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A unifying picture of generalized thermodynamic uncertainty relations*

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Abstract. The thermodynamic uncertainty relation is a universal trade-off relation connecting the precision of a current with the average dissipation at large times. For continuous time Markov chains (also called Markov jump processes) this relation is valid in the time-homogeneous case, while it fails in the time-periodic case. The latter is relevant for the study of several small thermodynamic systems. We consider here a time-periodic Markov chain with continuous time and a broad class of functionals of stochastic trajectories, which are general linear combinations of the empirical flow and the empirical density. Inspired by the analysis done in our previous work Barato *et al* (2018 *New J. Phys.* **20** 103023), we provide general methods to get local quadratic bounds for large deviations, which lead to universal lower bounds on the ratio of the diffusion coefficient to the squared average value in terms of suitable universal rates, independent of the empirical functional. These bounds are called 'generalized thermodynamic uncertainty relations' (GTUR's), being generalized versions of the thermodynamic uncertainty relation to the time-periodic case

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and to functionals which are more general than currents. Previously, GTUR's in the time-periodic case have been obtained in Barato *et al* (2018 *New J. Phys.* **20** 103023); Koyuk *et al* (2019 *J. Phys. A: Math. Theor.* **52** 02LT02); Proesmans and Van den Broeck (2017 *Europhys. Lett.* **119** 20001). Here we recover the GTUR's in Barato *et al* (2018 *New J. Phys.* **20** 103023); Koyuk *et al* (2019 *J. Phys. A: Math. Theor.* **52** 02LT02) and produce new ones, leading to even stronger bounds and also to new trade-off relations for time-homogeneous systems. Moreover, we generalize to arbitrary protocols the GTUR obtained in Proesmans and Van den Broeck (2017 *Europhys. Lett.* **119** 20001) for time-symmetric protocols. We also generalize to the time-periodic case the GTUR obtained in Garrahan (2017 *Phys. Rev.* E **95** 032134) for the so called dynamical activity, and provide a new GTUR which, in the time-homogeneous case, is stronger than the one in Garrahan (2017 *Phys. Rev.* E **95** 032134). The unifying picture is completed with a comprehensive comparison between the different GTUR's.

Keywords: large deviations in non-equilibrium systems, stochastic thermodynamics

Contents

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1. Introduction

Stochastic thermodynamics [46, 47] generalizes thermodynamics to small nonequilibrium systems, such as molecular motors, colloidal heat engines and quantum dots. Thermal fluctuations in these systems are relatively large and cannot be neglected. In the last decades, some universal relations concerning fluctuations in small nonequilibrium systems have been obtained. These relations mainly correspond to the so called fluctuations theorems (see [46] and references therein) and to the more recent thermodynamic uncertainty relations and their generalizations. Fluctuation theorems, initially developed for dynamical systems [19], provide constraints on the entropy probability distribution which generalize the second law of thermodynamics. On the other hand, the original *thermodynamic uncertainty relation* (TUR) introduced in [3] is a universal inequality that relates the precision of any current, such as the number of consumed ATP and the velocity of a molecular motor or the electron flux in a quantum dot, with the entropy production that quantifies energy dissipation. More precisely, the ratio of the asymptotic diffusion coefficient of any current to its squared asymptotic value is lower bounded by the inverse average entropy production rate. Possible applications of the TUR include the inference of enzymatic schemes in single molecule experiments [2], a bound on the efficiency of molecular motors depending only on the fluctuations of the displacement of the motor [38], a universal relation between power and efficiency for heat engines in a stationary state [41], and design principles in nonequilibrium self-assembly [35]. More generally, the TUR can be derived from a parabolic bound on large deviations (LD) proposed in [22, 37]. The proof of this bound, which has been obtained in [22], comes from the explicit form derived in [6, 7, 32] of the rate functional associated with the so called 2.5 level LDs.

Several works about the TUR and about quadratic bounds on LD rate functionals have already been produced (see for example [1, 2, 8–13, 16, 20, 21, 24–26, 28–31, 34–36, 38–44] and references therein). In particular, the TUR applies to systems driven by a fixed thermodynamic force. Mathematically, these systems can be described as time-homogenous Markov chains, i.e. with time-independent transition rates, or time-homogeneous diffusions as in [23, 34, 43]. A different way to drive a system out of equilibrium is through an external periodic protocol. Several artificial molecular pumps [17] and colloidal heat engines [33] constitute experimental examples of such periodically driven systems. A continuous–time Markov chain with time-periodic transitions rates is a standard mathematical framework to describe these systems [4].

As shown in [4], there is a fundamental difference between systems driven by a fixed thermodynamic force and periodically driven systems concerning the TUR. The original TUR from [3] that involves the entropy production does not apply to periodically driven systems. However, more recently, bounds on current fluctuations that generalize the TUR to periodically driven systems have been obtained in [1, 29, 44]. In this work we focus on *generalized thermodynamic uncertainty relations* (GTUR's). In a very broad sense, given a class $\mathcal{C}$ of empirical functionals (i.e. functionals of the stochastic trajectory as detailed in section 2.2), by GTUR we mean a lower bound on the ratio of the asymptotic diffusion coefficient to the squared asymptotic value of the empirical functional which holds *uniformly*. This means that the lower bounding quantity depends only on the Markov process itself and the class $\mathcal{C}$ of functionals under consideration, but does not depend on the specific empirical functional in $\mathcal{C}$.

A summary of the GTUR's developed so far (see [1, 29, 44]) is as follows. A first GTUR for periodically driven systems has been provided in [44]. This result is restricted to protocols that are time-symmetric under time reversal and to the class of empirical functionals fulfilling an antisymmetry relation. The resulting lower bound is in terms of the averaged entropy production rate, although in a form different from the standard TUR. A second contribution has come from our previous work [1]. There we have presented a very general method to get local quadratic upper bounds on the LD rate function of currents, and therefore lower bounds on the ratio of the asymptotic diffusion coefficient to the squared asymptotic value. As an application, we have obtained several specific classes of lower bounds (see [1, equations (55),(56),(61),(72),(73),(74)]), which hold for generic currents, also with time-dependent increments (the increment is the variation of the current due to a transition). When restricting to time-independent increments several lower bounds provided in [1] become uniform w.r.t. the possible increments and therefore are GTUR's, in the sense specified above (see e.g. [1, equations (26),(27)]). Another GTUR has been derived in [29] for a class of empirical functionals given by a current and a generic term that is linear in the fractions of time spent in a state, the so called empirical density (or measure).

Part of our main results are an extension of the analysis performed in [1]. We consider a quite broad class of empirical functionals. This class includes currents, which are the standard observables that appear in the TUR, an observable known as activity that has symmetric increments [20] (in contrast to currents that have antisymmetric increments) and the empirical density. In fact, our GTUR's are generalizations of the TUR in two senses: we consider time-periodic Markov chains and empirical functionals more general than currents. For instance one of our GTUR's is a generalization to the time-periodic case of the bound found in [20] related to the dynamical activity. We remark that, even for currents and time-homogeneous processes, some of our GTUR's are different and tighter than the usual TUR (similarly, one of our GTUR's is tighter than the bound found in [20] related to the dynamical activity). Finally, these GTUR's should not be confused with the generalizations of the TUR to finite time in time-homogeneous, time-inhomogeneous or time-periodic systems obtained in [11–13, 28, 40].

We provide general methods to produce local quadratic upper bounds on the LD rate function of the empirical functionals (see theorems 2–4). These methods rely on the LD principles obtained in [5] and work whenever one can exhibit a suitable mathematical object, that we call here *legal input*. By choosing suitable legal inputs we get the different GTUR's listed in section 3 as (GTUR 1), (GTUR 2),...,(GTUR 6). In this way we recover the results of [1, 29] but also go further, exhibiting new GTUR's which are sometimes even stronger of the existing ones (for example, (GTUR 4) provides always a stronger lower bound than the GTUR in [29]).

The GTUR in [44] is of a different nature (see section 5) and it does not enter in the above general scheme. Our unifying picture is completed with a generalization of this GTUR to the case of general protocols that can be time-asymmetric (see (GTUR 7) in section 3). This GTUR applies to a class of functionals that fulfills an antisymmetry relation. Interestingly, the average entropy production rate that appears in the bound for the case of symmetric protocols is substituted in our generalization by an average naive entropy production rate analyzed in [5] and recalled in sections 3.3 and 5. This rate equals the rate of entropy production plus a rate that becomes zero if the protocol is symmetric.

All our results apply as well to time-homogeneous Markov chains with continuous time, since they are a special case of periodically driven systems. In particular, our GTUR's include the original TUR from [3] and imply a generalization of the bound on the fluctuations of activity derived in [20].

Outline of the paper. The paper is organized according to the following scheme.

- **Notation and general framework:** in section 2 we fix the notation, describe the model and the empirical functionals we will focus on.
- **Main results**. They are shared in three parts, corresponding to sections 3–5. In section 3 we present our main GTUR's, denoted by (GTUR 1), (GTUR 2),..., (GTUR 7). In section 4 we optimize some GTUR's with respect to the parameters appearing there and make comparisons between GTUR's. In section 5 we extend the results of [44] to generic protocols (see theorem 1, implying (GTUR 7)).
- **Examples**. In section 6 we discuss in detail two examples.
- **Proofs.** They are shared in four parts, corresponding to sections 7–10. In section 7 we provide an overview on the methods used to derive the GTUR's listed in section 3. In sections 8 and 9 we provide general methods (see theorems 2–4 there) to get local/global quadratic upper bounds on the LD rate function and derive all the GTUR's listed in section 3, apart from (GTUR 7),

as well as some other lower bounds on the ratio between speed and precision (see corollaries 8.2, 9.2 and 9.6). In section 10 we derive the results concerning optimization and comparison presented in section 4.

- **Conclusion**. In section 11 we briefly report on the obtained results.
- **Appendixes**. In appendix A we collect some general remarks and in appendix B we give for completeness the proof of theorem 1, which follows the main arguments presented in [44].

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2. Notation and general framework

2.1. Models and notation

We consider a continuous-time Markov chain $X(t)$ with finite state space V and time-periodic jump rates $w_{ij}(t)$ with period τ:

$$\mathbb{P}(X(t+\mathrm{d}t)=j\,|\,X(t)=i)=w_{ij}(t)\mathrm{d}t, \qquad w_{ij}(t+\tau)=w_{ij}(t) \qquad \forall i,j\in V,\ \forall t\geqslant 0.$$

The transition graph associated with the Markov chain $X(t)$ is denoted (V,E), with vertex set V and set of oriented edges E. Our main technical assumptions are the following:

(i) the graph (V,E) is strongly connected;
(ii) for each $(i,j)\in E$ it holds $w_{ij}(t)>0$ for all t, while for each $(i,j)\notin E$ it holds $w_{ij}(t)=0$ for all t.

We recall that item (i) is equivalent to the fact that, given arbitrary states $i,j\in V$, there exists a path from i to j respecting the edge orientation.

Denoting by $P_i(t)$ the probability that the Markov chain is at state i at time t, the time evolution of $P_i(t)$ is given by the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}P_i(t)=\sum_{j:j\neq i}\left[P_j(t)w_{ji}(t)-P_i(t)w_{ij}(t)\right]. \tag{2.1}$$

The asymptotic properties related to this equation are as follows (see e.g. [5] for details). In the long time limit, $P_i(t)$ tends to an invariant time-periodic distribution $\pi_i(t)=\pi_i(t+\tau)$. The distribution $\pi(t)$ can be characterized as the unique invariant distribution of the discrete-time Markov chain $\big(X(t+n\tau)\big)_{n\geqslant 0}$. Other important quantities are the asymptotic elementary flow $\mathcal{Q}_{ij}(t)$ and current $\mathcal{J}_{ij}(t)$ along the edge (i,j), which are given by

$$\begin{cases}\mathcal{Q}_{ij}(t):=\pi_i(t)w_{ij}(t),\\ \mathcal{J}_{ij}(t):=\pi_i(t)w_{ij}(t)-\pi_j(t)w_{ji}(t)=\mathcal{Q}_{ij}(t)-\mathcal{Q}_{ji}(t).\end{cases} \tag{2.2}$$

Note that $\pi_i(t)>0$ for all $t>0$ and $i\in V$. Moreover $\mathcal{Q}_{ij}(t)>0$ for all $t>0$ if $(i,j)\in E$, while $\mathcal{Q}_{ij}(t)=0$ for all $t>0$ if $(i,j)\notin E$.

From equation (2.1) we get the continuity equation

$$\partial_t \pi_i(t) + \sum_{j:j\neq i} \mathcal{Q}_{ij}(t) - \sum_{j:j\neq i} \mathcal{Q}_{ji}(t) = 0 \qquad \forall i \in V, \tag{2.3}$$

which is equivalent to

$$\partial_t \pi_i(t) + \sum_{j:j\neq i} \mathcal{J}_{ij}(t) = 0 \qquad \forall i \in V. \tag{2.4}$$

The continuity equation (2.3) can be rewritten with a div operator in the form

$$\partial_t \pi(t) + \mathrm{div}\, \mathcal{Q}(t) = 0, \tag{2.5}$$

where $\pi(t)$ and $\mathrm{div}\,\mathcal{Q}(t)$ are vectors with components $\pi_i(t)$ and $\mathrm{div}_i\,\mathcal{Q}(t) := \sum_j \mathcal{Q}_{ij}(t) - \sum_j \mathcal{Q}_{ji}(t)$.

Time independent transition rates $w_{ij}(t) = w_{ij}$ correspond to a particular case of our theory. In this case, we have a steady state characterized by the asymptotic distribution π, which fulfills the continuity equation

$$\sum_{j:j\neq i} \mathcal{Q}_{ij} - \sum_{j:j\neq i} \mathcal{Q}_{ji} = 0 \qquad \forall i \in V, \tag{2.6}$$

where $\mathcal{Q}_{ij} = \pi_i w_{ij}$.

Finally, when the graph (V, E) contains an edge (i, j) if and only if it contains the edge (j, i), we denote by σ the average entropy production rate. In particular, we have

$$\sigma = \frac{1}{2} \sum_{(i,j)\in E} \frac{1}{\tau} \int_0^\tau \mathcal{J}_{ij}(t) \ln \frac{\mathcal{Q}_{ij}(t)}{\mathcal{Q}_{ji}(t)} \mathrm{d}t. \tag{2.7}$$

When the transition rates are time-independent, the above identity simply reads

$$\sigma = \frac{1}{2} \sum_{(i,j)\in E} \mathcal{J}_{ij} \ln \frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}. \tag{2.8}$$

Let us introduce the notations for time average and scalar products used in this paper. In what follows, when referring to a time-periodic function $f(t)$, we understand that its period equals τ. Moreover, we denote by $\overline{f}$ the average of f over a period, i.e.

$$\overline{f} := \frac{1}{\tau} \int_0^\tau f(t) \mathrm{d}t.$$

The scalar product of two vectors $a(t)$ and $b(t)$ with entries parameterized by $i \in V$ is given by

$$\langle a(t), b(t) \rangle := \sum_{i\in V} a_i(t) b_i(t);$$

while, if $a(t)$ and $b(t)$ are matrixes with entries parameterized by $(i, j) \in V \times V$, their scalar product is given by

$$\langle a(t), b(t) \rangle := \sum_{(i,j)\in V\times V} a_{ij}(t) b_{ij}(t).$$

Finally, in what follows Markov chains will always be considered as time-continuous (i.e. as Markov jump processes), also when not explicitly stated.

2.2. Empirical functionals

We describe now the class of empirical functionals on which we will focus and state the associated large deviation principle. Given a time-periodic matrix $\alpha(t) = \big(\alpha_{ij}(t) \,:\, (i,j) \in V \times V\big)$ and a time-periodic vector $\gamma(t) = \big(\gamma_i(t) \,:\, i \in V\big)$ we consider the empirical functional $Y^{(n)}_{\alpha,\gamma}$ defined as

$$Y^{(n)}_{\alpha,\gamma} := \frac{1}{n\tau} \sum_{\substack{t\in(0,n\tau]:\\ X(t-)\neq X(t+)}} \alpha_{X(t-),X(t+)}(t) + \frac{1}{n\tau}\int_0^{n\tau} \gamma_{X(t)}(t)\mathrm{d}t. \tag{2.9}$$

For example, if all components of $\gamma(t)$ are zero and the increments $\alpha_{ij}(t)$ are antisymmetric, i.e. $\alpha_{ij}(t) = -\alpha_{ji}(t)$, then $Y^{(n)}_{\alpha,\gamma}$ is a current, which is a key observable in stochastic thermodynamics. If the components of $\alpha(t)$ are zero, the component $\gamma_i(t) = 1$ and the other components of $\gamma(t)$ are zero, then $Y^{(n)}_{\alpha,\gamma}$ is the fraction of time spent in state i.

Note that, as $n \to \infty$, $Y^{(n)}_{\alpha,\gamma}$ has the following asymptotics (see [5, proposition 7.3]):

$$Y^{(n)}_{\alpha,\gamma} \to y_{\alpha,\gamma} := \overline{\langle \alpha, \mathcal{Q}\rangle} + \overline{\langle \gamma, \pi\rangle}. \tag{2.10}$$

In particular, if $\alpha_{ij} = \ln(w_{ij}/w_{ji})$ and $\gamma = 0$, then $y_{\alpha,\gamma}$ equals the average entropy production rate σ in (2.7).

As a byproduct of the large deviation (LD) principle given by [5, theorem 2] and the contraction principle (see e.g. [14, 15, 27, 48]), $Y^{(n)}_{\alpha,\gamma}$ satisfies an LD principle as $n \to \infty$ with speed $n\tau$. Calling $I_{\alpha,\gamma}$ its rate functional, roughly it holds

$$\mathbb{P}(Y^{(n)}_{\alpha,\gamma} \approx y) \asymp \mathrm{e}^{-n\tau I_{\alpha,\gamma}(y)}, \qquad y \in \mathbb{R},\ n \gg 1. \tag{2.11}$$

We point out that $I_{\alpha,\gamma}(y) \geqslant 0$ and $I_{\alpha,\gamma}(y) = 0$ if and only if $y = y_{\alpha,\gamma}$. This corresponds to the fact that $y_{\alpha,\gamma}$ is the typical value and different values of the functional are exponentially unlikely.

To describe the variational characterization of the LD rate functional $I_{\alpha,\gamma}$, we introduce the function $\Phi(q,p)$ defined for $q,p \geqslant 0$ as

$$\Phi(q,p) := q\ln(q/p) - q + p, \tag{2.12}$$

with the convention that $\Phi(0,p) := p$ and $\Phi(q,0) = +\infty$ for $q > 0$. Then, it holds

$$I_{\alpha,\gamma}(y) = \inf\{I(Q,\rho) \,:\, (Q,\rho) \in \mathcal{F}_{\alpha,\gamma,y}\}, \tag{2.13}$$

where

$$I(Q,\rho) := \sum_{(i,j)\in E} \overline{\Phi\big(Q_{ij}(t), \rho_i(t)w_{ij}(t)\big)} \tag{2.14}$$

and $\mathcal{F}_{\alpha,\gamma,y}$ denotes the family of pairs $(Q,\rho) = (Q(t),\rho(t))_{t\geqslant 0}$ such that

(i) $Q(t)$ is a time-periodic flow, i.e. $Q(t) = Q(t+\tau)$ and $Q(t)$ is a non-negative function on $V \times V$ which is zero outside E for each time t;

(ii) $\rho(t)$ is a time-periodic probability measure on V;

(iii) the continuity equation $\partial_t \rho(t) + \operatorname{div} Q(t) = 0$ is satisfied, where $\operatorname{div}_i Q(t) := {}_j Q_{ij}(t) - \sum_j Q_{ji}(t)$;

(iv) $y = \overline{\langle \alpha, Q \rangle} + \overline{\langle \gamma, \rho \rangle}$.

We point out that one recovers from (2.13) that $I_{\alpha,\gamma}(y_{\alpha,\gamma}) = 0$ since, denoting by $\mathcal{Q} = (\mathcal{Q}(t))_{t \geqslant 0}$ and $\pi = (\pi(t))_{t \geqslant 0}$ the asymptotic flow and density, respectively, it holds $I(\mathcal{Q}, \pi) = 0$ in addition to (2.10).

Formula (2.14) corresponds to the joint LD rate functional of the empirical flow and measure. To recall their definition, given $t \geqslant 0$ we denote by $[t]$ the only number in $[0, \tau)$ such that $t - [t]$ is a multiple of τ. Then the empirical flow $Q^{(n)}$ is defined as the measure on $E \times [0, \tau)$ given by

$$Q^{(n)}(i, j, A) := \frac{1}{n} \sharp \left\{ t \in (0, n\tau] : X(t-) = i,\ X(t+) = j,\ [t] \in A \right\},$$

where $\sharp$ denotes the cardinality of the set. On the other hand, the empirical measure $\rho^{(n)}$ is defined as the measure on $V \times [0, \tau)$ such that

$$\rho^{(n)}(i, A) := \frac{1}{n} \int_0^{n\tau} 1\left(X(t) = i,\ [t] \in A\right) \mathrm{d}t,$$

where $1(\cdot)$ denotes the characteristic function (i.e. the function equals 1 if the event under consideration takes place, otherwise it equals zero). Note that, given a time-periodic flow $Q = (Q(t))_{t \geqslant 0}$, we can think of Q as the measure on $E \times [0, \tau)$ with weights $(i, j, \mathrm{d}t) \mapsto Q_{ij}(t)\mathrm{d}t$. Given a time-periodic probability measure $\rho = (\rho(t))_{t \geqslant 0}$ on V we can think of ρ as the measure on $V \times [0, \tau)$ with weights $(i, \mathrm{d}t) \mapsto \rho_i(t)\mathrm{d}t$. In [5, theorem 2] it is proved that the pair $\left(Q^{(n)}, \pi^{(n)}\right)$ satisfies a LD principle with speed $n\tau$ and rate functional $I(Q, \rho)$ given by (2.14) if $(Q, \rho) = (Q(t), \rho(t))_{t \geqslant 0}$ satisfies the above conditions (i), (ii), (iii). If these conditions are not fulfilled, then $I(Q, \rho)$ equals infinity. Since

$$Y^{(n)}_{\alpha,\gamma} = \frac{1}{\tau} \sum_{i,j} \int_{[0,\tau)} \alpha_{ij}(t) Q^{(n)}(i, j, \mathrm{d}t) + \frac{1}{\tau} \sum_i \int_{[0,\tau)} \gamma_i(t) \rho^{(n)}(i, \mathrm{d}t), \tag{2.15}$$

(2.13) follows from the contraction principle and the above LD principle for $\left(Q^{(n)}, \pi^{(n)}\right)$.

The asymptotic diffusion coefficient $D_{\alpha,\gamma}$ associated with $Y^{(n)}_{\alpha,\gamma}$ is defined as

$$2D_{\alpha,\gamma} := \lim_{n \to \infty} n\tau \operatorname{Var}\left(Y^{(n)}_{\alpha,\gamma}\right). \tag{2.16}$$

This quantity can be obtained from the rate functional $I_{\alpha,\gamma}$ by the identity

$$2D_{\alpha,\gamma} = \frac{1}{I''_{\alpha,\gamma}(y_{\alpha,\gamma})}, \tag{2.17}$$

where $I''_{\alpha,\gamma}$ denotes the second derivative of $I_{\alpha,\gamma}$. We point out that in the mathematical literature the asymptotic diffusion coefficient is defined without the factor 2 in the lhs of (2.16).

Formula (2.17) can be applied when the rate function $I_{\alpha,\gamma}$ is twice differentiable around its minimum point $y_{\alpha,\gamma}$. If the set $\mathcal{F}_{\alpha,\gamma,y}$ defined after (2.14) is non-empty for any real value y, then the differentiability could be proved using the smoothness of the function (2.12) on points with strictly positive coordinates and the linearity of the constraint (iv) in the definition of $\mathcal{F}_{\alpha,\gamma,y}$. There are however exceptional cases when this does not happen. As an example consider the case when $\gamma \equiv 0$ and $\alpha_{ij} = f_j - f_i$ for fixed time-independent constants $(f_i)_{i\in V}$. Given $(Q,\rho) \in \mathcal{F}_{\alpha,\gamma,y}$ we deduce that $\operatorname{div} \overline{Q} = 0$ by integrating the continuity equation $\partial_t \rho(t) + \operatorname{div} Q(t) = 0$ on a period and using that $\rho(t)$ is periodic. Due to the gradient representation $\alpha_{ij} = f_i - f_j$ and since $\operatorname{div} \overline{Q} = 0$, by a discrete integration by parts we obtain that $\langle \alpha, \overline{Q} \rangle = 0$. We get therefore that $\mathcal{F}_{\alpha,\gamma,y} = \emptyset$ for any $y \neq 0$ (indeed, property (iv) in the definition of $\mathcal{F}_{\alpha,\gamma,y}$ cannot be fulfilled for $y \neq 0$). As a consequence $I_{\alpha,\gamma}(y) = +\infty$ for $y \neq 0$ and $I_{\alpha,\gamma}(0) = 0$, hence $I_{\alpha,\gamma}$ is not differentiable. In this case formula (2.17) cannot be applied. See also remark 9.1 for another exceptional class.

3. Main results I: (GTUR 1), (GTUR 2),...,(GTUR 7)

In this section we present our main GTUR's, given by inequalities (GTUR 1), (GTUR 2),...,(GTUR 7) below. For the reader's convenience, these GTUR's are summarized in tables 1 and 2. Apart from (GTUR 7), which is a generalization of the result derived in [44], their derivation is obtained by extending the methods and ideas from [1]. We refer to sections 7–9 for the proofs and further comments.

From now on, without further mention, we restrict to the case that the asymptotic value $y_{\alpha,\gamma}$ of the empirical functional $Y^{(n)}_{\alpha,\gamma}$ is non zero (see remark 8.1 for the case $y_{\alpha,\gamma} = 0$).

3.1. GTUR with generic increments

From corollary 8.2, which contains a more general result, we obtain:

GTUR 1. If the increments α are time-independent (i.e. $\alpha_{i,j}(t) \equiv \alpha_{i,j}$) and $\gamma \equiv 0$, then

$$\frac{D_{\alpha,0}}{y^2_{\alpha,0}} \geqslant \frac{1}{\widehat{\sigma}}, \tag{GTUR 1}$$

where

$$\widehat{\sigma} := 2 \sum_{(i,j)\in E} (\overline{\mathcal{Q}}_{ij})^2 \overline{\frac{1}{\mathcal{Q}_{ij}}}. \tag{3.1}$$

For the case of time-homogeneous Markov chains, $\widehat{\sigma} = 2\sum_{(i,j)\in E} \mathcal{Q}_{ij}$, and this GTUR becomes [20, equation (19)]. Hence, (GTUR 1) is a generalization of this inequality to time-periodic Markov chains. The quantity $\sum_{(i,j)\in E} \mathcal{Q}_{ij}$, which is the rate of average number of transitions, is known as *mean dynamical activity*. For time-periodic Markov chains, due to Jensen's inequality, we have the bound $\widehat{\sigma} \geqslant 2\sum_{(i,j)\in E} \overline{\mathcal{Q}}_{ij}$, i.e. $\widehat{\sigma}/2$ is larger than the dynamical activity.

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From corollary 8.3 we obtain:

GTUR 2. For generic increments α, it holds

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \frac{1}{C(p)}, \tag{GTUR 2}$$

where $p = (p_i)_{i \in V}$ is any probability on V with $\langle \overline{\gamma}, p \rangle = 0$ and

$$C(p) := 2 \sum_{(i,j)\in E} p_i^2 \overline{\left(\frac{w_{ij}^2}{\mathcal{Q}_{ij}} \right)} = 2 \sum_{(i,j)\in E} p_i^2 \overline{\left(\frac{w_{ij}}{\pi_i} \right)}. \tag{3.2}$$

Note that the above probability p is time-independent. This novel GTUR is valid for generic linear functionals of the form (2.9), including the case $\alpha = 0$, which corresponds to functionals that depend only on the empirical density.

3.2. GTUR with antisymmetric increments

In this subsection we assume, without further mention, that

$$(y, z) \in E \Leftrightarrow (z, y) \in E.$$

For the particular case of antisymmetric increments $\alpha_{i,j}(t) = -\alpha_{j,i}(t)$, we have the following GTUR's.

First, from corollary 9.2, which contains a more general result, we obtain:

GTUR 3. If α is time-independent and antisymmetric and $\gamma \equiv 0$, then

$$\frac{D_{\alpha,0}}{y^2_{\alpha,0}} \geqslant \frac{1}{\widetilde{\sigma}}, \tag{GTUR 3}$$

where

$$\widetilde{\sigma} := \sum_{(i,j)\in E} (\overline{\mathcal{J}}_{ij})^2 \overline{\frac{1}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}}}. \tag{3.3}$$

This GTUR corresponds to the first bound in [1, equation (27)].

Second, from corollary 9.3, we obtain:

GTUR 4. For generic antisymmetric increments α, it holds

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \frac{1}{C_{\mathrm{a}}(p)}, \tag{GTUR 4}$$

where $p = (p_i)_{i \in V}$ is any probability on V with $\langle \overline{\gamma}, p \rangle = 0$ and

$$C_{\mathrm{a}}(p) := \sum_{(i,j)\in E} \overline{\left(\frac{\left(p_i w_{ij} - p_j w_{ji}\right)^2}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}} \right)}. \tag{3.4}$$

The above GTUR for $\gamma \equiv 0$ has been obtained also in [11] by applying the Cramér–Rao bound. The bound is not explicitly pointed out in [11], but one gets it by combining (5), (A.22) and (A.23) there.

Third, from corollary 9.6, which contains a more general result, we obtain:

GTUR 5. If α is time-independent and antisymmetric and $\gamma \equiv 0$, then

$$\frac{D_{\alpha,0}}{y_{\alpha,0}^2} \geqslant \frac{1}{\sigma^*}, \tag{GTUR 5}$$

where

$$\sigma^* := \frac{1}{2} \sum_{(i,j)\in E} (\overline{\mathcal{J}}_{ij})^2 \overline{\left(\frac{1}{\mathcal{J}_{ij}} \ln \frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}} \right)}. \tag{3.5}$$

This GTUR corresponds to the second bound in [1, equation (27)] (see [1, section 3.4] for a physical interpretation of σ^*). Furthermore, due to the inequality $\sigma^* \geqslant \widetilde{\sigma}$, which has been proved in [1], (GTUR 5) can be also derived directly from (GTUR 3). The original TUR for time-homogeneous Markov chains is a particular case of (GTUR 5). For a time-homogeneous Markov chain σ^* becomes the average entropy production rate σ in (2.8).

Fourth, from corollary 9.7, we obtain:

GTUR 6. For generic antisymmetric increments α, it holds

$$\frac{D_{\alpha,\gamma}}{y_{\alpha,\gamma}^2} \geqslant \frac{1}{C_{\mathrm{a}}^*(p)}, \tag{GTUR 6}$$

where $p = (p_i)_{i\in V}$ is any probability on V with $\langle \overline{\gamma}, p\rangle = 0$ and

$$C_{\mathrm{a}}^*(p) := \frac{1}{2} \sum_{(i,j)\in E} \overline{\left(\frac{\left(p_i w_{ij} - p_j w_{ji}\right)^2}{\mathcal{J}_{ij}} \right) \ln \frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}}. \tag{3.6}$$

This GTUR, for the particular case $\overline{\gamma} = 0$ (which is equivalent to the fact that $\gamma_i(t) = \frac{\mathrm{d}}{\mathrm{d}t} g_i(t)$ for periodic functions g_i), has been obtained in [29] with a different derivation (see [29, equations (14)–(16)]).

The inequality (GTUR 6) can be derived by the general method presented in theorem 4 as well as directly from (GTUR 4) by the bound (9.30) presented in section 9.5.

3.3. GTUR with naive entropy production

Our last GTUR follows from theorem 1, which contains more general results:

GTUR 7. If $\alpha_{i,j}(t) = -\alpha_{j,i}(\tau - t)$ and $\gamma_i(t) = -\gamma_i(\tau - t)$ for any i, j and $t \in [0, \tau]$, then

$$\frac{D_{\alpha,\gamma}}{y_{\alpha,\gamma}^2} \geqslant \frac{\tau}{\mathrm{e}^{\tau\sigma_{\mathrm{naive}}} - 1}, \tag{GTUR 7}$$

where

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$$\sigma_{\text{naive}} := \frac{1}{\tau}\sum_{(i,j)\in E}\int_0^\tau \pi_i(s)\left[w_{ij}(\tau-s)-w_{ij}(s)\right]\mathrm{d}s + \frac{1}{\tau}\sum_{(i,j)\in E}\int_0^\tau \pi_i(s)w_{ij}(s)\ln\frac{w_{ij}(s)}{w_{ji}(\tau-s)}\mathrm{d}s. \tag{3.7}$$

The above result is a generalization to arbitrary protocols of [44, equation (2)], which only applies to symmetric protocols.

When the quantity $\tau\sigma_{\text{naive}}$ is small (for example when τ is small and σ_{naive} is of a given order of magnitude as in section 6.2), then the inverse rate given by the rhs of (GTUR 7) is well approximated by $1/\sigma_{\text{naive}}$. Note that for symmetric protocols $\sigma_{\text{naive}} = \sigma$. In the limit $\tau \to 0$ (GTUR 7) can be applied only to currents with time-independent increments (due to the constraints $\alpha_{i,j}(t) = -\alpha_{j,i}(\tau - t)$ and $\gamma_i(t) = -\gamma_i(\tau - t)$) and it reduces to the classical thermodynamic uncertainty relation $D_{\alpha,0}/y^2_{\alpha,0} \geqslant 1/\sigma$.

We refer to section 5 for further discussions on σ_{naive}, (GTUR 7) and its extensions.

3.4. Comments on the weights γ

We observe that (GTUR 2), (GTUR 4) and (GTUR 6) are uniform among the weights γ such that $\langle\gamma, p\rangle = 0$ for some probability measure p on V, i.e. the quantity lower bounding the ratio $D_{\alpha,\gamma}/y^2_{\alpha,\gamma}$ does not depend on the specific γ with $\langle\gamma, p\rangle = 0$. We remark that one cannot find a GTUR uniform among all possible weights γ's. Indeed, if we consider new weights γ' defined as $\gamma'_i = \gamma_i + c$ for some fixed constant c, we get $y_{\alpha,\gamma'} = y_{\alpha,\gamma} + c$, while $D_{\alpha,\gamma'} = D_{\alpha,\gamma}$. In particular the ratio of the asymptotic diffusion coefficient to the squared asymptotic value can be made arbitrarily small by playing with c. On the other hand, if we take $\gamma' = c\gamma$ for some $c \neq 0$, we have $y_{\alpha,\gamma'} = c\, y_{\alpha,\gamma}$, while $D_{\alpha,\gamma} = c^2 D_{\alpha,\gamma'}$, thus implying that $D_{\alpha,\gamma}/y^2_{\alpha,\gamma} = D_{\alpha,\gamma'}/y^2_{\alpha,\gamma'}$. As a consequence GTUR's are automatically uniform among proportional γ's. In (GTUR 2), (GTUR 4) and (GTUR 6) one goes further replacing proportionality by the weaker condition $\langle\overline{\gamma}, p\rangle = 0$.

We also observe that, given γ, the existence of a probability measure p such that $\langle\overline{\gamma}, p\rangle = 0$ is equivalent to the fact that the entries of $\overline{\gamma}$ are not all positive and not all negative. If for example the entries of γ are all positive, by taking a suitable constant c one can apply (GTUR 2), (GTUR 4) and (GTUR 6) to the weights α, γ' where $\gamma'_i = \gamma_i + c$, and then recover information on $Y^{(n)}_{\alpha,\gamma}$ by using that $Y^{(n)}_{\alpha,\gamma} = Y^{(n)}_{\alpha,\gamma'} - c$, $y_{\alpha,\gamma} = y_{\alpha,\gamma'} - c$, $D_{\alpha,\gamma} = D_{\alpha,\gamma'}$.

4. Main results II: optimization and comparisons

In this section we show three propositions. The first is concerned with the optimal p in the universal rate $C(p)$ in (GTUR 2). The second is concerned with the relation between (GTUR 2), (GTUR 4) and (GTUR 6). The third is concerned with the relation between (GTUR 1), (GTUR 3) and (GTUR 5). Finally, we conclude with some comparison between (GTUR 7) and some of the other GTUR's.

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We recall that (GTUR 2) holds for any choice of the increments α, antisymmetric or not. The following result shows the optimal bound that can be obtained in (GTUR 2) by taking the minimum among $p = (p_i)_{i\in V}$ of $C(p)$:

Proposition 4.1. *Setting*

$$A_i := \left[2 \sum_{j:(i,j)\in E} \overline{\left(\frac{w_{ij}}{\pi_i}\right)}\right]^{-1}, \tag{4.1}$$

the optimal bound in (GTUR 2) is the following:

(i) if $\overline{\gamma} = 0$, then

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \sum_i A_i; \tag{4.2}$$

(ii) if $\overline{\gamma} \neq 0$ and $\overline{\gamma}$ has neither all entries positive nor all entries negative, then

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \frac{\left(\sum_i A_i\right)\left(\sum_i A_i \overline{\gamma}_i^2\right) - \left(\sum_i A_i \overline{\gamma}_i\right)^2}{\sum_i A_i \overline{\gamma}_i^2}, \tag{4.3}$$

and the rhs of (4.3) is a positive number.

For the proof of the above proposition see section 10. We point out that the optimization among $p = (p_i)_{i\in V}$ for the other constants $C_{\mathrm{a}}(p)$ and $C^*_{\mathrm{a}}(p)$ appearing in (GTUR 4) and (GTUR 6), respectively, cannot be solved explicitly in the general case.

Remark 4.2. When the increments α are time-independent and $\gamma \equiv 0$, one can apply both (GTUR 1) and the optimal (GTUR 2) given by (4.2). If the asymptotic density $\pi(t)$ is time-independent as in the time-homogeneous case, or as in the time-periodic random walk on the ring considered in section 6.2, we can prove that (4.2) is stronger than (GTUR 1). We refer to section 10 for the derivation.

When α is antisymmetric, we can apply three p-dependent GTUR's, i.e. (GTUR 2), (GTUR 4) and (GTUR 6). Indeed, (GTUR 4) is the optimal one as follows from the next result:

Proposition 4.3. *Assume that $(i,j) \in E$ if and only if $(j,i) \in E$. Then for each probability measure $p = (p_i)_{i\in V}$ it holds $C^*_a(p) \geqslant C_a(p)$ and $C(p) \geqslant C_a(p)$. In particular, when α is antisymmetric, (GTUR 4) provides the optimal lower bound of $D_{\alpha,\gamma}/y^2_{\alpha,\gamma}$ between (GTUR 2), (GTUR 4) and (GTUR 6).*

For the proof of the above proposition see section 10. The optimality of (GTUR 4) stated in proposition 4.3 is also a consequence of a special alternative derivation of this bound by an optimization procedure (see remark 9.4).

Similarly to proposition 4.3 we have the following result for the universal constants in (GTUR 1), (GTUR 3) and (GTUR 5):

Proposition 4.4. *It holds $\sigma^* \geqslant \widetilde{\sigma}$ and $\widehat{\sigma} \geqslant \widetilde{\sigma}$. In particular, when α is antisymmetric and time-independent and $\gamma \equiv 0$, (GTUR 3) provides the optimal lower bound between (GTUR 1), (GTUR 3) and (GTUR 5).*

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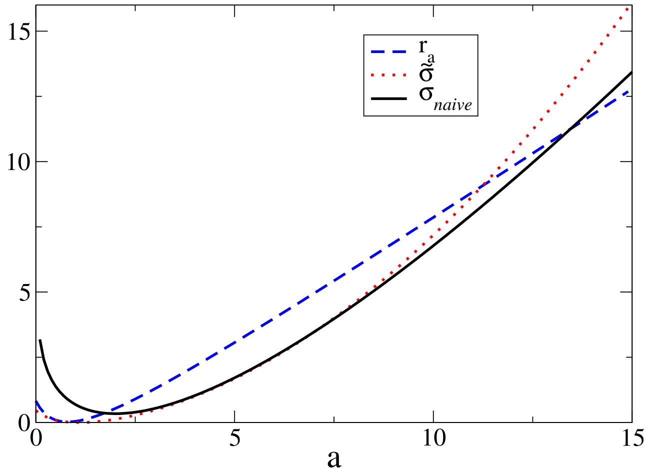

Figure 1. The constants r_{a}, $\widetilde{\sigma}$ and σ_{naive} as functions of the parameter a for the random walk on the ring in section 6.2 with fixed parameters $b = 1.7$, $c = 0.8$ and $d = 2$.

For the proof of the above proposition see section 10 (we recall that the bound $\sigma^* \geqslant \widetilde{\sigma}$ has been derived in [1]).

In section 6.2, considering the case of a random walk on the discrete ring, we show that the optimal bound (GTUR 4) of proposition 4.3 and the optimal bound (GTUR 3) of proposition 4.4 are non-comparable bounds (i.e. in some cases one is tighter, in other cases the other one is tighter). Similarly the bounds (GTUR 4) and (GTUR 7) are non-comparable, as well as the bounds (GTUR 3) and (GTUR 7). This is illustrated in figure 1 in section 6.2 and corresponds to the crossings of the plotted curves.

We collect the above comparative results in table 3.

We end this section with some remarks on (GTUR 7). If, in addition to (GTUR 7), it is possible to apply (GTUR 3) or (GTUR 4) (for example for currents with time-independent increments), then there is *a priori* no fixed order between the corresponding rates. This fact is demonstrated by an example in section 6.2.

Finally, (GTUR 7) does not provide a tight bound when the periodically driven Markov chain is obtained by a weak perturbation of a time-homogeneous Markov chain with continuous time. Indeed, suppose that the transition rates are given by $w_{ij}(t) = c_{ij} + \varepsilon d_{ij}(t)$, where c_{ij} are the transition rates of an irreducible time-homogeneous Markov chain and $d_{ij}(t)$ are genuinely time periodic, with period τ. Then, when $\varepsilon \to 0$, the value in the rhs of (GTUR 7) converges to $\tau(\mathrm{e}^{\tau\sigma} - 1)^{-1}$, which is smaller (and even much smaller for τ large) than $1/\sigma$ entering in the standard thermodynamic uncertainty relation. On the other hand, the rates $C(p)$, $C_{\mathrm{a}}(p)$, $C_{\mathrm{a}}(p^*)$, $\widehat{\sigma}$, $\widetilde{\sigma}$, σ^* behave well under perturbations.

5. Main results III: (GTUR 7) and its extensions

In this section we give further comments on σ_{naive}, (GTUR 7) and we generalize the results from [44] to general protocols that can be time-asymmetric. Our GTUR contains the rate σ_{naive} that becomes the average entropy production rate σ for the case of time-symmetric protocols, as pointed out in section 3.

The rate $\sigma_{\text{naive}} \geqslant 0$ is the asymptotic average value per unit time of the functional of the trajectories introduced in [5, section 4] and described as follows: the functional equals the logarithm of the ratio of the weight of the forward trajectory to the weight of the backward trajectory, without reversal of the protocol. This situation is different from the average entropy production rate $\sigma \geqslant 0$, for which the reversed trajectory with reversed protocol is considered. The subscript in σ_{naive} indeed refers to the fact that this quantity is obtained by the naive procedure that does include the reversal of the protocol for the reversed trajectory.

Furthermore, the quantity σ_{naive} can be written as $\sigma_{\text{naive}} = \sigma + \sigma_{\text{asy}}$, where

$$\sigma_{\text{asy}} := \sum_{(i,j)\in E} \overline{\mathcal{Q}_{ij}(A_{ij} - 1 - \ln A_{ij})}, \tag{5.1}$$

and $A_{ij}(t) := w_{ij}(\tau - t)/w_{ij}(t)$. This decomposition has a nice physical interpretation, the average entropy production rate σ quantifies energy dissipation and σ_{asy} is zero if the protocol is symmetric. We point out that $-\sigma \leqslant \sigma_{\text{asy}} \leqslant \sigma_{\text{naive}}$ and that σ_{asy} can have arbitrary sign, as demonstrated with an explicit calculation in section 6.2.

We now present our generalization of the results in [44] (see theorem 1 below), which in particular implies (GTUR 7). We denote by Θ_τ the set of all possible paths of the Markov chain up to time τ (Θ_τ is given by the piecewise-constant paths $\Gamma : [0, \tau] \to V$). Note that τ is both the period and the length of the paths. We write $\mathcal{R}_\tau : \Theta_\tau \to \Theta_\tau$ for the time-reflection around $\tau/2$ and we denote by P the probability measure on Θ_τ given by the law of the random path $(X(t))_{0\leqslant t\leqslant\tau}$ when the Markov chain has initial distribution $\pi(0)$. Similarly to [5] we introduce the average entropy flow from naive reversal defined as the entropy $H[P\,|\,P\circ\mathcal{R}_\tau]$ of P w.r.t. $P\circ\mathcal{R}_\tau$ (note that $\mathcal{R}_\tau = \mathcal{R}_\tau^{-1}$), i.e.

$$H[P\,|\,P\circ\mathcal{R}_\tau] = \int_{\Theta_\tau} P(d\Gamma) \ln \frac{\mathrm{d}P}{d(P\circ R_\tau)}(\Gamma), \tag{5.2}$$

where $P\circ\mathcal{R}_\tau(A) := P(\mathcal{R}_\tau(A))$. One gets (see [5, section 4])

$$H[P\,|\,P\circ\mathcal{R}_\tau] = \tau\sigma_{\text{naive}}, \tag{5.3}$$

where σ_{naive} is given by (3.7).

Given a function $F : \Theta_\tau \to \mathbb{R}$, we define the empirical functional $Y_F^{(n)}$ as

$$Y_F^{(n)} := \frac{1}{n}\sum_{j=0}^{n-1} F\left((X_{j\tau+s})_{0\leqslant s\leqslant\tau}\right). \tag{5.4}$$

We point out that the empirical functional $Y_{\alpha,\gamma}^{(n)}$ given in (2.9) can be written as $Y_{\alpha,\gamma}^{(n)} = Y_F^{(n)}$ by defining F as

$$F(\Gamma) := \frac{1}{\tau} \sum_{\substack{t\in(0,\tau]:\\ \Gamma(t-)\neq\Gamma(t+)}} \alpha_{\Gamma(t-),\Gamma(t+)}(t) + \frac{1}{\tau}\int_0^\tau \gamma_{\Gamma(t)}(t)\mathrm{d}t. \tag{5.5}$$

We remark that $Y_{\alpha,\gamma}^{(n)}$ is a linear functional of the empirical flow and density, while the empirical functional $Y_F^{(n)}$ in (5.4) is more general.

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Theorem 1 ([44] revisited). *Let $F : \Theta_\tau \to \mathbb{R}$ be antisymmetric, i.e. $F = -F \circ \mathcal{R}_\tau$. Then, as $n \to \infty$, $Y_F^{(n)}$ satisfies an LDP with speed n. Calling I_F the associated LD rate function, calling y_F the asymptotic value of $Y_F^{(n)}$ and assuming $y_F \neq 0$, it holds*

$$I_F''(y_F) \leqslant \frac{1}{2y_F^2}(\mathrm{e}^{\tau\sigma_{\text{naive}}} - 1). \tag{5.6}$$

As a consequence, one has the GTUR

$$\frac{D_F}{y_F^2} \geqslant \frac{1}{\mathrm{e}^{\tau\sigma_{\text{naive}}} - 1}, \tag{5.7}$$

where D_F is the asymptotic diffusion coefficient given by

$$2D_F := \lim_{n\to\infty} n\mathrm{Var}\left(Y_F^{(n)}\right). \tag{5.8}$$

We note that $y_F = E[F]$ and $2D_F = \mathrm{Var}(F)$, where the expectation and the variance are computed w.r.t. P.

We stress that theorem 1 holds for any protocol, but it is restricted to antisymmetric functionals F as in [44]. In appendix B we give for completeness the derivation of theorem 1. This proof follows the main steps of the one in [44], while some mathematical structures are investigated more carefully.

In order to apply theorem 1 to the functional $Y_{\alpha,\gamma}^{(n)} = Y_F^{(n)}$, with F defined in (5.5), we need that F is antisymmetric and this holds whenever

$$\begin{cases} \alpha_{i,j}(t) = -\alpha_{j,i}(\tau - t), \\ \gamma_i(t) = -\gamma_i(\tau - t), \end{cases} \tag{5.9}$$

for all $i, j \in V$ and all $t \in [0, \tau]$. If the weights are time independent, then (5.9) reduces to the fact that α is antisymmetric (i.e. $\alpha_{i,j} = \alpha_{j,i}$) and $\gamma \equiv 0$. Let us finally explain how to get (GTUR 7). By (2.16) and (5.8) we have

$$2D_{\alpha,\gamma} = \lim_{n\to\infty} n\tau\mathrm{Var}\left(Y_{\alpha,\gamma}^{(n)}\right) = \lim_{n\to\infty} n\tau\mathrm{Var}\left(Y_F^{(n)}\right) = 2\tau D_F, \tag{5.10}$$

while

$$y_{\alpha,\gamma} = y_F. \tag{5.11}$$

As a consequence, we get that $D_{\alpha,\gamma}/y_{\alpha,\gamma}^2 = \tau D_F/y_F^2$. As a byproduct with (5.7), we get the desired (GTUR 7).

6. Examples

We study here two specific examples, given by a periodically driven 2-state Markov chain and a periodically driven random walk on a ring. The latter is particularly relevant for the comparison of GTUR's.

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6.1. 2-state model

We consider a periodically driven 2-state Markov chain, which can be used e.g. to study a quantum dot. We take $V = \{0, 1\}$. Then the periodic stationary distribution $\pi_i(t)$ has the following form (see [5, section 6, [18, proposition 3.13]):

$$\pi_0(t) = \frac{e^{-C(t)}}{1 - e^{-C(\tau)}} \left[\int_0^t w_{10}(s) e^{C(s)} \, ds + e^{-C(\tau)} \int_t^\tau w_{10}(s) e^{C(s)} \, ds \right],$$
$$\pi_1(t) = \frac{e^{-C(t)}}{1 - e^{-C(\tau)}} \left[\int_0^t w_{01}(s) e^{C(s)} \, ds + e^{-C(\tau)} \int_t^\tau w_{01}(s) e^{C(s)} \, ds \right],$$

where

$$C(t) := \int_0^t [w_{01}(s) + w_{10}(s)] \, ds.$$

For simplicity we restrict below to $\overline{\gamma} = 0$.

When α is arbitrary, by proposition 4.1 we get the optimal (among $p = (p_0, p_1)$) (GTUR 2)

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \frac{1}{2} \left[\left(\overline{w_{01}/\pi_0} \right)^{-1} + \left(\overline{w_{10}/\pi_1} \right)^{-1} \right]. \tag{6.1}$$

When α is antisymmetric, by proposition 4.3 we know that (GTUR 4) is the optimal one between (GTUR 2), (GTUR 4) and (GTUR 6). One can optimize $C_a(p)$ among the probabilities $p = (p_0, p_1)$ as follows. Denoting the mean dynamical activity as $T(t)$, i.e.

$$T(t) := \mathcal{Q}_{01}(t) + \mathcal{Q}_{10}(t) = \pi_0(t) w_{01}(t) + \pi_1(t) w_{10}(t),$$

by straightforward computations we get

$$\min\{C_a(p) \,:\, p = (p_0, p_1)\} = 2 \frac{\overline{w^2_{01}/T} \cdot \overline{w^2_{10}/T} - \left(\overline{w_{01} w_{10}/T} \right)^2}{\overline{(w_{01} + w_{10})^2/T}}. \tag{6.2}$$

Note that, if one introduces on the fundamental period $[0, \tau]$ the probability measure

$$\nu(dt) := \left[\int_0^\tau \frac{1}{T(s)} ds \right]^{-1} \frac{1}{T(t)} dt,$$

then we can think of $w_{01}(t)$ and $w_{10}(t)$ as random variables on the probability space $([0, \tau], \nu)$ and the optimal constant given by the rhs of (6.2) equals

$$2 \frac{\mathrm{Cov}_\nu\big(w_{01}; w_{10}\big)}{\nu\big((w_{01} + w_{10})^2\big)}.$$

By (GTUR 4) we have, for α antisymmetric,

$$\frac{D_{\alpha,\gamma}}{y^2_{\alpha,\gamma}} \geqslant \frac{1}{2} \frac{\overline{(w_{01} + w_{10})^2/T}}{\overline{w^2_{01}/T} \cdot \overline{w^2_{10}/T} - \left(\overline{w_{01} w_{10}/T} \right)^2}. \tag{6.3}$$

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We recall that the GTUR's presented in section 3 are meaningful under the condition that $y_{\alpha,\gamma} \neq 0$. If one restricts to time-independent currents (i.e. $\alpha_{ij}(t) = \alpha_{ij}$, $\alpha_{ij} = -\alpha_{ji}$, and $\gamma \equiv 0$), then this condition fails, since $\overline{\mathcal{J}}_{01} = 0$ for all $t \geqslant 0$ (see remark 9.1 for a generalization).

6.2. Random walk on the ring

We consider a random walk on a ring with N sites, where $k_+(t)$ and $k_-(t)$ are the periodic probability rates to make a unitary jump clockwise and anticlockwise, respectively. In this case $\pi_i(t) = 1/N$ by symmetry.

Due to proposition 4.1, when α *is arbitrary and* $\overline{\gamma} = 0$, we have the optimal (GTUR 2)

$$\frac{D_{\alpha,\gamma}}{y_{\alpha,\gamma}^2} \geqslant \frac{1}{2} \frac{1}{\overline{k}_+ + \overline{k}_-} =: \frac{1}{r}. \tag{6.4}$$

By proposition 4.3, when α *is antisymmetric and* $\overline{\gamma} = 0$, (GTUR 4) is optimal among (GTUR 2), (GTUR 4) and (GTUR 6). By optimizing (GTUR 4) among the probability measures $p = (p_i)$, we get that the minimum is attained at the uniform probability and therefore we get the optimal (GTUR 4)

$$\frac{D_{\alpha,\gamma}}{y_{\alpha,\gamma}^2} \geqslant \frac{1}{2} \left[\overline{\left(\frac{(k_- - k_+)^2}{k_- + k_+} \right)} \right]^{-1} =: \frac{1}{r_{\mathrm{a}}}. \tag{6.5}$$

For this model we have

$$\widetilde{\sigma} = 2(\overline{k}_- - \overline{k}_+)^2 \overline{\frac{1}{k_- + k_+}} \tag{6.6}$$

and

$$\begin{aligned} \sigma_{\mathrm{naive}} &= \overline{k_+ \ln \frac{k_+}{k_-(\tau - \cdot)} + k_- \ln \frac{k_-}{k_+(\tau - \cdot)}} \\ &= \sigma + \overline{k_+ \ln \frac{k_-}{k_-(\tau - \cdot)} + k_- \ln \frac{k_+}{k_+(\tau - \cdot)}}. \end{aligned} \tag{6.7}$$

Above the function $k_\pm(\tau - \cdot)$ is defined as $t \mapsto k_\pm(\tau - t)$. If we take for example $k_+ \equiv 1$ we get $\sigma_{\mathrm{naive}} = \sigma + \overline{\ln \frac{k_-}{k_-(\tau - \cdot)}}$. This shows that there is not a fixed order between σ_{naive} and σ. Indeed, given a positive periodic function f, the random walk with rates $k_+ \equiv 1$ and $k_- = f$ and the random walk with rates $k_+ \equiv 1$ and $k_- = f(\tau - \cdot)$ have inverted ordering for σ and σ_{naive}. In particular, $\sigma_{\mathrm{asy}} = \sigma_{\mathrm{naive}} - \sigma$ can be positive and negative as well.

Let us now take the following time-symmetric protocol, where a, b, c, d are positive numbers:

$$k_+(t) = \begin{cases} a & \text{if } t \in [0, \tau/4) \\ b & \text{if } t \in [\tau/4, 3\tau/4) \\ a & \text{if } t \in [3\tau/4, \tau) \end{cases} \quad \text{and} \quad k_-(t) = \begin{cases} c & \text{if } t \in [0, \tau/4) \\ d & \text{if } t \in [\tau/4, 3\tau/4) \\ c & \text{if } t \in [3\tau/4, \tau) \end{cases}. \tag{6.8}$$

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Then we have

$$r = a + b + c + d, \tag{6.9}$$

$$r_{\mathrm{a}} = \frac{(a-c)^2}{a+c} + \frac{(b-d)^2}{b+d}, \tag{6.10}$$

$$\widetilde{\sigma} = \frac{1}{4}[(a+b)-(c+d)]^2 \left(\frac{1}{a+c} + \frac{1}{b+d}\right), \tag{6.11}$$

$$\sigma_{\mathrm{naive}} = \sigma = \frac{a-d}{2}\ln\frac{a}{d} + \frac{b-c}{2}\ln\frac{b}{c}. \tag{6.12}$$

Note that all the above quantities do not depend on the period τ.

Due to proposition 4.3 r is lower bounded by r_{a}. Due to proposition 4.4 $\widetilde{\sigma}$ lower bounds $\widehat{\sigma}$ and σ^*. We concentrate on the comparison between the constants $r_{\mathrm{a}}, \widetilde{\sigma}$ (which are optimal in the sense clarified by propositions 4.3 and 4.4) and σ_{naive}. As shown in figure 1, there is no fixed order either between r_{a} and σ_{naive} or between $\widetilde{\sigma}$ and σ_{naive}. Note that, for $\tau \to 0$, the universal constant $(\mathrm{e}^{\tau\sigma_{\mathrm{naive}}}-1)/\tau$ converges to σ_{naive}. As a consequence there is no optimality either between the GTUR (6.5) and (GTUR 7) or between (GTUR 3) and (GTUR 7). Figure 1 shows also that there is no fixed order between r_a and $\widetilde{\sigma}$, i.e. (GTUR 3) and (GTUR 4) are non-comparable bounds.

7. Proofs I: comments on the derivation of the GTUR's

We comment the methods used to derive the GTUR's, which are summarized in table 1.

(1) Due to (2.13) we have the upper bound

$$I_{\alpha,\gamma}(y) \leqslant I(Q,\rho) \text{ for any } (Q,\rho) \in \mathcal{F}_{\alpha,\gamma,y}, \tag{7.1}$$

where $I(Q,\rho)$ is the explicit function given in (2.14) and the set $\mathcal{F}_{\alpha,\gamma,y}$ is defined after (2.14).

(2) We assume to have an y-parameterized pair $(Q_y,\rho_y) \in \mathcal{F}_{\alpha,\gamma,y}$ such that (Q_y,ρ_y) differs from $(\mathcal{Q},\pi)$ by a term proportional to $y - y_{\alpha,\gamma}$.

(3) Plugging the above y-parameterized pair (Q_y,ρ_y) in the inequality (7.1) and taking a 2nd order Taylor expansion of the explicit function $y \mapsto I(Q_y,\rho_y)$ around $y_{\alpha,\gamma}$, one gets a quadratic local bound of $I_{\alpha,\gamma}$ at $y_{\alpha,\gamma}$ (see theorem 2 in section 8). A lower bound for the ratio $D_{\alpha,\gamma}/y^2_{\alpha,\gamma}$ can then be obtained by (2.17).

(4) By exhibiting different choices of (Q_y,ρ_y) satisfying the above general conditions, we obtain (GTUR 1) and (GTUR 2).

(5) When α is antisymmetric $Y^{(n)}_{\alpha,\gamma}$ can be expressed as a linear function of the empirical density and current, whose LD principle has been derived in [5] with an explicit LD rate functional I_*. The above strategy can be implemented working with currents (J) instead of flows (Q). Hence, we get a general result given by theorem 3, which is the analogous of theorem 2. Indeed, by a different approach, we show that theorem 3 can be even derived from theorem 2. By exhibiting different choices of (J_y, ρ_y) satisfying our general conditions, we get (GTUR 3) and (GTUR 4).

(6) (GTUR 6) is a consequence of a general result detailed in theorem 4. This theorem can be obtained along the above scheme, with the exception that one uses an upper bound of the LD rate function I_* by a suitable function proposed by [22] and afterwards applies a 2nd order Taylor expansion to this function. We also show that indeed theorem 4 can also be obtained as corollary of theorem 3.

(7) (GTUR 7) is a special case of a more general result given in theorem 1 in section 5 and its derivation follows very closely the one in [44]. The trajectory of the Markov chain on the time interval $[0, n\tau]$ can be thought of as a concatenation of paths on the fundamental periods $[0, \tau]$, $[\tau, 2\tau]$,.., $[(n-1)\tau, n\tau]$. One obtains a LD principle for the frequencies of these paths. On the other hand, the empirical functional $Y^{(n)}_{\alpha,\gamma}$ can be expressed as a linear functional of the above frequencies and by contraction one gets a new variational characterization for $I_{\alpha,\gamma}$. By playing with suitable inputs in the variational characterization, one finally gets the resulting quadratic local upper bounds on $Y^{(n)}_{\alpha,\gamma}$ and, as a byproduct with (2.17), (GTUR 7).

8. Proofs II: local bounds on $I_{\alpha,\gamma}$ and GTUR's for $Y^{(n)}_{\alpha,\gamma}$ with generic α

Our first aim is to describe a general method to get local quadratic upper bounds on $I_{\alpha,\gamma}$ around its minimum point $y_{\alpha,\gamma}$, thus leading also to lower bounds on $D_{\alpha,\gamma}$ via (2.17). This method is an extension of the one used for the empirical currents in [1, section 4.3].

It is convenient to introduce the concept of *generalized flow*, which is defined as a flow without the restriction of non-negativity. In other words, we will call generalized flow any function $k : V \times V \to \mathbb{R}$ which is zero outside E. If k is non-negative, then k is a flow. The divergence of k is defined as

$$\mathrm{div}_i k := \sum_j k_{ij} - \sum_j k_{ji}. \tag{8.1}$$

Due to (2.13) one has

$$I_{\alpha,\gamma}(y) \leqslant I(Q, \rho), \qquad \forall (Q, \rho) \in \mathcal{F}_{\alpha,\gamma,y}, \tag{8.2}$$

where the set $\mathcal{F}_{\alpha,\gamma,y}$ is defined after in (2.14). Moreover, the function $\Phi(q, p)$ defined in (2.12) satisfies the following bound obtained by a Taylor's expansion around the arbitrary diagonal point (a, a):

Table 1. Summary of GTUR's written as $D_{\alpha,\gamma}/y^2_{\alpha,\gamma} \geqslant$ lowerbound (see also table 2). The GTUR's are valid for the linear functionals $Y^{(n)}_{\alpha,\gamma}$ that fulfill the conditions on the third column.

GTUR	Lower bound	Restrictions on $Y^{(n)}_{\alpha,\gamma}$
GTUR 1	$1/\widehat{\sigma}$	$\alpha_{ij}(t) = \alpha_{ij}$ and $\gamma_i(t) = 0$
GTUR 2	$1/C(p)$	$\langle \overline{\gamma}, p \rangle = 0$
GTUR 3	$1/\widetilde{\sigma}$	$\alpha_{ij}(t) = \alpha_{ij}$, $\alpha_{ij} = -\alpha_{ji}$ and $\gamma_i(t) = 0$
GTUR 4	$1/C_a(p)$	$\alpha_{ij}(t) = -\alpha_{ji}(t)$ and $\langle \overline{\gamma}, p \rangle = 0$
GTUR 5	$1/\sigma^*$	$\alpha_{ij}(t) = \alpha_{ij}$, $\alpha_{ij} = -\alpha_{ji}$ and $\gamma_i(t) = 0$
GTUR 6	$1/C^*_a(p)$	$\alpha_{ij}(t) = -\alpha_{ji}(t)$ and $\langle \overline{\gamma}, p \rangle = 0$
GTUR 7	$\tau/\left(\mathrm{e}^{\tau\sigma_{\mathrm{naive}}} - 1\right)$	$\alpha_{ij}(t) = -\alpha_{ji}(\tau - t)$ and $\gamma_i(t) = -\gamma_i(\tau - t)$

Table 2. Summary of the constants appearing in the GTUR's.

Symbol	Definition
$\widehat{\sigma}$	$2\sum_{(i,j)\in E} \left(\overline{\mathcal{Q}}_{ij}\right)^2 \overline{(1/\mathcal{Q}_{ij})}$
$C(p)$	$2\sum_{(i,j)\in E} p_i^2 \overline{(w_{ij}/\pi_i)}$
$\widetilde{\sigma}$	$\sum_{(i,j)\in E} (\overline{\mathcal{J}}_{ij})^2\, \overline{1/(\mathcal{Q}_{ij} + \mathcal{Q}_{ji})}$
$C_{\mathrm{a}}(p)$	$\sum_{(i,j)\in E} \overline{\left((p_i w_{ij} - p_j w_{ji})^2/(\mathcal{Q}_{ij} + \mathcal{Q}_{ji})\right)}$
σ^*	$\frac{1}{2}\sum_{(i,j)\in E} (\overline{\mathcal{J}}_{ij})^2 \overline{\left(\frac{1}{\mathcal{J}_{ij}} \ln \frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}\right)}$
$C^*_{\mathrm{a}}(p)$	$\frac{1}{2}\sum_{(i,j)\in E} \overline{\left((p_i w_{ij} - p_j w_{ji})^2/\mathcal{J}_{ij}\right) \ln \frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}}$
σ_{naive}	$\sum_{(i,j)\in E} \overline{\pi_i \left[w_{ij}(\tau - \cdot) - w_{ij} + w_{ij} \ln \frac{w_{ij}}{w_{ji}(\tau - \cdot)}\right]}$

$$\Phi(q, p) = \frac{1}{2a}(p - q)^2 + o\left((q - a)^2 + (p - a)^2\right). \tag{8.3}$$

Due to (2.10), when y is close to the asymptotic value $y_{\alpha,\gamma}$, it is natural to look for pairs $(Q, \rho) \in \mathcal{F}_{\alpha,\gamma,y}$ which are obtained as perturbation of $(\mathcal{Q}, \pi)$. To this aim, it is convenient to use the representation

$$\begin{cases} Q = \mathcal{Q} + \frac{y - y_{\alpha,\gamma}}{y_{\alpha,\gamma}} R, \\ \rho = \pi + \frac{y - y_{\alpha,\gamma}}{y_{\alpha,\gamma}} m. \end{cases} \tag{8.4}$$

We assume $y_{\alpha,\gamma} \neq 0$ in this equation. For the case $y_{\alpha,\gamma} = 0$, the equation has to be modified, as explained in remark 8.1 below.

Note that $(Q, \rho) \in \mathcal{F}_{\alpha,\gamma,y}$ if and only if the following properties are satisfied by the pair (R, m):

Table 3. Implications between GTUR's. Lines, from top to bottom, correspond respectively to proposition 4.1—(i), proposition 4.1—(ii), remark 4.2, proposition 4.3 and proposition 4.4. Recall that (GTUR 3) and (GTUR 4) are non-comparable and the same holds for the pairs (GTUR 3) and (GTUR 7), (GTUR 4) and (GTUR 7).

SET-UP	HIERARCHY OF GTUR's
$\bar{\gamma}_i = 0$	(4.2) is the optimal (GTUR 2)
$\begin{cases} \bar{\gamma}_i \neq 0 \\ \bar{\gamma} \notin (0,+\infty)^V \\ \bar{\gamma} \notin (-\infty,0)^V \end{cases}$	(4.3) is the optimal (GTUR 2)
$\begin{cases} \pi_i(t) = \pi_i \\ \alpha_{ij}(t) = \alpha_{ij} \\ \gamma_i(t) = 0 \end{cases}$	Optimal (GTUR 2) (4.2) $\Rightarrow$ (GTUR 1)
$\alpha_{ij}(t) = -\alpha_{ji}(t)$	$\begin{cases} \text{(GTUR 4)} \Rightarrow \text{(GTUR 2)} \\ \text{(GTUR 4)} \Rightarrow \text{(GTUR 6)} \end{cases}$
$\begin{cases} \alpha_{ij}(t) = \alpha_{ij} \\ \alpha_{ij} = -\alpha_{ji} \\ \gamma_i(t) = 0 \end{cases}$	$\begin{cases} \text{(GTUR 3)} \Rightarrow \text{(GTUR 1)} \\ \text{(GTUR 3)} \Rightarrow \text{(GTUR 5)} \end{cases}$

(P1) $R = \big(R(t)\big)_{t\geqslant 0}$ is a time-periodic generalized flow and therefore $R(t) : V \times V \to \mathbb{R}$ is zero outside E for all $t \geqslant 0$;

(P2) $m = \big(m(t)\big)_{t\geqslant 0}$ is time-periodic and $m(t) : V \to \mathbb{R}$ satisfies $\sum_i m_i(t) = 0$ for all $t \geqslant 0$;

(P3) $\partial_t m(t) + \operatorname{div} R(t) = 0$,

(P4) $y_{\alpha,\gamma} = \overline{\langle \alpha, R\rangle} + \overline{\langle \gamma, m\rangle}$;

(P5) the functions in the rhs of (8.4) take non-negative values.

We point out that, given R, m satisfying (P1) and (P2), since $\mathcal{Q}_{ij}(t) > 0$ for all $(i,j) \in E$ and $\pi_i(t) > 0$ for all $i \in V$, property (P5) is satisfied for y sufficiently close to $y_{\alpha,\gamma}$. Since our bounds are local for y close to $y_{\alpha,\gamma}$, we will disregard (P5) in what follows.

Theorem 2. *For any pair (R, m) fulfilling the above properties (P1),…,(P4) the following local quadratic upper bound holds:*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{2}\frac{(y-y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2} \sum_{(i,j)\in E} \overline{\left(\frac{\big(R_{ij}-m_i w_{ij}\big)^2}{\mathcal{Q}_{ij}}\right)} + o\left((y-y_{\alpha,\gamma})^2\right). \qquad (8.5)$$

In particular, we have the lower bound

$$2D_{\alpha,\gamma} \geqslant y^2_{\alpha,\gamma} \left\{ \sum_{(i,j)\in E} \overline{\left(\frac{\left(R_{ij} - m_i w_{ij}\right)^2}{\mathcal{Q}_{ij}} \right)} \right\}^{-1} . \tag{8.6}$$

We point out that, since (8.4) defines a bijection $(R, m) \mapsto (Q, \rho)$, one would get an identity in (8.5) and (8.6) by optimizing among (R, m) in the above theorem.

Proof. From (2.14) and (8.3) by setting $a = \mathcal{Q}_{ij}(t)$, we have

$$\begin{aligned} I(Q,\rho) := & \sum_{(i,j)\in E} \overline{\Phi\big(Q_{ij}(t), \rho_i(t) w_{ij}(t)\big)} \\ = & \sum_{(i,j)\in E} \overline{\left(\frac{\left(Q_{ij} - \rho_i w_{ij}\right)^2}{2\mathcal{Q}_{ij}} + \mathcal{E}_{ij} \right)} \\ = & \frac{1}{2} \frac{(y - y_{\alpha,\gamma})^2}{y^2_{\alpha,\gamma}} \sum_{(i,j)\in E} \overline{\left(\frac{\left(R_{ij} - m_i w_{ij}\right)^2}{\mathcal{Q}_{ij}} + \mathcal{E}_{ij} \right)}, \end{aligned} \tag{8.7}$$

where the error term $\mathcal{E}_{ij}(t)$ is given by

$$\mathcal{E}_{ij}(t) = o\left((Q_{ij}(t) - \mathcal{Q}_{ij}(t))^2 \right) + o\left((\rho_i(t) - \pi_i(t))^2 \right) = o\left((y - y_{\alpha,\gamma})^2\right). \tag{8.8}$$

Equations (8.7) and (8.8) imply (8.5). Finally, (8.6) follows from (8.5) by means of (2.17). □

Remark 8.1. When $y_{\alpha,\gamma} = 0$ the above arguments remain valid by making the following changes. Formula (8.4) becomes $Q = \mathcal{Q} + yR, \rho = \pi + ym$. In (P4) one replaces $y_{\alpha,\gamma}$ with 1. In (P5) the $y_{\alpha,\gamma}$'s on the numerator are 0 while the ones on the denominator become 1. Then theorem 2 remains valid by replacing $y_{\alpha,\gamma}$ with 1 in the denominator of (8.5) (the $y_{\alpha,\gamma}$ in the numerator is zero) and in (8.6).

Theorem 2 provides a very general method from which several local quadratic bounds and GTUR's can be derived by inserting different choices of (R, m). To get sharp and interesting bounds it is important to select special perturbations (R, m) fulfilling the above properties (P1)–(P4). We discuss below some special choices, leading to some corollaries of theorem 2. This is of course not a complete list and one can find other choices in [1].

A first class of choices, closely related to the ones in [1, section 4.5], is given in the following corollary:

Corollary 8.2. *Suppose that $\mathcal{K}(t) = (\mathcal{K}_{ij}(t))$ is a time-periodic generalized flow with* $\operatorname{div} \mathcal{K} = 0$ *and such that $\overline{\langle \alpha, \mathcal{K} \rangle} \neq 0$. Then it holds*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4} \frac{\widehat{\sigma}}{\overline{\langle \alpha, \mathcal{K} \rangle}^2} (y - y_{\gamma,\alpha})^2 + o\big((y - y_{\gamma,\alpha})^2\big) \tag{8.9}$$

and

$$D_{\alpha,\gamma} \geqslant \frac{\overline{\langle \alpha, \mathcal{K} \rangle}^{\,2}}{\widehat{\sigma}}, \tag{8.10}$$

where

$$\widehat{\sigma} := 2 \sum_{(i,j)\in E} \overline{\left(\frac{\mathcal{K}_{ij}^2}{\mathcal{Q}_{ij}} \right)}. \tag{8.11}$$

Proof. It is enough to apply theorem 2 with $R := (y_{\alpha,\gamma}/\overline{\langle \alpha, \mathcal{K} \rangle})\mathcal{K}$ and $m = 0$. □

We collect some comments on the above corollary 8.2.

- A possible choice of $\mathcal{K}$ is given by $\mathcal{K} = \overline{\mathcal{Q}}$ when $\langle \overline{\alpha}, \overline{\mathcal{Q}} \rangle \neq 0$.
- When $\gamma \equiv 0$ and α is time-independent we have that $y_{\alpha,\gamma} = \overline{\langle \alpha, \mathcal{Q} \rangle} = \langle \alpha, \overline{\mathcal{Q}} \rangle$. In particular, by taking $\mathcal{K} = \overline{\mathcal{Q}}$ in the above corollaries 8.2, (8.10) becomes (GTUR 1) valid whenever $\langle \alpha, \overline{\mathcal{Q}} \rangle \neq 0$.
- Another possible choice for $\mathcal{K}$ is given by $\mathcal{K}_{ij}(t) = \mu_i(t) w_{ij}(t)$, where $\mu_i(t)$ denotes the so-called accompanying distribution, i.e. the invariant distribution for the time-homogeneous Markov chain with time-independent rates $w_{ij}(t)$ (t thought of as frozen). For this second choice we also refer to [1, section 4.5].
- The property of being a time periodic generalized flow with zero divergence is preserved by linear combinations. In particular, one can also take $\mathcal{K}_{ij} = c_1 \overline{\mathcal{Q}}_{ij} + c_2 \mu_i(t) w_{ij}(t)$, for any fixed $c_1, c_2 \in \mathbb{R}$.
- Given the model, one can look for more efficient choices of $\mathcal{K}$ by using Schnakenberg's cycle theory [7, 45] to build divergence-free flows, and afterwards by trying to optimize among these flows. Note that non-trivial divergence-free flows on the graph (V, E) always exist.

We are not going to discuss in detail the possible optimization problems related to the last comment above, concerning Schnakenberg's cycle theory, since this approach is very model-dependent. We consider in the next section just one special case where an argument of this type works naturally (see first proof of theorem 3).

In [29] the authors consider functionals of the form (2.9) with α antisymmetric and γ not arbitrary, but of the form

$$\gamma_i(t) = \frac{\mathrm{d}}{\mathrm{d}t} g_i(t) \qquad \forall i \in V, \tag{8.12}$$

for some periodic function g_i. The above form (8.12) is equivalent to the property

$$\overline{\gamma}_i = 0 \qquad \forall i \in V. \tag{8.13}$$

In the following result we consider general weights α and we weaken condition (8.13) on γ.

Corollary 8.3. *Suppose that the entries of* $\overline{\gamma}$ *are not all strictly positive, and not all strictly negative. Fix any time-independent probability measure* $p = (p_i)_{i \in V}$ *on* V *with* $\langle p, \overline{\gamma} \rangle = 0$. *Recall the constant* $C(p)$ *defined in (3.2). Then we have the upper bound*

$$I_{\alpha,\gamma}(y) \leqslant \frac{C(p)}{4} \frac{(y - y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2} + o\left((y - y_{\alpha,\gamma})^2\right). \tag{8.14}$$

As a consequence we have (GTUR 2).

Proof. We take

$$R(t) := \mathcal{Q}(t), \qquad m(t) := \pi(t) - p.$$

Properties (P1), (P2), (P3) are satisfied (recall the continuity equation (2.5)). Due to (2.10) and (8.13) we have

$$\overline{\langle \alpha, R \rangle} + \overline{\langle \gamma, m \rangle} = y_{\alpha,\gamma} - \langle \overline{\gamma}, p \rangle = y_{\alpha,\gamma}.$$

Hence, also property (P4) is satisfied. Note that

$$R_{ij}(t) - m_i(t) w_{ij}(t) = \mathcal{Q}_{ij}(t) - (\pi_i(t) - p_i) w_{ij}(t) = p_i w_{ij}(t).$$

By plugging the above identity in (8.5) and (8.6) we get (8.14). (GTUR 2) then follows due to (2.17). □

Remark 8.4. We would like to point out that the art of finding good bounds is related to the art of finding good perturbations (m, R) and this is essentially the art of finding periodic solutions of the continuity equation in condition (P3). We briefly discuss in appendix A two possible approaches.

9. Proofs III: local bounds on $I_{\alpha,\gamma}$ and GTUR's for $Y_{\alpha,\gamma}^{(n)}$ with antisymmetric α

In all this section we will assume, without further mention, that

$$\begin{cases} \alpha \text{ is antisymmetric, i.e. } \alpha_{ij}(t) = -\alpha_{ji}(t), \\ (i, j) \in E \text{ if and only if } (j, i) \in E. \end{cases}$$

Below we provide two general methods to get local quadratic bounds on $I_{\alpha,\gamma}$ (see theorems 3 and 4) and we discuss some corollaries. We prove theorem 3 using two approaches. For the first proof, we start with theorem 2 and perform an optimization among flows. Hence, theorem 3 can be seen as corollary of theorem 2. For the second proof, we use the LD rate functional associated with the empirical current and empirical measure from [5]. Also for theorem 4 we provide two alternative derivations. In one derivation we get theorem 4 from theorem 3. As a consequence, both theorems 3 and 4 follow from theorem 2.

9.1. Preliminaries and theorem 3

In what follows, we call *current* any function $d: V \times V \to \mathbb{R}$ which is zero outside E and antisymmetric, i.e. $d_{ij} = -d_{ji}$ $\forall i, j$. We order the elements of V (arbitrarily) and write $<$ for the order relation. Given $a: V \times V \to \mathbb{R}$, we define

$$\langle\langle a, d \rangle\rangle := \sum_{(i,j)\in E: i<j} a_{ij} d_{ij}.$$

Note that, when also a is antisymmetric, we have $\langle\langle a, d\rangle\rangle = \frac{1}{2}\langle a, d\rangle$. Finally, we define the divergence of a current d by

$$\mathrm{div}_i\, d = \sum_j d_{ij}. \tag{9.1}$$

We point out that the divergence of a current is defined differently from the divergence of a generalized flow (see (8.1)). This definition guarantees that, if k is a generalized flow and d is the current $d_{ij} := k_{ij} - k_{ji}$, then $\langle\langle d', d\rangle\rangle = \langle d', k\rangle$ for any current d'.

Due to the antisymmetry of the increments α_{ij}, the LD rate functional $I_{\alpha,\gamma}$ admits an alternative variational characterization, in addition to (2.13), in terms of the empirical current and density [5], as explained below. We consider the function

$$\psi(j, g, a) := \sqrt{g^2 + a^2} - \sqrt{j^2 + a^2} + j\left[\sinh^{-1}(j/a) - \sinh^{-1}(g/a)\right], \tag{9.2}$$

$\sinh^{-1}(x)$ denoting the hyperbolic arcsinus. Then it holds

$$I_{\alpha,\gamma}(y) = \inf\{I_*(J,\rho)\ :\ (J,\rho) \in \mathcal{F}^*_{\alpha,\gamma,y}\}, \tag{9.3}$$

where now

$$I_*(J,\rho) := \sum_{(i,j)\in E: i<j} \overline{\Psi\big(J_{ij}(t), G_{ij}(t), a_{ij}(t)\big)}, \tag{9.4}$$

$$G_{ij}(t) := \rho_i(t) w_{ij}(t) - \rho_j(t) w_{ji}(t), \tag{9.5}$$

$$a_{ij}(t) := 2\sqrt{\rho_i(t)\rho_j(t) w_{ij}(t) w_{ji}(t)}, \tag{9.6}$$

and $\mathcal{F}^*_{\alpha,\gamma,y}$ denotes the family of pairs $(J,\rho) = (J(t),\rho(t))_{t\geqslant 0}$ such that

(i) $J(t)$ is a time-periodic current, i.e. $J(t) = J(t+\tau)$ and $J(t)$ is an antisymmetric function on $V \times V$ which is zero outside E for each time t;

(ii) $\rho(t)$ is a time-periodic probability measure on V;

(iii) the continuity equation $\partial_t \rho(t) + \mathrm{div}\, J(t) = 0$ is satisfied (see (9.1));

(iv) $y = \overline{\langle\langle \alpha, J\rangle\rangle} + \overline{\langle \gamma, \rho\rangle}$.

According to [5, theorem 3], formula (9.4) with the restrictions (i), (ii) and (iii) is the joint LD rate function for the empirical current and measure with speed $n\tau$. The empirical current $J^{(n)}$ is defined as the measure on $E \times [0,\tau)$ given by $J^{(n)}(i,j,\mathrm{d}t) := Q^{(n)}(i,j,\mathrm{d}t) - Q^{(n)}(j,i,\mathrm{d}t)$ (see section 2.2). Formula (9.4) can be

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deduced directly by contraction starting from the joint LD rate functional for the empirical measure and flow discussed in section 2.2. As in (2.15) we have

$$Y^{(n)}_{\alpha,\gamma} = \frac{1}{\tau} \sum_{(i,j)\in E: i<j} \int \alpha_{ij}(t) J^{(n)}(i,j,\mathrm{d}t) + \frac{1}{\tau} \sum_i \int \gamma_i(t) \rho^{(n)}(i,\mathrm{d}t), \tag{9.7}$$

thus allowing to derive the LD principle for $Y^{(n)}_{\alpha,\gamma}$ from the LD principle of $\left(J^{(n)},\rho^{(n)}\right)$ by contraction. We point out that the asymptotic pair $(\mathcal{J},\pi)$ belongs to $\mathcal{F}^*_{\alpha,\gamma,y}$ with $y = y_{\alpha,\gamma}$ and that it fulfills the identity $I_*(\mathcal{J},\pi) = 0$.

As in section 8, from now on we assume that $y_{\alpha,\gamma} \neq 0$.

Remark 9.1. Suppose that the transition graph (V,E) has the property that (i) for each edge in E also the reversed edge belongs to E, (ii) the non-oriented graph obtained from (V,E) by disregarding the edge orientation is a tree. In this case, being divergence-free, $\overline{\mathcal{J}}$ must be zero and, as a consequence, $y_{\alpha,0} = 0$ for currents with time-independent increments. Moreover, reasoning as in the last paragraph of section 2, one can show that the set $\mathcal{F}^*_{\alpha,\gamma,y}$ defined after (9.6) is empty for $y \neq 0$, thus implying that $I_{\alpha,\gamma}(y) = +\infty$ for $y \neq 0$ and $I_{\alpha,\gamma}(0) = 0$.

As in section 8 we consider pairs (J,ρ) written as perturbations of the stationary pair $(\mathcal{J},\pi)$ as follows:

$$\begin{cases} J = \mathcal{J} + \frac{y-y_{\alpha,\gamma}}{y_{\alpha,\gamma}} Z, \\ \rho = \pi + \frac{y-y_{\alpha,\gamma}}{y_{\alpha,\gamma}} m. \end{cases} \tag{9.8}$$

To assure that $(J,\rho) \in \mathcal{F}^*_{\alpha,\gamma,y}$, the pair (Z,m) must satisfy the following properties:

(P1*) $Z = \left(Z(t)\right)_{t\geqslant 0}$ is a time-periodic current (in particular $Z(t): V\times V \to \mathbb{R}$ is antisymmetric and is zero outside E for all $t \geqslant 0$);

(P2*) $m = \left(m(t)\right)_{t\geqslant 0}$ is time-periodic and $m(t): V \to \mathbb{R}$ satisfies $\sum_i m_i(t) = 0$ for all $t \geqslant 0$;

(P3*) $\partial_t m + \operatorname{div} Z(t) = 0$ (see (9.1));

(P4*) $y_{\alpha,\gamma} = \overline{\langle\langle \alpha, Z\rangle\rangle} + \overline{\langle \gamma, m\rangle}$;

(P5*) it holds $\pi_i(t) + \frac{y-y_{\alpha,\gamma}}{y_{\alpha,\gamma}} m_i(t) \geqslant 0$ for all $t \geqslant 0$ and $i \in V$.

Since $\pi_i(t) > 0$ for any t, condition (P5*) is satisfied for y near enough to $y_{\alpha,\gamma}$. As a consequence, in what follows we disregard condition (P5*).

We can finally state our general method to get local quadratic bounds on $I_{\alpha,\gamma}$:

Theorem 3. *For any pair (Z,m) fulfilling the above properties (P1*),…,(P4*) the following local quadratic upper bound holds:*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{2}\frac{(y-y_{\alpha,\gamma})^2}{y^2_{\alpha,\gamma}} \sum_{(i,j)\in E: i<j} \overline{\left(\frac{\left(Z_{ij} - (m_i w_{ij} - m_j w_{ji})\right)^2}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}}\right)} + o\left((y-y_{\alpha,\gamma})^2\right). \tag{9.9}$$

In particular, we have the lower bound

$$2D_{\alpha,\gamma} \geqslant y^2_{\alpha,\gamma} \left\{ \sum_{(i,j)\in E: i<j} \overline{\left(\frac{\left(Z_{ij} - (m_i w_{ij} - m_j w_{ji})\right)^2}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}} \right)} \right\}^{-1}. \tag{9.10}$$

We point out that, since (9.8) defines a bijection $(Z, m) \mapsto (J, \rho)$, one would get an identity in (9.9) and (9.10) by optimizing among (Z, m) in the above theorem.

9.2. First proof of theorem 3

The proof relies on theorem 2 and an optimization procedure in the same spirit of the last comment on corollary 8.2.

Let (Z, m) be a pair fulfilling properties (P1*),...,(P4*) and let R' be the time-periodic generalized flow given by $R'_{ij}(t) := Z_{ij}(t)/2$. Note that the pair (R', m) satisfies properties (P1),...,(P4) in section 8. We take $R = (R(t))_{t\geqslant 0}$ as $R(t) := R'(t) + S(t)$, where $S(t)$ is a generic time-periodic symmetric generalized flow, i.e. $S_{i,j}(t) = S_{j,i}(t)$ for all i, j, t. Since $\operatorname{div} S(t) = 0$ and $\langle \alpha(t), S(t)\rangle = 0$ by the antisymmetry of α, also the pair (R, m) satisfies conditions (P1),..,(P4) and therefore theorem 2 applies to (R, m).

We optimize the upper bound (8.5) in theorem 2 over the symmetric generalized flows S. For the optimization, the basic computation that we need is the following. We consider some fixed numbers r_k, a_k, q_k, $k = 1, 2$ and compute

$$\inf_{s\in\mathbb{R}} \left[\frac{(r_1 + s - a_1)^2}{q_1} + \frac{(r_2 + s - a_2)^2}{q_2} \right]. \tag{9.11}$$

The function is minimized at

$$s^* = \frac{c_1}{c_1 + c_2}(a_1 - r_1) + \frac{c_2}{c_1 + c_2}(a_2 - r_2),$$

where $c_k := q_k^{-1}$. The minimal value is given by

$$\frac{\left[(r_1 - r_2) - (a_1 - a_2)\right]^2}{q_1 + q_2}. \tag{9.12}$$

Let us come back to the upper bound (8.5) in theorem 2. Independently for each pair of edges (i, j) and (j, i), we can evaluate

$$\inf_{s\in\mathbb{R}} \left\{ \frac{\left(R'_{ij}(t) + s - m_i(t) w_{ij}(t)\right)^2}{\mathcal{Q}_{ij}(t)} + \frac{\left(R'_{ji}(t) + s - m_j(t) w_{ji}(t)\right)^2}{\mathcal{Q}_{ji}(t)} \right\},$$

where s has to be thought as the value $S_{ij}(t) = S_{ji}(t)$. According to (9.12) the above infimum is indeed attained at a suitable value $S^*_{ij}(t)$ and equals

$$\frac{\left[\left(R'_{ij}(t) - R'_{ji}(t)\right) - \left(m_i(t) w_{ij}(t) - m_j(t) w_{ji}(t)\right)\right]^2}{\mathcal{Q}_{ij}(t) + \mathcal{Q}_{ji}(t)}. \tag{9.13}$$

As a consequence, by taking $R(t) = R'(t) + S^*$ the resulting bound (8.5) reduces to (9.9) since $Z_{ij}(t) := R'_{ij}(t) - R'_{ji}(t)$. Finally, (9.10) follows from (9.9) and (2.17).

9.3. Second proof of theorem 3

We follow the same arguments of theorem 2 but applied to the functional (9.4). We first consider the Taylor's expansion up to the second order of the function $\Psi(j,g,a)$ around the point $(x-y, x-y, 2\sqrt{xy})$ with $x, y \geqslant 0$. By writing

$$\begin{cases} j = x - y + \delta j, \\ g = x - y + \delta g, \\ a = 2\sqrt{xy} + \delta a, \end{cases} \tag{9.14}$$

we have (after cumbersome but straightforward computations) that

$$\begin{aligned} \psi(j,g,a) &= \frac{1}{2}\frac{1}{x+y}(j-g)^2 + o\big((\delta j)^2\big) + o\big((\delta g)^2\big) + o\big((\delta a)^2\big) \\ &= \frac{1}{2}\frac{1}{x+y}(\delta j - \delta g)^2 + o\big((\delta j)^2\big) + o\big((\delta g)^2\big) + o\big((\delta a)^2\big). \end{aligned} \tag{9.15}$$

By (9.5) and (9.6) we can write

$$J_{ij}(t) = \mathcal{Q}_{ij}(t) - \mathcal{Q}_{ji}(t) + \frac{y - y_{\alpha,\gamma}}{y_{\alpha,\gamma}} Z_{ij}(t), \tag{9.16}$$

$$G_{ij}(t) = \mathcal{Q}_{ij}(t) - \mathcal{Q}_{ji}(t) + \frac{y - y_{\alpha,\gamma}}{y_{\alpha,\gamma}} \big[m_i(t)w_{ij}(t) - m_j(t)w_{ji}(t)\big], \tag{9.17}$$

$$a_{ij}(t) = 2\sqrt{\mathcal{Q}_{ij}(t)\mathcal{Q}_{ji}(t)} + \delta a_{ij}(t) \tag{9.18}$$

where $\delta a_{ij}(t) = O\big(|y - y_{\alpha,\gamma}|\big)$ (i.e. $|\delta a_{ij}(t)| \leqslant C|y - y_{\alpha,\gamma}|$ for y near to $y_{\alpha,\gamma}$). Due to the above identities, applying (9.15) with $x = \mathcal{Q}_{ij}(t)$ and $y = \mathcal{Q}_{ji}(t)$ we get

$$\begin{aligned} &\psi\big(J_{ij}(t), G_{ij}(t), a_{ij}(t)\big) \\ &= \frac{1}{2}\frac{(y - y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2} \frac{\big[Z_{ij}(t) - \big(m_i(t)w_{ij}(t) - m_j(t)w_{ji}(t)\big)\big]^2}{\mathcal{Q}_{ij}(t) + \mathcal{Q}_{ji}(t)} + o\left((y - y_{\alpha,\gamma})^2\right). \end{aligned} \tag{9.19}$$

From this equation together with (9.3) and (9.4) we get (9.9). Finally, (9.10) follows from (9.9) by (2.17).

9.4. Corollaries to theorem 3

Likewise the previous section we have also the following results.

Corollary 9.2. *Suppose that* $\mathcal{K}(t) = \big(\mathcal{K}_{ij}(t)\big)$ *is a time-periodic current with* $\operatorname{div}\mathcal{K} = 0$ *and such that* $\overline{\langle\langle \alpha, \mathcal{K}\rangle\rangle} \neq 0$. *Then it holds*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4}\frac{\widetilde{\sigma}}{\overline{\langle\langle \alpha, \mathcal{K}\rangle\rangle}^2}(y - y_{\gamma,\alpha})^2 + o\big((y - y_{\gamma,\alpha})^2\big) \tag{9.20}$$

and

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$$D_{\alpha,\gamma} \geqslant \frac{\overline{\langle\langle \alpha, \mathcal{K} \rangle\rangle}^2}{\widetilde{\sigma}}, \tag{9.21}$$

where

$$\widetilde{\sigma} := 2 \sum_{(i,j)\in E: i<j} \overline{\frac{\mathcal{K}_{ij}^2}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}}}. \tag{9.22}$$

We point out that corollary 9.2 was also obtained in [1] and it is an immediate consequence of theorem 3 with $Z := \left(y_{\alpha,\gamma} / \overline{\langle\langle \alpha, \mathcal{K} \rangle\rangle} \right) \mathcal{K}$ and $m = 0$.

As in section 8 we can collect some comments on the above corollary 9.2.

- A possible choice of $\mathcal{K}$ is given by $\mathcal{K} = \overline{\mathcal{J}}$ when $\langle\langle \overline{\alpha}, \overline{\mathcal{J}} \rangle\rangle \neq 0$.
- When $\gamma \equiv 0$ and α is time-independent we have that $y_{\alpha,\gamma} = \overline{\langle\langle \alpha, \mathcal{J} \rangle\rangle} = \langle\langle \alpha, \overline{\mathcal{J}} \rangle\rangle$. In particular, by taking $\mathcal{K} = \overline{\mathcal{J}}$ in the above corollary 9.2, (9.21) becomes (GTUR 3) valid whenever $\langle \alpha, \overline{\mathcal{J}} \rangle \neq 0$.
- Another possible choice for $\mathcal{K}$ is given by $\mathcal{K}_{ij}(t) = \mu_i(t) w_{ij}(t) - \mu_j w_{ji}(t)$, where $\mu_i(t)$ denotes the so-called accompanying distribution (see section 8). For this second choice we also refer to [1, section 4.5].
- The property of being a time periodic current with zero divergence is preserved by linear combinations. In particular, one can also take $\mathcal{K}_{ij} = c_1 \overline{\mathcal{J}}_{ij} + c_2 \left(\mu_i(t) w_{ij}(t) - \mu_j(t) w_{ji}(t) \right)$, for any fixed $c_1, c_2 \in \mathbb{R}$ (see [1, section 4.5] for further discussions).
- Given the model, one can look for more efficient choices of $\mathcal{K}$ by using Schnakenberg's cycle theory [7, 45] to build divergence-free currents, and afterwards by trying to optimize among these currents. We recall that any divergence-free current $\mathcal{K}$ must be zero if the graph (V, E) is a tree after replacing pairs of oriented edges (i, j) and (j, i) by the unoriented edge $\{i, j\}$. In this case corollary 9.2 becomes empty.

Corollary 9.3. *Suppose that the entries of $\overline{\gamma}$ are not all strictly positive, and not all strictly negative. Fix any time-independent probability measure $p = (p_i)_{i\in V}$ on V with $\langle p, \overline{\gamma} \rangle = 0$. Recall the definition of $C_{\mathrm{a}}(p)$ in (3.4). Then we have the upper bound*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4} \frac{(y - y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2} C_{\mathrm{a}}(p) + o\left((y - y_{\alpha,\gamma})^2 \right). \tag{9.23}$$

As a consequence we have (GTUR 4).

The above result follows from theorem 3 by taking $Z(t) := \mathcal{J}(t)$ and $m(t) := \pi(t) - p$.

Remark 9.4. Note that both corollaries 9.2 and 9.3 could be derived respectively from corollaries 8.2 and 8.3 by an optimization over symmetric generalized flows as in the first proof of theorem 3. In particular, in the case of an antisymmetric α, the bounds discussed in this section are better than the corresponding ones discussed in the previous section, since they are obtained by an optimization procedure. We recall that we have proved in a direct way this issue (see proposition 4.3 and its proof in section 10).

9.5. Theorem 4 and its corollaries

In theorem 4 below we present another general method to produce quadratic bounds on the LD rate functional $I_{\alpha,\gamma}$. We provide two simple derivations of this theorem. The first one is inspired by the approach followed in [1, section 4.1]. The second one, based on theorem 3, shows indeed that the bounds provided by theorem 3 are better than the ones provided by theorem 4 (see remark 9.5 below). Nevertheless, the interest to theorem 4 comes from the fact that it allows (see the corollaries below) to get GTUR's with constants resembling in their form to the average entropy production rate σ.

Theorem 4. *For any pair (Z,m) fulfilling properties (P1*),...,(P4*) the following local quadratic upper bound holds:*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4}\frac{(y-y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2}\sum_{(i,j)\in E:i<j}\overline{\left(\frac{\left(Z_{ij}-(m_iw_{ij}-m_jw_{ji})\right)^2}{\mathcal{J}_{ij}}\ln\frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}\right)}+o\left((y-y_{\alpha,\gamma})^2\right). \tag{9.24}$$

In particular, we have the lower bound

$$D_{\alpha,\gamma} \geqslant y_{\alpha,\gamma}^2\left\{\sum_{(i,j)\in E:i<j}\overline{\left(\frac{\left(Z_{ij}-(m_iw_{ij}-m_jw_{ji})\right)^2}{\mathcal{J}_{ij}}\ln\frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}\right)}\right\}^{-1}. \tag{9.25}$$

First proof. We have (recall (9.3) and (9.5))

$$I_{\alpha,\gamma}(y)\leqslant I_*(J,\rho)\leqslant\frac{1}{4}\sum_{(i,j)\in E:i<j}\frac{1}{\tau}\int_0^\tau\frac{[J_{ij}(t)-G_{ij}(t)]^2}{G_{ij}(t)}\ln\frac{\rho_i(t)w_{ij}(t)}{\rho_j(t)w_{ji}(t)}\mathrm{d}t, \tag{9.26}$$

for any pair (J,ρ) in $\mathcal{F}^*_{\alpha,\gamma,y}$. The second bound in (9.26) follows from equation (12) in [22], implying that

$$\Psi\big(J_{ij}(t),G_{ij}(t),a_{ij}(t)\big)\leqslant\frac{1}{4}\frac{[J_{ij}(t)-G_{ij}(t)]^2}{G_{ij}(t)}\ln\frac{\rho_i(t)w_{ij}(t)}{\rho_j(t)w_{ji}(t)}.$$

We take the pair (J,ρ) as in (9.8). