.6}$$

It is clear that if our mapping were integrable, then $e^i{}_{(a,bc)} = e^i{}_{a,bc}$ and the index symmetrization in (5.4b) would become redundant, implying $A^\epsilon_{n,n-1} = \bar{A}^\epsilon_{n,n-1}$. Therefore, in view of (5.6), as far as trivial coordinate transformations are concerned, one could have used the naive transformation of the measure in (2.5) based on

$$\mathrm{d}^r q^i = \det(e^i{}_{a(n)})\, \mathrm{d}^r q^a = \sqrt{\frac{L}{L'(q^a_{(n)})}}\, \mathrm{d}^r q^a$$

which follows directly from (3.1). However, for the non-integrable mapping under consideration, it follows from (5.4b) and (5.5b) that to the lowest order

$$A^\epsilon_{n,n-1} - \bar{A}^\epsilon_{n,n-1} = -\tfrac{1}{6} R_{bc(n-1)} \Delta q^b_{(n)} \Delta q^c_{(n)}$$

with the Ricci tensor defined by (3.8). Substituting this in (5.6) yields via (5.1) for the transformed normalization condition

$$\begin{aligned} 1 &= \int W_<(q^a, t; q'^a, t')\, \mathrm{d}^r q^a \\ &= \lim_{\substack{N\to\infty \\ (\epsilon\to 0)}} (4\pi\epsilon k)^{-rN/2} \left\{ \prod_{n=1}^N \int \frac{\mathrm{d}^r \Delta q^a_{(n)}}{\sqrt{L'(q^a_{(n)})}} \right\} \exp \sum_{n=1}^N \left\{ -\frac{\epsilon}{k} \mathcal{L}^\epsilon_<(q^a_{(n)} - \Delta q^a_{(n)}, q^a_{(n)}) \right. \\ &\quad \left. -\tfrac{1}{6} R_{bc}(q^a_{(n)} - \Delta q^a_{(n)}) \Delta q^b_{(n)} \Delta q^c_{(n)} \right\} \end{aligned} \tag{5.7}$$

with $q^a = q^a_{(0)}$ and $q'^a = q^a_{(N)}$ and $\mathcal{L}^\epsilon_<$ given by (4.4a), of course. The appearance of the curvature term in the above is a manifestation of the non-integrable coordinate transformation. This term, being evaluted at the prepoint, gives the overall contribution to the effective thermodynamic Lagrangian and may be calculated perturbatively in the standard manner, as follows. In (5.7) we expand the exponential and write each single integral as

$$(4\pi\epsilon k)^{-r/2}\int \frac{\mathrm{d}^r\Delta q^a_{(n)}}{\sqrt{L'(q^a_{(n)})}}\, \mathrm{e}^{-G^\epsilon_n/k}\left(1-\frac{1}{6}R_{bc(n)}\Delta q^b_{(n)}\Delta q^c_{(n)}+\cdots\right)$$

where

$$G^\epsilon_n = \frac{1}{4\epsilon}\,\ell_{ab(n)}(\Delta q^a_{(n)}-\epsilon\chi^a_{(n)})(\Delta q^b_{(n)}-\epsilon\chi^b_{(n)})$$

is the Gaussian part of the action $\epsilon\mathcal{L}^\epsilon_<(q^a_{(n)}-\Delta q^a_{(n)}, q^a_{(n)})$. Evaluating the above integral using the well known results for Gaussian moments (listed in the appendix) gives the expression $(1-(k/3)\epsilon R_{(n)}+\mathrm{O}(\epsilon^2))$ with the scalar curvature R defined as in (3.8). This can also be thought of as coming from an integral

$$\lim_{\epsilon\to 0}(4\pi\epsilon k)^{-r/2}\int \frac{\mathrm{d}^r\Delta q^a_{(n)}}{\sqrt{L'(q^a_{(n)})}}\exp\left\{-\frac{\epsilon}{k}\mathcal{L}^\epsilon_<(q^a_{(n)}-\Delta q^a_{(n)}, q^a_{(n)})-\frac{k}{3}\epsilon R(q^a_{(n)}-\Delta q^a_{(n)})\right\}.$$

