On the use of stochastic differential geometry for non-equilibrium thermodynamic modeling and control

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Abstract

We discuss the relevance of geometric concepts in the theory of stochastic differential equations for applications to the theory of non-equilibrium thermodynamics of small systems. In particular, we show how the Eells–Elworthy–Malliavin covariant construction of the Wiener process on a Riemann manifold provides a physically transparent formulation of optimal control problems of finite-time thermodynamic transitions. Based on this formulation, we turn to an evaluative discussion of recent results on optimal thermodynamic control and their interpretation.

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1. Introduction

Stochastic differential equations [1] provide a widely applied mathematical model for non-equilibrium dynamics. In particular, they are well adapted to the description of kinetics and finite-time thermodynamics of small systems such as bio-molecules, RNA and other molecular scale ‘machines’; see e.g. [2] for a review of theoretical and experimental aspects.

The application of stochastic differential equations to non-equilibrium phenomena bears a natural relation to geometry in an at least twofold way. First, even when a stochastic differential equation is used to model processes evolving in a flat Euclidean space, in arbitrary coordinates the scale of the noise in the stochastic differential equation imposes a Riemannian or sub-Riemannian metric (if there are constraints on the admissible directions of motion such as conditioning a set of variables to be the derivatives of other ones) on the space. The second way geometry sets in is more distinctive of applications to non-equilibrium physics. It originates from the use of second derivatives of thermodynamic potentials to impose a Riemannian metric on the set of equilibrium states. The consequent notion of thermodynamic length has then been exploited to characterize optimal processes in macroscopic and, very recently, microscopic, nano-scale processes (see [3, 4] for references and discussion).
In the present contribution, we show how a coordinate-independent geometric formalism may ease the analysis of control problems arising in the study of finite-time thermodynamics of small systems. By doing so, we derive two new results. First, we prove that the thermodynamic entropy production provides, independently of the frame reference adopted to describe a physical transition, a well-defined information-theoretic quantifier of the irreversibility of the transition. Second, we prove that entropy production minimizers in the class of differentiable protocols must satisfy a covariant Monge–Kantorovich optimal mass transport problem. This result extends to diffusions over Riemann manifolds the recently discovered refinement of the second law of thermodynamics for Langevin stochastic processes describing mesoscopic systems driven by conservative forces and interacting with thermal noise [5].

Although the required mathematical tools are well known in stochastic analysis (see e.g. [1, 6–8]), we are not aware of any previous application to stochastic thermodynamics. In what follows, we will generically denote by $\mathcal{M}$ a complete connected Riemannian manifold. We will also imply some further technical assumptions to guarantee probability conservation (see e.g. [9] for a concise discussion). In practice, our main focus here will be on the covariance of physical laws so that $\mathcal{M}$ can be thought of as $\mathbb{R}^d$ endowed with a Riemannian metric. In order to simplify the notation, thermodynamic expressions will be evaluated at unit temperature.

The outline of this paper is as follows. In section 2, we recall the covariant construction of a Wiener process on a Riemann manifold by means of the development map. In applications, a diffusion process is most often defined by assigning or measuring its ‘macroscopic’ observables, i.e. the drift, and the diffusion tensor. The development map then has a twofold use. First, it shows that in order to write the stochastic differential equations governing the diffusion, it is sufficient to compute the square root of the diffusion tensor in just one point rather than on the full $\mathcal{M}$ as non-covariant Itô or Stratonovich constructions otherwise require. Second, it allows us to derive a covariant form of Girsanov formula expressing the density of the diffusion process with respect to that of the Wiener process on $\mathcal{M}$. In section 3, we need the covariant Girsanov formula in order to show that the thermodynamic entropy production by a diffusion process during a finite-time transition between assigned states specifies the Kullback–Leibler divergence [10] between two probability measures. The first probability measure is obviously that of the original ‘physical’ diffusion process. The second probability measure describes the statistics of an auxiliary diffusion process obtained from the physical one by composing a time-reversal transformation in the spaces of measures of Markov processes with a deterministic time-reversal transformation of the drift field. The generically non-vanishing divergence between these two probability measures is a natural quantifier of the irreversibility induced by thermal fluctuations. In section 4, we use this result to attain a coordinate-independent derivation of the first two laws of thermodynamics. In section 5, we discuss the mathematical well-posedness of the minimization during a finite-time transition of thermodynamic functionals related to the entropy production such as heat and work. We show that the result of section 3 readily yields lower bounds for these functionals without directly invoking fluctuation-theorem-like arguments [11]. This is important because the notion of ‘optimal control’ depends upon the class of ‘admissible controls’. In other words, the possibility of determining a minimizer as the solution of a partial differential equation specifying the extremal of a variational problem is subordinate to the differentiability and boundary conditions imposed on the variations. The set of conditions required for the derivation of fluctuation relations may, however, a priori not define a class of admissible protocols that are natural for the formulation of an optimal control problem. Thus, the solution of the Monge–Kantorovich optimal mass transport problem we derive in section 5 minimizes the entropy production over the class of at least twice-differentiable protocols, driving in finite time the probability density of the system from one state to another. Generically, protocols
in this class are not in local equilibrium, in a sense which will be made mathematically precise with the state probability measure at the ends of the control horizon. In consequence, the optimization in the class of differentiable protocols provides only a lower bound for smooth transformations between equilibria. It is, however, important to stress that such a lower bound does not apply if protocols with 'jumps' are included in the class of admissible controls. In section 5, we explain the relevance of these observations for the problem of determining the optimal work protocol. We refer the reader to [12] for optimal control of thermodynamic transition described by Markov jump processes. We conclude section 5 by discussing the relation of a viscous regularization of the Monge–Kantorovich equations with the 'Schrödinger' diffusion problem [13]. To render the above considerations more transparent, we apply them in section 6 to a simple analytically tractable example.

2. Geometry and the development map

Differential geometry is most naturally formulated in the language of first-order forms. For this reason, the Stratonovich calculus [1] is commonly considered to have an edge on the Itô calculus when it comes to identifying geometric structures. Let us therefore start by considering a diffusion process \( \xi \equiv \{ \xi_t; t \in [t_0, t_1] \} \) specified by stochastic differential equations in the sense of Stratonovich

\[
\frac{d\xi_t}{dt} = \xi_t + \xi_t \circ \frac{d\beta_t}{dt}
\]

(1)
in a coordinate neighborhood \( U \subset \mathbb{R}^d \) centered e.g. around the initial condition \( \xi_{t_0} = x_0 \). The symbol \( \circ \) pinspoints the Stratonovich prescription. In (1), \( \beta_t : U \times [t_0, t_1] \to \mathbb{R}^d \) is some smooth map; Einstein convention is implied on the Latin indices \( i = 1, \ldots, d \) to pair the elements of a collection of \( d \)-independent one-dimensional Euclidean Wiener processes (Brownian motions) \( \beta_t = \{ \beta_t^i; t \in [t_0, t_1] \} \) to \( d \)-orthonormal frame fields \( \{ e_i \}_{i=1}^d \) specifying a basis for \( T_x \mathbb{R}^d \). Let us also endow \( U \) with a strictly positive, time-independent metric tensor \( g \) and require that for any \( x \in U \),

\[
\langle e_i, e_j \rangle_g := g_{ij} \quad (i, j = 1, 2)
\]

(2)

which is equivalent to

\[
e_i \otimes e_i = g^{-1}.
\]

(3)
The hypothesis of time independence of the metric tensor is physically relevant and will also serve to neaten the formalism. The extension to the time-dependent case is, however, straightforward and is of common use, for example, in the inquiry of Ricci flows; see e.g. [14, 15] for details. From (1), we can write for any \( x \in U \) the generator of the stochastic process \( x \) acting on any scalar function \( f : U \to \mathbb{R} \):

\[
\mathcal{L}_x f = \left( \mathcal{B}_x \cdot \partial_x + \frac{1}{2} \sum_{i} \xi_i \cdot \partial_x e_i \cdot \partial_x \right) f
\]

(4)

\( \mathcal{B}_x \equiv B^{ij} \partial_x^i \partial_x^j \), and \( A : \mathcal{B} \equiv \text{Tr} A^T \mathcal{B} \). The last equality in (4) motivates the identification of the inverse of the metric as the diffusion tensor of the process \( \xi \). A diffusion process is fully specified by the knowledge of the conditional expectation of its increments up to second order. Under the present hypotheses, these expectation values are

\[
\lim_{dt \downarrow 0} \mathbb{E}_{x,t} \left[ \frac{\xi_{t+dt} - \xi_t}{dt} \right] = \left( \mathcal{B}_x + \frac{1}{2} \sum_{i} \xi_i \cdot \partial_x e_i \right) (x, t) := B_t(x, t)
\]

(5)

the 'Itô drift', and

\[
\lim_{dt \downarrow 0} \mathbb{E}_{x,t} \left[ \frac{(\xi_{t+dt} - \xi_t) \otimes (\xi_{t+dt} - \xi_t)}{dt} \right] = g^{-1}(x)
\]

(6)
the diffusion tensor. It is therefore physically justified to take (5) and (6) as the data specifying a stochastic differential equation. We are now in the position to pinpoint two disadvantages related to the use of (1). For any \( O \in O(d) \), the group of orthogonal matrices, the vector-valued Wiener processes \( \bar{\beta} := [\bar{\beta}_1, \ldots, \bar{\beta}_d] \) and \( \Omega \beta \) are statistically equivalent. Let us denote with \( O(M) \) the collection of \( d \)-tuples \( \{x, e_1(x), \ldots, e_d(x)\} \) attached to any \( x \in M \). In the language of differential geometry, this collection forms the ‘bundle’ of orthonormal frames specified by the triple \( (O(M), O(d), M) \) [16, 1]. Since only (6) is observable, any element of the bundle must provide an equivalent description of the statistics of the process \( \xi \). Equation (1), however, is not invariant for different choices of orthonormal frames in the bundle. More explicitly, the same statistics can be equivalently described by the Stratonovich drift \( b_S \) or by its ‘gauge’ transform

\[
\bar{b}_S[O] = b_S - \frac{1}{2} (\Omega_{ij} \cdot \partial_s \Omega_{ij}) e_i.
\]  

This was already noted long ago in connection with the inquiry of the covariant path-integral representation of stochastic processes and Euclidean quantum mechanics over curved manifolds (see e.g. [17–19] for a more complete list of references; see also [20] for a discussion of gauge transformations in non-equilibrium thermodynamics). A second disadvantage is that the natural, coordinate-independent, definition of the generator of \( \xi \) acting on scalar functions is [21, 22]

\[
\mathcal{L} = (b \cdot \partial_s + \frac{1}{2} \Delta_{LB}) f
\]

with \( \Delta_{LB} \) being the Laplace–Beltrami operator and \( b \) a vector field which we will refer to as the covariant drift. In general, it is not possible to identify globally on \( M \) the Stratonovich drift with the covariant one, i.e. \( b_S = b \) unless the integrability condition

\[
\partial_s (v_1 \cdot e_i) = v_2 \cdot \partial_s (v_1, e)_g
\]

is satisfied for any constant vectors \( v_1, v_2 \). To interpret (9), we observe that it is satisfied if there exists a collection of scalar functions \( \{G_i\}_{i=1}^d \) such that

\[
\partial_s G_i = g \cdot e_i
\]

whence it follows that

\[
\langle e_i, d\xi_s \rangle_g = dG_i(\xi_s)
\]

meaning that there exists a change of variables turning in (4) the frame fields \( \{e_i\}_{i=1}^d \) into the canonical basis of \( \mathbb{R}^d \). In other words, (10) states the existence of a privileged choice of global coordinates for which the noise becomes additive. In general, however, (9) is not satisfied since

\[
\Delta_{LB} f = g^{-1} : \partial_s \otimes \partial_s f - (\Gamma : g^{-1}) \cdot \partial_s f
\]

with \( \Gamma \) being the Christoffel symbols of the Levi-Civita connection on \( M \). In [22], Itô gave the expression in local coordinates of a stochastic differential equation (in the Itô sense) associated with (8):

\[
d\xi_s = (b - \frac{1}{2} \Gamma : g^{-1}) \, dt + e_i d\beta_{i,s}.
\]

A straightforward calculation then shows that (1) is equivalent to (13) if (9) is satisfied. The conclusion is that the Stratonovich equation (1) does not provide a coordinate-independent description of the dynamics. Furthermore, the inspection of (13) shows that the ‘Itô drift’ cannot transform as a vector field under the general change of coordinates. The Eells–Elworthy–Malliavin development map (see e.g. [1, 7, 8] for rigorous and pedagogic derivations) obviates these disadvantages. The idea is that a Wiener process can be pathwise-constructed on \( M \) by
'rolling' the manifold along the realizations of a Euclidean Brownian motion. Mathematically, this means that the Wiener process should be constructed as the solution of the system of Stratonovich differential equations:

\[
\begin{align*}
\text{d} \omega_t &= e^{-i \cdot} \text{d} \beta_t; \\
\text{d} e_{i,t} &= -\Gamma : e_{i,t} \otimes \text{d} \omega_t. 
\end{align*}
\]

As above, \( [\beta_t]_{t=0}^t \) are a collection of independent Wiener processes. Were they constant vectors, (14) could be couched in the form of a geodesic equation. Furthermore, upon converting (14a) into the Itô representation, we recover (13) for the vanishing covariant drift. An important further consequence of (14a) is that we can identify a stochastic process \( \xi \) as a local \( M \)-valued martingale if in any local chart it satisfies \([23, 1, 6]\)

\[
\begin{align*}
\text{d} \xi_t + \frac{1}{2} \text{d} \xi_t \otimes \text{d} \xi_t \equiv \text{d} \xi_t + \frac{1}{2} \Gamma : g^{-1} \text{d} t = \text{local Euclidean martingale}. 
\end{align*}
\]

In other words, the time integral of (15) is the proper quantity to check in order to verify whether a process is driven by a drift field. Three remarks are in order before concluding this short discussion of background results from the stochastic analysis. First, (14) admits a straightforward extension to diffusion processes on \( M \) driven by a drift field (semi-martingales). This is done simply by introducing a drift term into (14a). The drift specified in this way transforms under a general change of variables as an ordinary vector field. We do not need to take this step here explicitly since we can combine the Girsanov formula and the development map (14) to take drift terms into account. In particular, following [16], we can write the Girsanov formula in an explicitly covariant form using the equality

\[
\begin{align*}
\frac{d P_\xi}{d P_\omega}(\omega) &= e^{-\int \langle b, e_i ; t \rangle g^{-1/2} \text{d} t} \\
\frac{d P_\xi}{d P_a}(a) &= e^{\int \langle b, e_i ; t \rangle g^{-1/2} \text{d} t},
\end{align*}
\]

for

\[
\nabla \cdot b = \frac{1}{\sqrt{|g|}} \partial^\rho (\sqrt{|g|} b^\rho).
\]

