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Document Version
Publisher's PDF, also known as Version of record

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Abstract. We consider fluxes and forces in Markov chains. In physics, the concept of so-called iso-surfaces has recently been introduced. In generic cases, there are infinitely many associated iso-dissipation forces. We first show that this is due to different notions of duality, each giving rise to dual force. We then study Hamiltonians associated to variational formulations of Markov processes, and develop different decompositions for them.

1. Introduction

Many processes in nature are directional in time, with diffusion being a simple but prominent example. In this article, we call these processes non-reversible, for reasons explained below. Further examples of non-reversible processes are drift-diffusion processes,

$$\partial_t \rho = -\mathrm{div}(f\rho) + \Delta\rho, \tag{1}$$

where ρ is a density and f is a field. Here the nature of the field f matters: if $f = \nabla V$ for some potential V, then the evolution can be understood in terms of an underlying free energy. If f is not a gradient vector field, i.e., no such V exists, then significant qualitative changes occur. These changes can have practical applications. For example, a system governed by a free energy converges under suitable conditions to equilibrium. Non-gradient terms change the rate of convergence, and can be used to accelerate the convergence (see, e.g., [1] for an analysis on the level of Markov chains). This is sometimes visualised with milk being dropped in a cup of coffee: The milk will diffuse, and the mixture which will eventually reach equilibrium (the homogeneous mixture of milk and coffee) without interference, but will reach equilibrium much faster if stirred by a spoon.

This analogy can only lead so far. A more careful analysis reveals that processes can often be decomposed in different components, which often satisfy suitable orthogonality relations. The understanding of such splits help to understand acceleration of convergence to equilibrium. For example, one can think of convergence to equilibrium as decreasing the free energy, thus undergoing a suitable gradient descent. If this takes place in a shallow part of the energy landscape, then the convergence will be slow. If there is an additional drift "orthogonal" to the gradient descent, then this can lead to steeper regions being reached, where convergence is faster.

The situation gets even more complicated in processes out of equilibrium. One can think of a one-dimensional bar with both ends held at different systems. Then a cost is required to

maintain the steady state, unlike the maintenance of the steady state in equilibrium. This cost is sometimes called housekeeping heat. The analysis of such phenomena is a very active field in stochastic thermodynamics. An example is recent work by Dechant, Sasa and Ito [2, 3] on the geometric decomposition of entropy production in housekeeping, excess and coupling.

There are various levels on which non-reversible processes can be looked at – on the continuum scale in form of a partial differential equation as in (1), or on the scale of underlying Markov processes. We will largely focus on Markov processes. One reason is that their structure is remarkable in the following sense: The evolution can be described in terms of forces F and fluxes j, and the relation between them is always the same (equation (3) below); the rates, which differentiate different Markov processes, enter through the mobility (equation (4) below). The price to pay is that the force-flux relations on the level of Markov chains are necessarily nonlinear. Section 2 summarises these classic results. The focus on Markov chains also explains the slightly unusual terminology "non-reversible": This is to avoid the term "irreversible", which has a different meaning for Markov processes.

1.1. Outline of the paper

The paper combines two thrusts of investigation presented in Section 2 and Section 3. In both sections, we use the knowledge that the most likely evolution of a Markov chain can (in suitable situations) be described by a variational principle, a so-called large deviation principle. There, the pathwise evolution appears as minimiser of a functional. The functional is called rate functional and the integrand is here denoted as Lagrangian. It is the Lagrangian functional that plays a central role in both sections.

In Section 2, we first summarise some key notions for the description of Markov processes in terms of forces and fluxes. We then explain the non-uniqueness of the so-called iso-dissipation force recently introduced in the physics literature [4] in a mathematical way. The iso-dissipation force is related to the force of the system through an equation involving a dissipation potential of the Lagrangian functional, see (10) below. This characterisation allows us to identify an iso-dissipation force to a dual force and, using this relation, to show its non-uniqueness.

In Section 3, we consider the Legendre dual of the Lagrangian, thus a Hamiltonian. The central results of this section are various decompositions of the Hamiltonian into reversible and irreversible components. We also discuss an application of these splittings to diffusive processes in terms of the Fokker-Planck equation. Here we start from a general decomposition of the Hamiltonian into two Hamiltonians and obtain a general decomposition for the Lagrangian valuated at 0, see Proposition 3.3. The decomposition may come from different ways that have been studied in the literature, such as from a decomposition of fluxes and forces [5, 6, 7, 8], hydrodynamic limits of many-particle systems [9] (which often impose some specific structures on the functionals) or from a symmetric-antisymmetric decomposition of the generator [10].

2. Orthogonality of forces and decomposition of the entropy production

In this paper, we consider an ergodic Markov process $(X_t)_{t\geq 0}$ with generator $\mathcal{L}$ and a unique invariant measure π. The time evolution of the probability density ρ_t of X_t can be written in terms of the master equation (also called Fokker-Planck or forward Kolmogorov equation),

$$\dot{\rho}_t = \mathcal{L}'(\rho_t) \tag{2a}$$
$$= -\mathrm{div}[j(\rho_t)] \tag{2b}$$
$$= -\mathrm{div}[a(\rho_t)\phi(F(\rho_t))], \tag{2c}$$

where $\mathcal{L}'$ denotes the adjoint (with respect to the L^2 inner product) generator of $\mathcal{L}$, j is the flux (current), a is the mobility and F is the force.