Thus equation (5.7) reduces to

$$1=\int W_<(q^a,t;q'^a,t')\,\mathrm{d}^r q^a$$

$$=\lim_{\substack{N\to\infty\\(\epsilon\to 0)}}(4\pi\epsilon k)^{-rN/2}\left\{\prod_{n=1}^{N}\int\frac{\mathrm{d}^r\Delta q^a_{(n)}}{\sqrt{L'(q^a_{(n)})}}\right\}$$

$$\times\exp\sum_{n=1}^{N}-\frac{\epsilon}{k}\left\{\mathcal{L}^\epsilon_<(q^a_{(n)}-\Delta q^a_{(n)}, q^a_{(n)})+\frac{k^2}{3}R(q^a_{(n)}-\Delta q^a_{(n)})\right\}.$$

Finally, restoring the integration volume $\mathrm{d}^r q^a_{(n)}$, we get

$$W_<(q^a,t;q'^a,t')=\lim_{\substack{N\to\infty\\(\epsilon\to 0)}}\frac{(4\pi\epsilon k)^{-rN/2}}{\sqrt{L'(q'^a)}}\left\{\prod_{n=1}^{N-1}\int\frac{\mathrm{d}^r q^a_{(n)}}{\sqrt{L'(q^a_{(n)})}}\right\}$$

$$\times\exp\sum_{n=1}^{N}-\frac{\epsilon}{k}\left\{\mathcal{L}^\epsilon_<(q^a_{(n-1)}, q^a_{(n)})+\frac{k^2}{3}R(q^a_{(n-1)})\right\}. \qquad (5.8)$$

This may be written in the continuum limit as

$$W_<(q^a,t;q'^a,t')=\frac{1}{\sqrt{L'(q'^a)}}\int_{q^a(t)=q^a}^{q^a(t')=q'^a}\mathrm{d}[q^a(t)]\,\exp\left\{-\frac{1}{k}\int_t^{t'}\mathrm{d}t\,\mathcal{L}'(\dot q^a(t),q^a(t))\right\} \qquad (5.9a)$$

where, as usual, the notation for the measure is symbolic and

$$\mathcal{L}'(\dot q^a,q^a)=\frac{1}{4}\,\ell_{ab}(\dot q^a-\chi^a)(\dot q^b-\chi^b)+\frac{k}{2}\,\chi^a_{;a}+\frac{k^2}{3}\,R \qquad (5.9b)$$

is the thermodynamic Lagrangian in the curved configuration space of far from equilibrium situations. Our result (5.9a,b) for the conditional probability agrees, upto differences in notation, with that obtained by Grabert and Green via stochastic considerations.

6. The Fokker–Planck equation in curved configuration space

We shall now use the path integral representation of the previous section to derive the Fokker–Planck equation in the curved state space of nonlinear irreversible processes. First, we shall cast the nonlinear conditional probability in a form suitable for our purpose.

We have from (5.2) and (5.4*a*) that

$$\mathrm{d}^r \Delta q^i_{(n)} = \sqrt{\frac{L}{L'(q^a_{(n-1)})}}\mathrm{e}^{A^\epsilon_{n,n-1}}\,\mathrm{d}^r \Delta q^a_{(n)}$$

Substituting this together with (4.4*a*) in the normalization condition (5.1), gives the transformed conditional probability in the form

$$W_<(q^a,t;q'^a,t') = \lim_{\substack{N\to\infty\\(\epsilon\to 0)}} \frac{(4\pi\epsilon k)^{-r/2}}{\sqrt{L'(q^a)}}\left\{\prod_{n=1}^{N-1}\int\frac{(4\pi\epsilon k)^{-r/2}}{\sqrt{L'(q^a_{(n)})}}\mathrm{d}^r q^a_{(n)}\right\}$$

$$\times\exp\sum_{n=1}^{N}\left\{-\frac{\epsilon}{k}\mathcal{L}^\epsilon_<(q^a_{(n-1)},q^a_{(n)})+A^\epsilon_{n,n-1}\right\}$$

so that the short-time conditional probability becomes

$$W_<(q^a,t;q^a_{(1)},t_1) = \lim_{\epsilon\to 0}\frac{(4\pi\epsilon k)^{-r/2}}{\sqrt{L'(q^a)}}\exp\left\{-\frac{\epsilon}{k}\mathcal{L}^\epsilon_<(q^a,q^a_{(1)})+A^\epsilon_{1,0}\right\} \tag{6.1}$$

where, of course as before, $q^a = q^a_{(0)}$. Now the system evolves backward in time according to

$$\Omega(q^a,t) = \int W_<(q^a,t;q^a_{(1)},t_1)\;\Omega(q^a_{(1)},t_1)\;\mathrm{d}^r q^a_{(1)}$$

which can be written, on using (6.1) and (4.4*a*, *b*), as

$$\Omega(q^a,t) = \lim_{\epsilon\to 0}\frac{(4\pi\epsilon k)^{-r/2}}{\sqrt{L'(q^a)}}\int \mathrm{d}^r\;\Delta q^a_{(1)}\mathrm{e}^{-G^\epsilon_0/k}\;I^\epsilon(\Delta q^a_{(1)}) \tag{6.2a}$$

where

$$I^\epsilon(\Delta q^a_{(1)}) = \Omega(q^a+\Delta q^a_{(1)},t+\epsilon)\exp\left\{-\frac{\epsilon}{k}\;H^\epsilon(\Delta q^a_{(1)})+A^\epsilon_{1,0}\right\} \tag{6.2b}$$

and

$$G^\epsilon_0 = \frac{1}{4\epsilon}\;\ell_{ab(0)}(\Delta q^a_{(1)}-\epsilon\chi^a_{(0)})(\Delta q^b_{(1)}-\epsilon\chi^b_{(0)}) \tag{6.2c}$$

is the Gaussian part of $\epsilon\mathcal{L}^\epsilon_<$ in (6.1) as prescribed by (4.4*a*). We proceed by expanding $I^\epsilon(\Delta q^a_{(1)})$ in terms of $\Delta q^a_{(1)}$, thereby reducing the integral in (6.2*a*) to a summation involving various Gaussian moments which are then to be evaluated in a straightforward manner. In this expansion, we need only keep terms which will finally contribute linearly in ϵ as higher order terms will be seen to vanish in the limit $\epsilon\to 0$. Since there is no risk of confusion, we drop suffices for simplicity so that

$$I^\epsilon(\Delta q^a) = \left[\Omega(q^a,t+\epsilon)+\Delta q^a\partial_a\Omega(q^a,t+\epsilon)+\tfrac{1}{2}\Delta q^a\Delta q^b\partial_a\partial_b\Omega(q^a,t+\epsilon)\right]$$

$$\times\Bigg[1+\Gamma_{ab}{}^a\Delta q^b+\frac{1}{4k}\;\Gamma_{bc}{}^a\;\chi_a\Delta q^b\Delta q^c$$

$$+\tfrac{1}{2}\left\{\Gamma_{(ab}{}^a{}_{,c)}+\Gamma_{d(c}{}^a\Gamma_{ab)}{}^d-\Gamma_{db}{}^a\Gamma_{ac}{}^d+\Gamma_{ab}{}^a\Gamma_{dc}{}^d\right\}\Delta q^b\Delta q^c$$

$$-\frac{1}{4\epsilon k}\Gamma_{abc}\Delta q^a\Delta q^b\Delta q^c - \frac{1}{4\epsilon k}\,\Gamma_{abc}\Gamma_{df}{}^d\Delta q^a\Delta q^b\Delta q^c\Delta q^f$$

$$-\frac{1}{4\epsilon k}\left\{\frac{1}{3}\,\ell_{ab}(\Gamma_{ed}{}^b{}_{,c} + \Gamma_{ed}{}^f\Gamma_{fc}{}^b) + \frac{1}{4}\,\Gamma_{cd}{}^b\Gamma_{eab}\right\}\Delta q^a\Delta q^c\Delta q^d\Delta q^e$$

$$\left.+\frac{1}{32\epsilon^2k^2}\,\Gamma_{abc}\Gamma_{def}\Delta q^a\Delta q^b\Delta q^c\Delta q^d\Delta q^e\Delta q^f\right] + \text{HOT}.$$

Denoting the second bracket collectively by $[\cdots]$, the above can be further reduced to

$$I^\epsilon(\Delta q^a) = \Omega(q^a, t+\epsilon)[\cdots] + \left(\Delta q^d + \Gamma_{ab}{}^a\Delta q^b\Delta q^d - \frac{1}{4\epsilon k}\Gamma_{abc}\Delta q^a\Delta q^b\Delta q^c\Delta q^d\right)$$

$$\times\partial_d\Omega(q^a, t+\epsilon) + \tfrac{1}{2}\Delta q^a\Delta q^b\partial_a\partial_b\Omega(q^a, t+\epsilon) + \text{HOT}. \tag{6.3}$$

These are all the terms that contribute linearly in ϵ, after having computed the Gaussian moments as prescribed by (6.2*a*). To this end, we invoke the results of the appendix again to obtain

$$\Omega(q^a, t) = \lim_{\epsilon\to 0}\Big[\Omega(q^a, t+\epsilon) + \epsilon(\chi^c - k\,\ell^{ab}\Gamma_{ab}{}^c)\,\partial_c\Omega(q^a, t+\epsilon)$$

$$+\epsilon k\,\ell^{ab}\partial_a\partial_b\Omega(q^a, t+\epsilon) + O(\epsilon^2)\Big]$$

or

$$-\partial_t\Omega(q^a, t) = \left\{k\,\ell^{ab}\partial_a\partial_b + (\chi^c - k\,\ell^{ab}\Gamma_{ab}{}^c)\,\partial_c\right\}\,\Omega(q^a, t). \tag{6.4}$$

This is sometimes called the backward Kolmogorov equation. The equivalence of (6.4) with the forward Kolmogorov equation (the Fokker–Planck equation)

$$\partial_t\Omega(q^a, t) = k\,\partial_a\partial_b(\ell^{ab}\Omega(q^a, t)) - \partial_c\left\{(\chi^c - k\,\ell^{ab}\Gamma_{ab}{}^c)\,\Omega(q^a, t)\right\} \tag{6.5}$$

is well known [11]. Using the prepoint form for the action, one can only derive the backward equation systematically. The Fokker–Planck equation cannot be obtained directly but only through invoking the well known equivalence between the solutions of the two equations [11].

Our Fokker–Planck equation (6.5) coincides with that quoted by Grabert and Green. However, the lack of distinction between the forward and backward time evolution makes their work less systematic in this respect.

Appendix. Gaussian moments

These, denoted below by $\langle\cdots\rangle$, are given by

$$\langle 1\rangle = \left\{L(4\pi\epsilon k)^r\right\}^{-1/2}\int \mathrm{d}^r\Delta q^i\ \exp\left\{\frac{1}{4\epsilon k}\,\ell_{ij}(\Delta q^i - \epsilon\chi^i)(\Delta q^j - \epsilon\chi^j)\right\} = 1$$

$$\langle\Delta q^i\rangle = \epsilon\chi^i$$

$$\langle\Delta q^i\Delta q^j\rangle = 2\epsilon k\,\ell^{ij} + \epsilon^2\,\chi^i\chi^j$$

$$\langle\Delta q^{i_1}\Delta q^{i_2}\cdots\Delta q^{i_{2n-1}}\rangle = \sum\langle\Delta q^{i_1}\Delta q^{i_2}\rangle\cdots\langle\Delta q^{i_{2n-3}}\Delta q^{i_{2n-2}}\rangle\langle\Delta q^{i_{2n-1}}\rangle$$

$$\langle\Delta q^{i_1}\Delta q^{i_2}\cdots\Delta q^{i_{2n}}\rangle = \sum\langle\Delta q^{i_1}\Delta q^{i_2}\rangle\cdots\langle\Delta q^{i_{2n-1}}\Delta q^{i_{2n}}\rangle.$$

Here, summation is over all possible combinations of such terms.

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