The symbol \( \nabla \) betokens here and in what follows the covariant derivative operation compatible with the metric \( g \). The stochastic integral in the first row of (16) is in Itô sense. The use of the time-symmetric Stratonovich integral in the second row of (16) exhibits the fact that the argument of the exponential transforms indeed as a scalar under a change of coordinates. Second, if the metric is time dependent, we must include a drift term \( 1/2 \partial_t g^{-1} \) in (14b) to preserve the metric compatibility of the connection. Finally [21], the adjoint of (8)

\[
\mathcal{L}^\dagger f = -\nabla \cdot bf + \frac{1}{2} \Delta_{\text{LB}} f
\]

is defined with respect to the invariant Riemann volume:

\[
\text{d}^\star \text{d} \equiv \text{d}^\star x \sqrt{\det g(x)}.
\]

The covariant density \( k \) is then related to the transition probability density with respect to the Lebesgue measure \( p \) by the equation

\[
p(x_2, t_2 | x_1, t_1) = \sqrt{\det g(x_2)} k(x_2, t_2 | x_1, t_1)
\]

for any coordinates \( x_i, i = 1, 2 \) in a local chart \( U \), and any \( t_2 \geq t_1 \) in \([t_0, t_f]\).
3. Kullback–Leibler divergence and time reversal

Our aim is now to derive, with the help of the development map, the covariant expression of time-reversal relations which can be used as bridge relations between the theory of stochastic processes and finite-time thermodynamics of small systems. Under rather general smoothness assumptions [24, 25], if we know the probability \( m = \sqrt{|G|} n \) and the transition probability densities \( p = \sqrt{|G|} k \) of a semi-martingale process \( \xi \) in the full-time horizon \([t_0, t_1]\), we can construct the time-reversed time evolution by requiring for any \( t_0 \leq t_1 \leq t_2 \leq t_1 \)

\[
n(x_2, t_2) \\ k^{(r)}(x_1, t_1 | x_2, t_2) = k(x_2, t_2 | x_1, t_1) n(x_1, t_1).
\]

(21)

If \( \xi \) is adapted to an \( M \)-valued Wiener process (14), we can use the Girsanov formula (16) to evaluate averages of non-anticipative functionals of \( \xi \) as averages with respect to \( \omega \). As noted in [26], we can also take advantage of the invariance under time reversal of the Wiener process to express the density of a \( \text{backward} \) process \( \xi = (\xi_t : t \in [t_0, t_1]) \)

\[
\frac{dP^\xi}{dP_\omega}(\omega) = e^{\int_0^{t_1} \left[ b_\omega(x_t, \hat{d} \xi_t) - \frac{1}{2} g_\omega \left( x_t, \hat{d} \xi_t \right)^2 \right] (\omega, t) = e^{\int_0^{t_1} \left[ b_\omega(x_t, \xi_t) + \frac{1}{2} g_\omega \left( x_t, \xi_t \right)^2 \right] (\omega, t).}
\]

(22)

The symbol \( \hat{\cdot} \) appearing in the first row of (22) indicates that the stochastic integral is defined as averages with respect to \( \omega \). In other words, the first stochastic integral in (22) is an Itô integral with respect to the filtration of the ‘future’, while the second is a Stratonovich integral. The requirement \( \hat{\xi} \overset{\text{law}}{=} \xi \) translates into

\[
n(\omega_t, t_2) \\ \frac{dP^\xi}{dP_\omega}(\omega) = n(\omega_t, t_1) \\ \frac{dP^\xi}{dP_\omega}(\omega)
\]

(23)

whence we immediately recover the classical result

\[
b(x, t) = \hat{b}(x, t) + g^{-1} \cdot \partial_x n(x, t).
\]

(24)

Both sides of the equation are now well-defined vector fields. We thus see that the same probability measure admits a forward and backward dynamics representation in terms of two different drift vector fields. A natural question is how it is possible to compare quantitatively the stochastic time-reversal operation defined by (23) with the deterministic counterpart specified by the inversion of the sign of the drift. This question can be answered by considering a forward, auxiliary process \( \bar{\xi} \) absolutely continuous with respect to \( \xi \) defined by the replacement

\[
b(\cdot, \cdot) \mapsto \bar{b}(\cdot, \cdot) := -b(\cdot, \cdot)
\]

(25)

in the stochastic differential equation driving \( \xi \). The rationale behind (25) is to combine the stochastic with the deterministic time reversal. As a consequence, for a gradient-type drift (see equation (33)) at equilibrium, (25) reduces to the identity \( b = \hat{b} \). A widely applied quantifier of the discrepancy between two probability measures is provided by their Kullback–Leibler divergence [10]. It is therefore natural to quantify the cost of (23) of the process \( \xi \) with respect to \( \bar{\xi} \):

\[
\mathcal{K}(P_\xi || P_{\bar{\xi}}) := E^{(\xi)} \ln \frac{dP_\xi}{dP_{\bar{\xi}}}(\xi) = E^{(\omega)} \ln \frac{dP_\xi}{dP_{\omega}}(\omega) \ln \left( \frac{dP_\xi}{dP_{\omega}} \frac{dP_\omega}{dP_{\bar{\xi}}} \right)(\omega).
\]

(26)

The notation \( E^{(\xi)}(\cdot) \) emphasizes that the average is with respect to the measure of \( \xi \) (\( \omega \)). The Kullback–Leibler divergence is by construction a positive-definite quantity. The direct evaluation of (26) yields

\[
\mathcal{K}(P_\xi || P_{\bar{\xi}}) = E^{(\xi)} \int_{t_0}^{t_1} \nabla_{\xi_t} \cdot (b + \hat{b}) \xi_t \hat{d} \xi_t + E^{(\xi)} \int_{t_0}^{t_1} d\xi_t \frac{\nabla_{\xi_t} \cdot (b + \hat{b}) + \| b \|^2_2 - \| \hat{b} \|^2_2}{2}.
\]

(27)
Upon inserting (24) into (27) and using the probability conservation and the covariant Fokker–Planck equation
\[(\partial_t - \mathcal{L}^\dagger)n = 0,\] we can prove that the Riemann integral in (27) vanishes. The integrand of the Stratonovich stochastic integral is instead proportional to the current velocity [24, 25] of the process \(\xi_t\):
\[v = \frac{b + \tilde{b}}{2}.\] The current velocity enjoys two important properties. First, for expectation values of Stratonovich line integrals it plays the same role as the Itô drift (5) for expectation values of Itô line integrals: for any smooth, mean square integrable vector field \(h\), the equality
\[E(\xi)\int_{t_0}^{t_f} \langle h \cdot d\xi \rangle_g = E(\xi)\int_{t_0}^{t_f} dt \langle h \cdot v \rangle_g\] holds true under the assumption that integrations by parts do not bring about boundary terms. Second, in terms of the current velocity, the covariant Fokker–Planck equation reduces to the deterministic mass conservation equation:
\[\partial_t n + \nabla \cdot v n = 0.\] Combining (30) with (24) and (28), we finally arrive at
\[K(P_\xi|P_{\xi_0}) = 2 E(\xi)\int_{t_0}^{t_f} dt \|v\|^2_g.\] The right-hand side of (32) is proportional to the ‘kinetic energy’ specified by the current velocity of the system. Its physical interpretation [27, 28] (see also [29–31]) is that of entropy production during the transformation. The way we arrived at (32) differs to some extent from that of [32–34]. There, the role of the Kullback–Leibler divergence is played by an ‘action functional’ defined by contrasting the forward dynamics with its path-space time reversed defined by inverting the arrow of time \(t \mapsto t + t_0 - t\), in analogy with what was done to prove fluctuation theorems in hyperbolic dynamics [35]. The entropy production relation can also be regarded as the continuum limit under diffusive scaling of the analogous relation found in [12] for Markov jump processes.

4. Stochastic thermodynamics

Let us now examine the consequences of (32) for optimal control in thermodynamic functionals. We thus consider a dynamical system driven by time-dependent gradient-like drift
\[b(x, t) = -g^{-1}(x) \cdot \partial_x U(x, t)\] which is a stylized model of a mechanical potential subject to an external control. The current velocity in such a case becomes
\[v(x, t) = -g^{-1}(x) \cdot \partial_x \left(U + \frac{1}{2} \ln n \right)(x, t).\] Drawing from [36], we define the work done on the system as
\[\mathcal{W}_{t_0, t_f} = E(\xi)\int_{t_0}^{t_f} dt \partial_x U(\xi_t, t) = E(\xi) U(\xi_t, t)|_{t_0}^{t_f} - E(\xi) \int_{t_0}^{t_f} \langle d\xi_t \circ g^{-1}(\xi) \cdot \partial_x U(\xi_t, t) \rangle_g.\]
If we require the first law of thermodynamics to hold true, we must identify the heat as
\[ Q_{t, t_o} = -\mathbb{E}^{(E)} \int_{t_o}^{t} (d\xi_t \circ g^{-1}(\xi_t) \cdot \partial_t U(\xi_t, t)) g. \] (36)

Under the present conventions, the local equilibrium condition is
\[ \nabla_x \cdot g^{-1} \cdot (n \partial_x U + \frac{1}{2} \partial_x n) = 0. \] (37)

Correspondingly, we define the osmotic velocity \([24, 25]\) as
\[ u(x, t) := \frac{1}{2} (b - \tilde{b})(x, t) = \frac{1}{2} g^{-1}(x) \cdot \partial_x \ln n(x, t) \] (38)

and the scalar (i.e. coordinate-independent) expression of the Gibbs–Shannon entropy:
\[ S(t) = -\frac{1}{2} \mathbb{E}^{(E)} \ln n(\xi_t, t) \equiv -\frac{1}{2} \int_M dM \psi (n \ln n)(x, t). \] (39)

Note that the definition (39) of the Gibbs–Shannon entropy differs from that given in [37, 28] by a prefactor \(\frac{1}{2}\) dictated by the convention adopted here for the diffusion tensor, and by an addend proportional to \(\ln \sqrt{|g|}\) which does not transform as a scalar under change of coordinates. If we now add and subtract the osmotic velocity to the integrand in (35) and (36), and use the probability conservation and the identity (30), we arrive at the manifestly coordinate-independent representations of the released heat:
\[ Q_{t, t_o} = -[S(t) - S(t_o)] + \mathbb{E}^{(E)} \int_{t_o}^{t} dt \|v\|^2_g. \] (40)

and of thermodynamic work
\[ W_{t, t_o} = \mathcal{F}(t) - \mathcal{F}(t_o) + \mathbb{E}^{(E)} \int_{t_o}^{t} dt \|v\|^2_g. \] (41)

In (41), the Helmholtz free energy of the system is
\[ \mathcal{F}(t) \equiv U(t) - S(t) = \mathbb{E}^{(E)} (U + \frac{1}{2} \ln n)(\xi_t, t) := -\mathbb{E}^{(E)} \psi (\xi_t, t). \] (42)

The advantage of introducing here the \textit{scalar} quantity \(\psi\) to denote the free energy density emerges when contrasting the definitions of the current and osmotic velocities with (33). We then recognize that the current velocity is the gradient of the Helmholtz free energy density:
\[ v(x, t) = g^{-1}(x) \cdot \partial_x \psi(x, t). \] (43)

It is worth noting that the Helmholtz free energy \(\psi\) density (42) coincides with the potential similarly denoted in [37] owing to a cancellation of terms proportional to \(\ln \sqrt{|g|}\) between the individually non-coordinate-independent expressions of the internal energy and the Gibbs–Shannon entropy thereby used. Similar considerations, exploiting the time independence of the Riemann metric, also guarantee that the expression for the released heat of [37] does coincide with the one given here. The same is true for the work whose expression (41) has been also obtained in [38] using, however, arguments valid only in the weak noise limit.

5. Optimal control

Expressions (40) and (41) evince that the current velocity formulation of Langevin thermodynamics is natural from the point of view of control theory. There are at least two kinds of considerations supporting this claim. First, by (31), the current velocity maps the original stochastic control problem into a deterministic control one. Such a mapping exists for any smooth diffusion but is of limited practical use if the drift is known \textit{a priori} and the problem is to derive the evolution of the density. It becomes useful for control purposes when
the drift is not known but must be determined by minimizing a ‘cost’ functional over a suitable space of admissible controls. The second consideration is that the functional dependence of the entropy production on the current velocity readily enforces the coercivity condition (see e.g. [39] p 33: convexity with growth faster than linear) which plays an important role in the variational calculus to prove the existence of extremal solutions. A direct consequence of these considerations is the recovery of Jarzynski’s

\[ \mathcal{W}_{t_0, t_f} \geq F(t_f) - F(t_0) \]  

and ‘finite-time Landauer’s’ [40] inequalities

\[ Q_{t_0, t_f} \geq -[S(t_f) - S(t_0)]. \]  

The interpretation of (45) as Landauer’s inequality stems from the identification of the heat release with the entropy variation of the environment. By (34), the current velocity vanishes at equilibrium. As a consequence, inequalities (44) and (45) become tight for transitions described by a jump between two ‘equilibrium’ states. Physically, jumps are mathematical mock-ups for transitions occurring at the fastest admissible timescale. As such, they are not suited to describe macroscopic control of a nano-system. It is therefore relevant to look for minima of thermodynamic indicators by restricting the space of admissible controls to those guaranteeing a smooth behavior of the current velocity. In order to achieve this goal, let us recall that given a forward Markov process \( \eta \), deterministic or stochastic, with the generator \( \mathcal{G} \) depending on a control \( u \), the canonical form of cost functionals considered in the control theory [39] is

\[ A(x, t) = E_{\eta, t}^{(u)} \Psi(\eta_t) + E_{\eta, t}^{(u)} \int_{t_0}^{t_f} dt L(\eta_t; \eta, u). \]  

Some regularity assumptions standing, it is a priori tenable to expect the ‘cost functional’ \( A \) to admit a minimum over the space of smooth controls \( u \) if the ‘running cost’ \( L \) depends coercively on \( u \) and the ‘terminal cost’ \( \Psi \) is some assigned function independent of \( u \). The minimum

\[ J_*(x, t) = \min_u A(x, t) \]  

is usually referred to as the ‘value function’. Under these hypotheses, the solution of the Hamilton–Jacobi–Bellman equation

\[ \partial_t J_* + \min_u \{ \mathcal{G}_u J_* + L \} = 0 \]  

\[ J_*(x, t_f) = \Psi(x) \]  

corresponding to the smallest value of \( A \) (in the case of multiple minima in (48a)) specifies the value of the optimal control \( u_* \) for any \( t \) in a closed horizon \([t_0, t_f]\) if the resulting \( \mathcal{G}_{u_*} \) is a well-defined generator of a Markov process. The properties that a solution of (48) must enjoy in order to satisfy such a self-consistency condition are determined by the so-called verification theorems [39, 41]. Linearity of the Kolmogorov pair of equations governing a Markovian dynamics extends (48) to expectations of \( A \) with respect to the measure of \( \eta \) evolving from non-localized initial density assigned at time \( t = t_0 \) [42]. Namely, if we denote variations with respect to the control \( u \) by a ‘prime symbol’, we can couch the variation of \( E^{(u)} A \) into the form

\[ (E^{(u)} A)'(\eta_{t_0}, t_f) = \int_\mathbb{M} d\mu_{t_0, t} (n_{t_0} \Psi)(x, t) + \int_{t_0}^{t_f} dt \int_\mathbb{M} d\mu_{t_0, t} \left( n_{t_0} L + n_{t_f} L' \right)(x, t). \]
If we now require the ‘dynamic programming’ (non-homogeneous backward Kolmogorov) equation to hold for any admissible control
\[(\partial_t + G_u)J + L = 0,\] (50)
we obtain for \(n'_\eta(\cdot, t_0) = 0\)
\[(E^{(\eta)}A)' = \begin{array}{l}
\int_M d^n_x [n'_\eta (\Psi - J)](x, t) + \\
\int_{t_0}^t dt \int_M d^n_x \left\{ (\partial_t - G^\dagger_u)n_\eta \right\} (x, t) \end{array}.\] (51)
The variation yields a stationary point if (48b) is satisfied, the probability density evolves for any \(u\) according to the dynamics specified by the adjoint action of \(G_u\) and the optimal control is fixed by the same condition as in (48a). If, furthermore, the generator is linear in the control \(u\), the convexity of \(L\) readily implies that the stationary point is a minimum
\[(E^{(\eta)}A)'' = \begin{array}{l}
\int_{t_0}^t dt \int_M d^n_x (n_\eta L'')(x, t) \geq 0.\end{array}\] (52)
The dynamic programming equation (50) has the hydrodynamic interpretation of a material derivative along the realizations of the Markov process \(\eta\). Requiring it to hold \textit{a priori} substantiates Bellman’s idea that optimal control stems from a condition imposed \textit{locally} during the time evolution [39, 41]. Within this framework, the probability evolution must be regarded as the adjoint transport equation which may be non-local owing to the boundary conditions and must hold in the same time horizon \([t_0, t_f]\) where (50) is defined. In [42], it was also shown that the above chain of steps also holds if the running cost \(L\) depends upon the derivatives of the control. This was originally exploited in [5] to unveil the relation between optimal thermodynamic control and hydrodynamic mass transport. The formulation in terms of the current velocity, however, renders this extension no longer required for thermodynamic control.

In the application of the control-theory toolkit to expressions such as (41), we are confronted with a subtle difficulty. While the entropy production specifies a well-defined coercive running cost, the interpretation of the terminal cost is more problematic. Namely, a candidate smooth optimal control must satisfy the stationarity condition
\[\partial_x J_\star + 2 g \cdot v = \partial_x (J_\star + 2 \psi) = 0\] (53)
and the terminal condition (we suppose that no optimization is carried out over the initial state)
\[J_\star (x, t_f) = \Psi(x)\] (54)
Contrasting (53) and (54) with (43), it is evident that the terminal condition cannot be interpreted as the end-horizon value of the free energy density of a smooth optimal protocol since in general, \(\psi(\cdot, t_f) \neq \Psi(\cdot)\). Furthermore, a process jumping at \(t_f^-\) from a state of non-vanishing current velocity cannot be considered optimal, independent of the prescription adopted for the probability density at time \(t_f\). Namely, if we enlarge the space of admissible protocols to encompass jump processes, we know \textit{a priori} that the infimum is attained by an instantaneous transition between ‘equilibria’. In the latter case, the current velocity and the running cost vanish identically in the full control horizon and the work coincides with the free energy difference. The conclusion is that the ‘optimal work’ protocol proposed in [43] cannot be justified using the Hamilton–Jacobi–Bellman theory and Langevin dynamics alone. It appears instead to describe an optimal control strategy if the Langevin dynamics is embedded into a higher order Markovian dynamics [37] following ideas closely reminiscent of the ‘valley method’ (see e.g. [44]). The ‘valley method’ is a technique which aims to justify the stationary
point approximation to path integrals when no exact classical field configuration can match the required boundary conditions. In the context of work optimization, the valley method has a simple physical interpretation: it penalizes protocols varying with large acceleration. Hence, it substantiates the role of inertia often invoked in heuristic arguments for deriving the qualitative behavior of the optimal protocol. Finally, it is worth stating clearly that if the terminal cost (54) is interpreted only as the variation of an external potential without an explicit relation with $\psi$ in the control horizon $[t_0, t_f]$, then the protocol found in [43] is optimal according to standard verification theorems (see e.g. the discussion in sections III.5– III.8 of [39]). In [37], it was then shown that the variation of the value function of the latter model across the control horizon coincides with the work done on the system in the valley model in the limit of vanishing inertia.

A control problem which lends itself to a more transparent physical interpretation is that of the minimization of the entropy production between assigned probability densities at the end of the control horizon. The analytic and numerical treatments of this problem have been inquired into in detail in [28]. It is worth drawing attention here to some aspects of this problem which are not discussed in [37, 28]. By (32), the problem can be equivalently formulated in terms of the minimization of the Kullback–Leibler divergence associated with a time-reversal operation. It is instructive to contrast thermodynamic entropy production minimization with the control problem defining the so-called Schrödinger diffusion; see e.g. [13, 45–47]. Given two probability densities at the end of a control horizon and a reference diffusion process, the Schrödinger diffusion problem determines the smoothly interpolating diffusion obtained from the reference process by a deformation of the drift under the requirement that the Kullback–Leibler divergence between the two processes be at a minimum value. If the reference process is the Wiener process, then the Schrödinger diffusion corresponds to treat an analogous quantity as the running cost instead of the entropy production, in which the current velocity is replaced by the forward drift of the process. Correspondingly, the associated control problem is converted from deterministic to stochastic. A widely used approach to deterministic control is to prove the existence and uniqueness of solutions in a viscosity sense [39]. In the simplest cases, this means constructing solutions as the inviscid limit of an ultraviolet regularization of the Hamilton–Jacobi equation by adding a Laplacian. The Monge–Ampère–Kantorovich method [48] applied in [28] to study the nucleation at the minimum entropy production is an example of this general ideology. This observation allows us also to attribute a direct physical interpretation to the regularized entropy production minimization problem. Namely, in the presence of any finite viscosity, we can interpret the minimizer of the Kullback–Leibler divergence (32) as the drift solving an associated Schrödinger diffusion problem.

6. An explicit example

We consider the minimization of the entropy production $E$ for $\mathcal{M} = \mathbb{R}^d$ endowed with a trivial metric tensor in a transition between two states, respectively, specified by densities $m_0$ and $m_f$ assigned at the end of a control horizon $[t_0, t_f]$. The viscosity solution of the corresponding Monge–Kantorovich problem is obtained as the limit for vanishing $\kappa$ of the system

$$\partial_t \psi + \frac{1}{2} \| \partial_q \psi \|^2 + \frac{\kappa}{2} \partial^2_q \psi = 0$$  \hspace{1cm} (55a)

$$\partial_t m + \frac{1}{\tau} \partial_q \left( m \partial_q \psi \right) = \frac{\kappa}{2} \partial^2_q m.$$  \hspace{1cm} (55b)
In (55), we rescaled the free energy density by a parameter $\tau$ which was set to unity in the previous sections. For any finite $\kappa$, we associate with (55) the Onsager–Machlup functional

$$\mathcal{O} = \int_{t_0}^{t_f} ds \left\{ \frac{\|\dot{\xi}_s - \frac{1}{2}\partial_q \psi\|^2}{2\kappa} + \frac{1}{2\tau} \dot{\psi}^2 \right\} = \frac{\psi(t_f) - \psi(t_0)}{\kappa \tau} + \int_{t_0}^{t_f} ds \frac{\|\dot{\xi}_s\|^2}{2\kappa}. $$

A straightforward Gaussian path-integral calculation (see e.g. [49] for details) allows us to prove

$$\partial_q \psi(q, t) = \int_{\mathbb{R}^{2d}} d^d q_f (\partial_q \psi)(q_f, t_f) e^{-\frac{\|q_f - q\|^2_{2(t_f - t)}}{2\kappa + \kappa\tau}}$$

which in the limit of vanishing $\kappa$ yields for all $t \in [t_0, t_f]$

$$\psi(q, t) = \sup_{q_f} \left\{ \psi(q_f, t_f) - \frac{\tau\|q_f - q\|^2_{t_f - t}}{2(t_f - t)} \right\}. $$

The map $\Phi(q, t; t_f)$ attaining the sup in (57) is usually referred to as the Lagrangian map. We can then couch the solution of (55) in the form

$$m(q, t) = m_t(\Phi(q, t; t_f))$$

for all $t \in [t_0, t_f]$ so that in particular, we must have

$$m_0(q) = m_0(\Phi(q, t_0; t_1)).$$

Solving the latter equation determines $\psi(q_f, t_f)$. If we now suppose

$$m_0(q) = \left( \frac{\beta}{2\pi \sigma_0^2} \right)^{d/2} \exp \left\{ -\beta \frac{\|q - q_0\|^2}{2\sigma_0^2} \right\}$$

$$m_t(q) = \left( \frac{\beta}{2\pi \sigma_t^2} \right)^{d/2} \exp \left\{ -\beta \frac{\|q - q_t\|^2}{2\sigma_t^2} \right\},$$

we see that a quadratic ansatz for $\psi(q_f, t_f)$ yields a linear Lagrangian map, the free parameters of which can be chosen such as to satisfy (59). Finally, we obtain for the entropy production

$$\mathcal{E} = 2 \int_{\mathbb{R}^{2d}} [m_t(q)\psi(q, t_f) - m_0(q)\psi(q, t_0)]$$

$$= \frac{\tau\|q_t - q_0\|^2}{(t_f - t_0)} + \frac{d\tau\|\sigma_t - |\sigma_0\|^2}{\beta(t_f - t_0)}. $$

7. Conclusions

In conclusion, we showed how a coordinate-independent formalism for stochastic differential equations provides a convenient formulation of control problems arising in stochastic thermodynamics. In doing so, we restricted our attention to time-independent diffusion tensors. This is not too restrictive under the hypothesis that mechanical forces and control parameters are most naturally encapsulated in the drift field, while the diffusion coefficient contains purely geometric information. We also analyzed how the local nature of the Bellman principle are most naturally encapsulated in the drift field, while the diffusion coefficient contains purely geometric information. We also analyzed how the local nature of the Bellman principle affects the optimal control equations. Preserving the adjoint structure of the Kolmogorov pair requires, for example, that jumps in the protocol which are governed by the backward Kolmogorov equation bring about jumps in the forward Kolmogorov equation governing the probability density evolution. Hence, it is an essential modeling question to assess a priori which is the physically relevant space of admissible protocols and whether and how to describe the procedures to switch on and off the optimal protocol at the end of the control horizon.
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