In (2b) and (2c) we use a, possibly nonlinear, relation between forces and fluxes

$$j(\rho) = a(\rho)\phi(F(\rho)),$$

for some function ϕ. For instance, for the spatially continuous setting of diffusion processes, j is linearly dependent on F,

$$j(\rho) = a(\rho)F(\rho),$$

while for spatially discrete Markov chains, the relation between j and F may be non-linear, and specifically of the form

$$j_{xy}(\rho) = a_{xy}(\rho) \sinh\left(\frac{1}{2}F_{xy}(\rho)\right), \tag{3}$$

where

$$a_{xy}(\rho) = 2\sqrt{\rho(x)r_{xy}\rho(y)r_{yx}}, \quad \text{and} \quad F_{xy}(\rho) = \log\frac{\rho(x)r_{xy}}{\rho(y)r_{yx}}, \tag{4}$$

with r_{xy} being the transition rate for jumps from state x to state y. This result goes back to Schnakenberg [11], see also [5]. We mention that for discrete Markov chains, the force-flux relation may also be linear [12, 13, 14].

The formulations (2a), (2b) and (2c) give rise to different ways of decomposing a non-reversible dynamics into symmetric and anti-symmetric parts studied in recent years:

(i) A decomposition of the generator [15, 10]: $\mathcal{L} = \mathcal{L}_S + \mathcal{L}_A$ (and thus of the dual operator $\mathcal{L}'$),

(ii) A decomposition of the fluxes [5]: $j = j_S + j_A$,

(iii) A decomposition of the forces [5, 6, 7]: $F = F_S + F_A$.

In this paper, we complement these decompositions by developing different splittings for Hamiltonians, that is, duals of Lagrangians appearing in a variational formulation of the Markov process. We now sketch this setting.

We now consider the process run $\mathcal{N}$ times and write $\hat{\rho}_t^{\mathcal{N}}$ for the associated density and $,\hat{j}^{\mathcal{N}}$ for the associated flux. Here $t \in [0, T]$ parametrises the path. Then under suitable technical assumptions a large deviation principle exists, see , e,.g., [5],

$$\text{Prob}\left((\hat{\rho}_t^{\mathcal{N}}, \hat{j}_t^{\mathcal{N}})_{t\in[0,T]} \approx (\rho_t, j_t)_{t\in[0,T]}\right) \asymp \exp\left\{-\mathcal{N}I_{[0,T]}\left((\rho_t, j_t)_{t\in[0,T]}\right)\right\}, \tag{5}$$

with *rate function* of the form

$$I_{[0,T]}\left((\rho_t, j_t)_{t\in[0,T]}\right) = I_0(\rho_0) + \frac{1}{2}\int_0^T \Phi(\rho_t, j_t, F(\rho_t))\mathrm{d}t, \tag{6}$$

where

$$\Phi(\rho, j, f) := \Psi(\rho, j) - \langle j, f \rangle + \Psi^*(\rho, f), \tag{7}$$

in which Ψ is a convex functional, Ψ^* is its Legendre dual, and $\langle j, f \rangle$ is a dual pairing between a current j and a force f. Here Ψ and hence Ψ^* depend on the process, in particular on the rates. While Φ is a function of density ρ, flux j and force f, the force in the physical system is given as a function of ρ, which we write as uppercase symbol $F(\rho_t)$. For ease of notation, we will only write the second argument in the functionals Ψ and Ψ^* if no confusion can arise. In this paper, $\mathcal{N}$ can be interpreted, for example, as the number of realisations of a stochastic process described by a Markov chain.

The dual pairing in the rate functional has a special meaning. Given a Markov process with flux j and a force F, the *entropy production rate* associated with the process is given by

$$e := 2\langle j, F \rangle \tag{8}$$

(the reason for calling this term entropy production rate is that an expansion of the rate functional yields for example for Brownian particles the entropy difference).

It is of significant current interest in physics to understand the roles of entropy and entropy production, in particular in processes out of equilibrium. For example, recently a connection between the response of a physical observable and the relative entropy has been established [16]. A natural way to understand entropy (production) is to split it in components. In [4], the authors introduce a decomposition of the force as $F = F_S + F_A$ where

$$F_S = \frac{F + F_{\mathrm{iso}}}{2}, \quad \text{and} \quad F_A = \frac{F - F_{\mathrm{iso}}}{2}. \tag{9}$$

In the formula above, F_{iso}, which is called an *iso-dissipation force*, is defined such that the identity

$$\Psi^*(F) = \Psi^*(F_{\mathrm{iso}}) \tag{10}$$

holds. Obviously this does not define F_{iso} uniquely, except for degenerate situations. In particular, if Ψ^* is continuous, convex and coercive, then $\{r \mid \Psi^*(r) = \Psi^*(F)\}$ is simply the boundary of the convex sublevel set. In this section, we provide another interpretation for iso-dissipation forces and its non-uniqueness, relating them to dual forces of dual processes.

The decomposition of the force (9) gives rise to a nonnegative decomposition of the entropy production [4, Section II C]

$$
\begin{aligned}
e = 2\langle j, f \rangle = 2\langle j, F_S \rangle + 2\langle j, F_A \rangle \\
= D[j\| - j_{\mathrm{iso}}] + D[j\|j_{\mathrm{iso}}],
\end{aligned}
\tag{11}
$$

where j_{iso} is the Legendre transform of F_{iso} (in suitable function spaces) and given two fluxes j_1, j_2, $D[j_1\|j_2]$ is the *Bregman divergence* between them,

$$D[j_1\|j_2] := \Psi(j_1) - \Psi(j_2) - \langle j_1 - j_2, \partial_{j_1}\Psi(j_2) \rangle \geq 0.$$

In addition, according to [4] there are infinitely many decompositions of the force (9) (and thus of the entropy production (11)), originating from different choices of iso-dissipation forces according to (10).

In the rest of this section, combining results from [17] and an adaption of arguments in [5], we provide a mathematical interpretation of iso-dissipation forces. The key idea is to link them to the dual force (associated to a dual process of the original one).

As in [17], we now consider the time-reversed path $(\rho_t^*, j_t^*)_{t\in[0,T]} = (\rho_{T-t}, -j_{T-t})_{t\in[0,T]}$, which defines an adjoint process. Then in the framework discussed in [5], the associated rate functional with adjoint force $F^*(\rho)$ is

$$I_{[0,T]}^*\big((\rho_t, j_t)_{t\in[0,T]}\big) = I_0(\rho_0) + \frac{1}{2}\int_0^T \Phi(\rho_t, j_t, F^*(\rho_t))\mathrm{d}t, \tag{12}$$

see [5]. Here, I_0 is the rate function associated with fluctuations of the density ρ, for a system in its steady state. That is, within the steady state, $\mathrm{Prob}(\hat{\rho}^{\mathcal{N}} \approx \rho) \asymp \exp(-\mathcal{N} I_0(\rho))$.

Then by [5, Proposition 3] we have

$$\Psi^*\big(\rho, F(\rho)\big) = \Psi^*\big(\rho, F^*(\rho)\big). \tag{13}$$

It follows from (13) and (10) that one can identify an iso-dissipation force with a dual force $F_{\mathrm{iso}} = F^*$.

We now show that mathematically there are infinitely many representations for the dual force F^*. Therefore, there are indeed infinitely many choices for an iso-dissipation force.

We define a time-reversal operation $\mathbb{T}_0$ which reverses time but does not change any coordinates or momenta. That is, for paths X on the time interval $[0, \tau]$, we take $(\mathbb{T}_0 X)_t = (X)_{\tau - t}$. Now define an adjoint dynamics [18] for which the path measure is $\mathcal{P}^*$, with

$$\mathrm{d}\mathcal{P}^*(X) = \mathrm{d}\mathcal{P}(\mathbb{T}_0 X). \tag{14}$$

Let $\mathbb{W}^*$ be the corresponding operator for the adjoint process. Then $\mathbb{W}^*$ satisfies

$$(\mathbb{W})_{y,x} \pi(x) = (\mathbb{W}^*)_{x,y} \pi(y). \tag{15}$$

Let μ be a measure which is absolutely continuous with respect to the invariant measure π. We denote by $h = \frac{\mathrm{d}\mu}{\mathrm{d}\pi}$ the corresponding Radon-Nikodym derivative. The following argument is adapted from [17]. Let $\mathbb{W}_\mu^+$ be the adjoint of $\mathbb{W}$ with respect to μ^{-1}, that is

$$\int f(y)(\mathbb{W}g)(y)\mu^{-1}(y)\mathrm{d}y = \int g(x)(\mathbb{W}_\mu^+ f)(x)\mu^{-1}(x)\mathrm{d}x.$$

The above equality can be rewritten as

$$\int \int f(y)(\mathbb{W})_{y,x} g(x)\mu^{-1}(y)\mathrm{d}x\mathrm{d}y = \int \int g(x)(\mathbb{W}_\mu^+)_{x,y} f(y)\mu^{-1}(x)\mathrm{d}x\mathrm{d}y,$$

which implies that

$$(\mathbb{W})_{y,x} \mu^{-1}(y) = (\mathbb{W}_\mu^+)_{x,y} \mu^{-1}(x). \tag{16}$$

From (15) and (16) we deduce that

$$(\mathbb{W}^*)_{x,y} = (\mathbb{W})_{y,x} \frac{\pi(x)}{\pi(y)} = \frac{\pi(x)}{\mu(x)} (\mathbb{W}_\mu^+)_{x,y} \frac{\mu(y)}{\pi(y)}.$$

Thus

$$\mathbb{W}^* = \mathbb{W}_\mu^* = h^{-1} \circ \mathbb{W}_\mu^+ \circ h. \tag{17}$$

Hence for each μ, (17) provides a representation of $\mathbb{W}^*$, which in turn gives rise to a dual force $F^* = F_\mu^*$. As a consequence, using the identification between an iso-dissipation force and a dual force discussed after (13), it follows that there are infinitely many iso-dissipation forces (and thus infinitely many different ways of decomposing the entropy production).

Example 2.1. *Consider the following non-reversible diffusion process*

$$\mathrm{d}X_t = f(X_t)\,\mathrm{d}t + \sqrt{2}\sigma\,\mathrm{d}W(t). \tag{18}$$

The associated Fokker-Planck equation is

$$\partial_t \rho = \mathbb{W}\rho = -\mathrm{div}(f\rho) + D\Delta\rho = -\mathrm{div}(\rho F(\rho)),$$

where $D = \sigma^2$ and

$$F(\rho) = f - D \log \nabla \rho.$$

Suppose the invariant measure is of the form $\mathrm{d}\pi(x) \propto e^{-U(x)}\mathrm{d}x$ (this is a common assumption in physics, with the difficulty that U is in general not known). Taking $\mu(dx) = \mathrm{d}x$, the corresponding adjoint process is

$$\partial_t \rho = \mathbb{W}^*\rho = -\mathrm{div}(f^*\rho) + D\Delta\rho = -\mathrm{div}(\rho F^*(\rho)),$$

where

$$f^*(\rho) = -(2D\nabla U + f), \quad and \quad F^*(\rho) = f^*(\rho) - D \log \nabla \rho.$$

Thus a decomposition of the force is

$$F_S(\rho) = \frac{F(\rho) + F^*(\rho)}{2} = -D\nabla U - D\log\nabla\rho$$

and

$$F_A(\rho) = \frac{F(\rho) - F^*(\rho)}{2} = f + D\nabla U.$$

While F_S and F_A are uniquely defined, there are infinitely many choices of F_{iso} giving rise to this decomposition, via (9). It is also constructive to use (10) where, in this example, Ψ^* is given explicitly in Section 3.2 below (see the last equation there).

3. Hamilton formulations for Markov chains

In this section we review the Hamiltonian viewpoint of the picture described above, and introduce splittings on the Hamiltonian level. As discussed in [5, Eq. (44)], the Hamiltonian associated with Markov chains is

$$\mathscr{H}(\rho,\xi) = \frac{1}{2}\left[\Psi^*(\rho, F(\rho) + 2\xi) - \Psi^*(\rho, F(\rho))\right]. \tag{19}$$

Let $\mathscr{L}$ be the Legendre dual of $\mathscr{H}$, that is

$$\mathscr{L}(\rho,j) = \sup_{\xi}\{\langle j,\xi\rangle - \mathscr{H}(\rho,\xi)\}.$$

Given the Hamiltonian $\mathscr{H}$ and the force F, we can also find the functional Ψ^* from (19) by

$$\Psi^*(\rho,\xi) = 2\left[\mathscr{H}\left(\rho, \frac{1}{2}(\xi - F(\rho))\right) - \mathscr{H}\left(\rho, -\frac{1}{2}F(\rho)\right)\right]. \tag{20}$$

Lemma 3.1. *The Hamiltonian being of the form* (19) *is equivalent to the Lagrangian being given by*

$$\mathscr{L}(\rho,j) = \frac{1}{2}\left[\Psi(\rho,j) - 2\langle j, F(\rho)\rangle + \Psi^*(\rho, F(\rho))\right]. \tag{21}$$

We note that (21) is precisely the form of the integrand of a rate functional we have encountered in (7), with the middle term being the entropy production rate.

Proof. This proof is adapted from [19] to be consistent with our definition (19) (in [19] the authors use a slightly different definition where there are no factors 1/2 and 2 on the right-hand

side of (19)). Suppose $\mathscr{H}$ is given as in (19). Then we get

$$
\begin{aligned}
\mathscr{L}(\rho, j) &= \sup_{\xi}\{\langle j, \xi\rangle - \mathscr{H}(\rho, \xi)\} \\
&= \sup_{\xi}\{\langle j, \xi\rangle - \frac{1}{2}\Psi^*(\rho, F(\rho) + 2\xi) + \frac{1}{2}\Psi^*(\rho, F(\rho))\} \\
&= \sup_{\xi}\{\langle j, \xi\rangle - \frac{1}{2}\Psi^*(\rho, F(\rho) + 2\xi)\} + \frac{1}{2}\Psi^*(\rho, F(\rho)) \\
&= \frac{1}{2}\sup_{\xi}\{\langle j, 2\xi\rangle - \Psi^*(\rho, F(\rho) + 2\xi)\} + \frac{1}{2}\Psi^*(\rho, F(\rho)) \\
&= \frac{1}{2}\sup_{\xi}\{\langle j, \xi\rangle - \Psi^*(\rho, F(\rho) + \xi)\} + \frac{1}{2}\Psi^*(\rho, F(\rho)) \\
&= \frac{1}{2}\sup_{\xi}\{\langle j, \xi - F(\rho)\rangle - \Psi^*(\rho, \xi)\} + \frac{1}{2}\Psi^*(\rho, F(\rho)) \\
&= \frac{1}{2}\sup_{\xi}\{\langle j, \xi\rangle - \Psi^*(\rho, \xi)\} - \langle j, F(\rho)\rangle + \frac{1}{2}\Psi^*(\rho, F(\rho)) \\
&= \frac{1}{2}\Psi(\rho, j) - \langle j, F(\rho)\rangle + \frac{1}{2}\Psi^*(\rho, F(\rho)).
\end{aligned}
$$

Similarly suppose $\mathscr{L}$ is given in (21) then one obtains (19). $\qquad\square$

3.1. Splittings of Hamiltonians

The question addressed in this section is: Given an evolution of a Markov process governed by a Lagrangian of the form (21), can this variational formulation be split in symmetric and asymmetric parts? For example, assume we consider a process with a given rate functional (21) and construct a second process with the same minimiser of the rate functional, where the rate functional is equal or higher than the one of the first process. This can be interpreted as acceleration of convergence to equilibrium: The equilibrium (minimiser) has not changed, but the steeper nature of the second functional can lead to faster convergence. For example, it is illuminating if a contribution due to an asymmetric term can be shown to increase the Lagrangian. If the functionals were quadratic, polarisation identities could be easily used. The situation with nonquadratic functionals $\Psi^\star$ is more complex (also on the level of the associated evolution equation, which is then nonlinear). We develop here splittings in the dual (Hamiltonian) picture, where information of this kind can be read off. While the splittings appear technical at first sight, we illustrate them with an example in Subsection 3.2.

We consider a general decomposition of the Hamiltonian $\mathscr{H}$ as a sum of two Hamiltonians and study its implications. The computations are formal, as we assume sufficient regularity and convexity conditions to ensure the existence of derivatives of the relevant functionals and to guarantee the existence of maximisers (minimisers) in the relevant suprema (infima). We first characterise the minimiser of $\mathscr{H}$. The following lemma is elementary and well-known. We include the proof for completeness.

Lemma 3.2. *Let $\mathscr{L}, \mathscr{H}$ be Legendre duals. Then $\min_{\xi} \mathscr{H}(\rho, \xi) = -\mathscr{L}(\rho, 0)$ is achieved at $\xi^* = \partial_j \mathscr{L}(\rho, 0)$.*

Proof. By definition of $\mathscr{H}$, we have

$$
\mathscr{H}(\rho, \xi) = \langle \xi, s_\xi\rangle - \mathscr{L}(\rho, s_\xi), \tag{22}
$$

where s_ξ satisfies

$$\xi = \partial_j \mathscr{L}(\rho, s_\xi). \tag{23}$$

The optimal ξ_{opt} is thus found through

$$\xi_{\mathrm{opt}} = \partial_j \mathscr{L}(\rho, s_{\xi_{\mathrm{opt}}}), \tag{24}$$

and

$$
\begin{aligned}
0 = {}& \partial_\xi \mathscr{H}(\rho, \xi_{\mathrm{opt}}) \\
= {}& s_{\xi_{\mathrm{opt}}} + \xi_{\mathrm{opt}} \partial_{\xi_{\mathrm{opt}}} s_{\xi_{\mathrm{opt}}} - \partial_j \mathscr{L}(\rho, s_{\xi_{\mathrm{opt}}}) \partial_{\xi_{\mathrm{opt}}} s_{\xi_{\mathrm{opt}}} \\
= {}& s_{\xi_{\mathrm{opt}}} + (\xi_{\mathrm{opt}} - \partial_j \mathscr{L}(z, s_{\xi_{\mathrm{opt}}})) \partial_{\xi_{\mathrm{opt}}} s_{\xi_{\mathrm{opt}}} \\
= {}& s_{\xi_{\mathrm{opt}}}.
\end{aligned}
$$

Hence $\xi_{\mathrm{opt}} = \partial_j \mathscr{L}(\rho, 0)$ and $\min_\xi \mathscr{H}(\rho, \xi) = \mathscr{H}(\rho, \xi_{\mathrm{opt}}) = -\mathscr{L}(\rho, 0)$ as claimed. □

We now give different decompositions of Hamiltonian $\mathscr{H}$. The first result provides a decomposition of the Hamiltonian $\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2$. The key idea is to relate the Legendre duality of the sum of two operators with the duality of each of them, which was studied for instance in [20]. We will apply this general result to the cases where $\mathscr{H}_1$ and $\mathscr{H}_2$ are constructed respectively from the reversible and irreversible parts of the underlying process.

Proposition 3.3. *Suppose that the Hamiltonian $\mathscr{H}$ can be decomposed as a sum of two Hamiltonians $\mathscr{H}_1$ and $\mathscr{H}_2$,*

$$\mathscr{H}(\rho, \xi) = \mathscr{H}_1(\rho, \xi) + \mathscr{H}_2(\rho, \xi), \tag{25}$$

where $\mathscr{H}_1(\rho, 0) = \mathscr{H}_2(\rho, 0) = 0$. Let $\mathscr{L}_1$, $\mathscr{L}_2$ and $\mathscr{L}$ be the Legendre transformation of $\mathscr{H}_1$, $\mathscr{H}_2$ and $\mathscr{H}$. Then we have

$$\mathscr{L}(\rho, j) = \mathscr{L}_1(\rho, \partial_\xi \mathscr{H}_1(\rho, \xi')) + \mathscr{L}_2(\rho, \partial_\xi \mathscr{H}_2(\rho, \xi')), \tag{26}$$

where each term on the right-hand side is non-negative and ξ' satisfies

$$\partial_\xi \mathscr{H}(\rho, \xi') = j. \tag{27}$$

As a consequence, we have the following decomposition

$$\mathscr{L}(\rho, 0) = \mathscr{L}_1(\rho, \partial_\xi \mathscr{H}_1(\rho, \xi^*)) + \mathscr{L}_2(\rho, \partial_\xi \mathscr{H}_2(\rho, \xi^*)), \tag{28}$$

where $\xi^* = \partial_j \mathscr{L}(\rho, 0)$, which is a solution of

$$\partial_\xi \mathscr{H}(\rho, \xi^*) = 0. \tag{29}$$

Note that $\mathscr{L}(\rho, 0)$ depends implicitly on ξ^*, which solves (29), via $\partial_\xi \mathscr{H}_1(\rho, \xi^*)$ and $\partial_\xi \mathscr{H}_2(\rho, \xi^*)$.

Proof. We express $\mathscr{L}$ in terms of $\mathscr{L}_1$ and $\mathscr{L}_2$. We have

$$
\begin{aligned}
\mathscr{L}(\rho, j) = {}& \sup_\xi \{\langle j, \xi \rangle - \mathscr{H}(\rho, \xi)\} \\
= {}& \sup_\xi \{\langle j, \xi \rangle - \mathscr{H}_1(\rho, \xi) - \mathscr{H}_2(\rho, \xi)\} \\
= {}& \langle j, \xi' \rangle - \mathscr{H}_1(\rho, \xi') - \mathscr{H}_2(\rho, \xi'), \tag{30}
\end{aligned}
$$

where ξ' solves for given j

$$j = \partial_\xi \mathscr{H}_1(\rho, \xi') + \partial_\xi \mathscr{H}_2(\rho, \xi') = \partial_\xi \mathscr{H}(\rho, \xi').$$

Let $s_1 := \partial_\xi \mathscr{H}_1(\rho, \xi')$, then $j - s_1 = \partial_\xi \mathscr{H}_2(\rho, \xi')$. Therefore

$$\mathscr{L}_1(\rho, s_1) = \langle s_1, \xi' \rangle - \mathscr{H}_1(\rho, \xi'), \quad \mathscr{L}_2(\rho, j - s_1) = \langle j - s_1, \xi' \rangle - \mathscr{H}_2(\rho, \xi'). \tag{31}$$

From (30) and (31), it follows that

$$\mathscr{L}(\rho, j) = \mathscr{L}_1(\rho, s_1) + \mathscr{L}_2(\rho, j - s_1) = \mathscr{L}_1(\rho, \partial_\xi \mathscr{H}_1(\rho, \xi')) + \mathscr{L}_2(\rho, \partial_\xi \mathscr{H}_2(\rho, \xi')),$$

which is (26). In addition, since $\mathscr{H}_1(\rho, 0) = \mathscr{H}_2(\rho, 0) = 0$ we have

$$\mathscr{L}_1(\rho, j) = \sup\{\langle j, \xi \rangle - \mathscr{H}_1(\rho, \xi)\} \geq \langle 0, s \rangle - \mathscr{H}_1(\rho, 0) = 0.$$

Similarly $\mathscr{L}_2(\rho, j) \geq 0$. Hence each term on the right-hand side of (26) is non-negative.

Applying (26) to $j = 0$, we obtain (28), where ξ^* solves the equation

$$\partial_\xi \mathscr{H}(\rho, \xi^*) = 0,$$

and according to Lemma 3.2, we get $\xi^* = \partial_j \mathscr{L}(\rho, 0)$.   □

Next we consider a number of applications of Proposition 3.3. In particular, we provide different decompositions of $\mathscr{L}(\rho, 0) = \sup_\xi(-\mathscr{H}(\rho, \xi))$, which is of particular interest since it gives the rate functional for the empirical occupation measures of the Markov process. The first application is a characterisation of the (Donsker-Varadhan) rate functional of reversible processes. Here we follow the definition of reversibility in [9], that is, given a functional $\mathcal{S} \in C^1$, we say that the Hamiltonian $\mathscr{H}$ is *reversible* with respect to $\mathcal{S}$ if $\mathscr{H}(\rho, \xi) = \mathscr{H}(\rho, d\mathcal{S}(\rho) - \xi)$ for all (ρ, ξ). In particular, when $\mathcal{S}$ is the relative entropy, then this is equivalent to the usual detailed balance condition and time-reversibility [19]. According to [9], the Legendre pair of functionals (Ψ, Ψ^*) associated to $\mathscr{H}$ as in (19) with $F(\rho) = d\mathcal{S}(\rho)$ are strictly convex, continuously differentiable, symmetric (in the second argument) and satisfy $\Psi(\rho, 0) = \Psi^*(\rho, 0) = 0$ if and only if $\mathscr{H}$ is reversible with respect to $\mathcal{S}$.

Lemma 3.4. *Suppose that* $\mathscr{H}(\rho, \xi) = \mathscr{H}_2(\rho, \xi)$, *where* $\mathscr{H}_2$ *is reversible with respect to some functional* $\mathcal{S}$. *Let* $\mathscr{L}_2$ *be the associated Lagrangian and* Ψ_2^* *be the dissipation potential associated to* $\mathscr{H}_2$ *and* $d\mathcal{S}$, *that is*

$$\Psi_2^*(\rho, \xi) = 2\left[\mathscr{H}_2(\rho, \tfrac{1}{2}(\xi - d\mathcal{S}(\rho)) - \mathscr{H}_2(\rho, -\tfrac{1}{2}d\mathcal{S}(\rho))\right]. \tag{32}$$

Then we have

$$\mathscr{L}_2(\rho, 0) = \frac{1}{2}\Psi_2^*(\rho, d\mathcal{S}(\rho)).$$

Proof. Since $\mathscr{H} = \mathscr{H}_2$ is reversible with respect to $\mathcal{S}$, we have

$$\mathscr{H}(\rho, \tfrac{1}{2}d\mathcal{S} - \xi) = \mathscr{H}(\rho, \xi + \tfrac{1}{2}d\mathcal{S}) \qquad \forall(\rho, \xi).$$

Taking the derivative with respect to ξ on both sides yields

$$\partial_\xi \mathscr{H}(\rho, \tfrac{1}{2}d\mathcal{S} - \xi) = -\partial_\xi \mathscr{H}(\rho, \xi + \tfrac{1}{2}d\mathcal{S}) \qquad \forall(\rho, \xi).$$

This implies that

$$\partial_\xi \mathscr{H}(\rho, \frac{1}{2} d\mathcal{S}) = 0.$$

Thus $\xi^* = \frac{1}{2} d\mathcal{S}$ is a solution to (29). Therefore,

$$\mathscr{L}_2(\rho, 0) = \frac{1}{2} \Psi_2^*(\rho, d\mathcal{S}(\rho)),$$

where the last equality is (21) with $j = 0$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Next, we consider a special case where $\mathscr{H}_2$ is independent of the second argument.

Lemma 3.5. *Suppose that*

$$\mathscr{H}(\rho, \xi) = \mathscr{H}_1(\rho, \xi) + \mathscr{H}_2(\rho). \tag{33}$$

Then the associated Lagrangian $\mathscr{L}$ is given by

$$\mathscr{L}(\rho, 0) = \mathscr{L}_1(\rho, 0) - \mathscr{H}_2(\rho). \tag{34}$$

Proof. Since $\mathscr{H}_2(\rho, \xi) = \mathscr{H}_2(\rho)$, $\mathscr{L}_2$ is defined only on $\mathrm{Dom}(\mathscr{L}_2) = \{0\}$ and $\mathscr{L}_2(\rho, 0) = -\mathscr{H}_2(\rho)$. Since $\partial_\xi \mathscr{H}_2(\rho, \xi) = 0$, it follows that $\partial_\xi \mathscr{H}(\rho, \xi^*) = \partial_\xi \mathscr{H}_1(\rho, \xi^*) = 0$. Thus

$$\mathscr{L}(\rho, 0) = \mathscr{L}_1(\rho, \partial_\xi \mathscr{H}_1(\rho, \xi^*)) + \mathscr{L}_2(\rho, \partial_\xi \mathscr{H}_2(\rho, \xi^*)) = \mathscr{L}_1(\rho, 0) + \mathscr{L}_2(\rho, 0)$$
$$= \mathscr{L}_1(\rho, 0) - \mathscr{H}_2(\rho).$$

Alternatively, this can be seen directly by

$$\mathscr{L}(\rho, 0) = \sup_\xi \{-\mathscr{H}(\rho, \xi)\} = \sup_\xi \{-\mathscr{H}_1(\rho, \xi) - \mathscr{H}_2(\rho)\} = \sup_\xi \{-\mathscr{H}_1(\rho, \xi)\} - \mathscr{H}_2(\rho)$$
$$= \mathscr{L}_1(\rho, 0) - \mathscr{H}_2(\rho).$$

$$\square$$

An example for (33) would be [1, Equations (18)–(20)]. Next, we consider a special case where $\mathscr{H}_1$ is linear with respect to the second argument and $\mathscr{H}_2$ is reversible. In this case, we will be able to determine $\partial_\xi \mathscr{H}_1(\rho, \xi^*)$ and $\partial_\xi \mathscr{H}_2(\rho, \xi^*)$ in (28) explicitly.

Lemma 3.6. *Suppose that*

$$\mathscr{H}(\rho, \xi) = \langle \mathcal{W}(\rho), \xi \rangle + \mathscr{H}_2(\rho, \xi), \tag{35}$$

where $\mathscr{H}_2(\rho, \xi)$ is symmetric around $d\mathcal{S}$. Let $\mathscr{L}_2(\rho, s)$ be the Legendre dual of $\mathscr{H}_2(\rho, \xi)$ and Ψ_2^* be the dissipation potential defined from $\mathscr{H}_2$ as in (32). Then we have

$$\mathscr{L}(\rho, 0) = \mathscr{L}_2(\rho, -\mathcal{W}(\rho)) = \frac{1}{2} \Psi_2(\rho, -\mathcal{W}(\rho)) + \frac{1}{2} \Psi_2^*(\rho, d\mathcal{S}(\rho)) + \langle \mathcal{W}(\rho), d\mathcal{S}(\rho) \rangle. \tag{36}$$

In particular, if $\langle d\mathcal{S}(\rho), \mathcal{W}(\rho) \rangle = 0$, then

$$\mathscr{L}(\rho, 0) = \Psi_2(\rho, -\mathcal{W}(\rho)) + \Psi_2^*(\rho, -\frac{1}{2} d\mathcal{S}(\rho)).$$

The decomposition of the form (35) has been studied in [9]. Typical applications of Lemma 3.6 are diffusion processes, see Section 3.2 below. We will apply this lemma to obtain a decomposition of the so-called Donsker-Varadhan rate functional for non-reversible diffusion processes, see Subsection 3.2.

Proof. This lemma is an application of Proposition 3.3, where $\mathscr{H}_1(\rho, \xi) = \langle \mathcal{W}(\rho), \xi \rangle$, thus $\mathscr{L}_1(\rho, \cdot)$ is defined only on $\mathrm{Dom}(\mathscr{L}_1) = \{\mathcal{W}(\rho)\}$ and $\mathscr{L}_1(\rho, \mathcal{W}(\rho)) = 0$. In addition, since $\partial_\xi \mathscr{H}_1(\rho, \xi^*) = \mathcal{W}(\rho)$, we have $\partial_\xi \mathscr{H}_2(\rho, \xi^*) = -\mathcal{W}(\rho)$. Thus

$$\mathscr{L}(\rho, 0) = \mathscr{L}_1(\rho, \mathcal{W}(\rho)) + \mathscr{L}_2(\rho, -\mathcal{W}(\rho)) = \mathscr{L}_2(\rho, -\mathcal{W}(\rho))$$
$$= \frac{1}{2}\Big[\Psi_2(\rho, -\mathcal{W}(\rho)) + \Psi_2^*(\rho, d\mathcal{S}(\rho)) + 2\langle \mathcal{W}(\rho), d\mathcal{S}(\rho) \rangle \Big],$$

where the last equality is (21) with $j = -\mathcal{W}(\rho)$ and $F(\rho) = d\mathcal{S}(\rho)$. We can also prove this directly as follows.

$$\mathscr{L}(\rho, 0) = \sup_\xi \{-\mathscr{H}(\rho; \xi)\} = \sup_\xi \{-\langle \mathcal{W}(\rho), \xi \rangle - \mathscr{H}_2(\rho, \xi)\}$$
$$= \mathscr{L}_2(\rho, -\mathcal{W}(\rho)),$$

where the second equation is by (35). □

3.2. Application to diffusion processes
As application, we consider general non-reversible diffusion process of the form (18), where the diffusion matrix may depend on the position,

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sqrt{2}\sigma(X_t)\,\mathrm{d}W(t).$$

Let μ be the invariant measure of the process and $\mathcal{S}_\mu(\rho)$ be the relative entropy between ρ and μ, and $D = \sigma\sigma^T$. Then, one has [19, 10] for the generator

$$\mathcal{L}_s\phi = \mathrm{div}(D\nabla\phi) + D\nabla\phi \cdot \nabla\log\mu,$$
$$\mathcal{L}_a\phi = \mathcal{L}\phi - \mathcal{L}_s\phi = b \cdot \nabla\phi - D\nabla\phi \cdot \nabla\log\mu,$$
$$\mathcal{L}_s'\rho = \mathrm{div}(D\nabla\rho) - \mathrm{div}(\rho D\nabla\log\mu) = \mathrm{div}\left[\rho D\nabla\left(\log(\rho/\mu)\right)\right] = \mathrm{div}\left[\rho D\nabla(\mathrm{d}\mathcal{S}_\mu(\rho))\right],$$
$$\mathcal{L}_a'\rho = \mathrm{div}(\rho D\nabla\log\mu - b\rho),$$

and furthermore

$$\mathscr{H}(\rho; \xi) = \int e^{-\xi}\mathcal{L}e^\xi\rho = (\xi, \mathcal{L}'\rho) + (D\nabla\xi \cdot \nabla\xi, \rho).$$

The symmetric Hamiltonian is given by

$$\mathscr{H}_s(\rho; \xi) = \int e^{-\xi}\mathcal{L}_s e^\xi\rho = (\xi, \mathcal{L}_s'\rho) + (D\nabla\xi \cdot \nabla\xi, \rho).$$

The dissipation potential associated to the symmetric Hamiltonian (with $F(\rho) = -\mathrm{d}\mathcal{S}_\mu(\rho)$) is given by

$$\Psi_s^*(\rho; \xi) = 2\left[\mathscr{H}_s\left(\rho; \frac{1}{2}(\xi + \mathrm{d}\mathcal{S}_\mu(\rho))\right) - \mathscr{H}_s\left(\rho; \frac{1}{2}\mathrm{d}\mathcal{S}_\mu(\rho)\right)\right]$$
$$= \frac{1}{2}(D\nabla\xi \cdot \nabla\xi, \rho).$$

Lemma 3.7. *Suppose that $\mathcal{L}_a$ satisfies a chain rule and that $\mathcal{L}_a'(\mu) = 0$. Let $\mathcal{S}_\mu(\rho)$ be the relative entropy between ρ and the invariant measure μ. Then*

$$\mathscr{L}(\rho, 0) = \mathscr{L}_s(\rho, -\mathcal{L}_a'(\rho)) = \frac{1}{2}\Psi_s(\rho, -\mathcal{L}_a'(\rho)) + \frac{1}{2}\Psi_s^*(\rho, d\mathcal{S}_\mu(\rho)). \tag{37}$$

Proof. Since $\mathcal{L}_a$ satisfies the chain rule, we can simplify $\mathscr{H}_a$ as

$$\mathscr{H}_a(\rho;\xi) = \left\langle e^{-\xi}\mathcal{L}_a e^{\xi}\right\rangle_\rho = \left\langle \mathcal{L}_a(\xi)\right\rangle_\rho = \langle \mathcal{L}_a'(\rho),\xi\rangle.$$

Since $\mathcal{L}_s$ is symmetric in L_μ^2, $\mathscr{H}_s$ is symmetric around $d\mathcal{S}_\mu(\rho)$ [19, 10]. Therefore, the above decomposition

$$\mathscr{H}(\rho,\xi) = \mathscr{H}_a(\rho;\xi) + \mathscr{H}_s(\rho,\xi) = \langle\mathcal{L}_a'(\rho),\xi\rangle + \mathscr{H}_s(\rho,\xi).$$

Furthermore, we have

$$\langle d\mathcal{S}_\mu(\rho),\mathcal{L}_a'(\rho)\rangle = \langle \log\frac{\rho}{\mu},\mathcal{L}_a'(\rho)\rangle = \langle \rho,\mathcal{L}_a\big(\log\frac{\rho}{\mu}\big)\rangle = \langle\rho,\frac{\mu}{\rho}\mathcal{L}_a(\frac{\rho}{\mu})\rangle$$

$$= \langle 1,\mu\mathcal{L}_a(\frac{\rho}{\mu})\rangle = \langle\frac{\rho}{\mu},\mathcal{L}_a'(\mu)\rangle = 0.$$

Hence, the above decomposition satisfies the assumptions in Lemma 3.6 with $\mathcal{W}(\rho) = \mathcal{L}_a'(\rho)$, $\mathscr{H}_2 = \mathscr{H}_s$ and $\mathcal{S} = \mathcal{S}_\mu$; therefore, the statement of this lemma follows from Lemma 3.6. $\square$

This lemma applies to the non-reversible diffusion process described above; we obtain the splitting

$$\mathscr{L}(\rho,0) = \frac{1}{2}\Psi_s(\rho,-\mathcal{L}_a'(\rho)) + \frac{1}{2}\Psi_s^*(\rho,d\mathcal{S}_\mu(\rho)) =$$
$$\frac{1}{2}\Psi_s(\rho,-\mathrm{div}(\rho D\nabla\log\mu - b\rho)) + \frac{1}{2}\Psi_s^*(\rho,d\mathcal{S}_\mu(\rho)),$$

where $\mathcal{S}_\mu$ is the relative entropy. This example is chosen for illustrative purposes only; as the dissipation potential $\Psi^\star$ and hence its Legendre dual are quadratic, splittings can be analysed using polarisation identities as mentioned at the beginning of Section 3.1. Yet, although the splittings developed in this paper are developed with nonquadratic dissipation potentials in mind, the results apply in the quadratic case as well. The interpretation of the result above is as follows: (37) is a statement about the stationary (equilibrium) state, $j = 0$. The result says that the functional depends there only on the symmetric part $\Psi_s^\star$; there is no contribution from the asymmetric part. So we see that the addition of the asymmetric part does not change the steady state. With additional arguments, it can be shown that away from $j = 0$, the (Donsker-Varadhan) rate functional associated with (37) increases when the non-reversible component is present [21, 22]. As discussed at the beginning of Section 3.1, this can be interpreted as the asymmetric process converging faster (or at least equally as fast) as the symmetric process.

4. Conclusion

In Section 2, we have shown that the non-uniqueness of the iso-dissipation force can be explained through different notions of duality. In Section 3, we have introduced different splittings of Hamiltonians associated to Markov processes through large deviation principles, and given an application to a diffusion process on the Fokker-Planck level.

It is natural to compare these decompositions to decompositions in terms of the generator; this is area of future research. Similar, the application of these splittings for different non-reversible processes remains to be investigated.

Acknowledgment

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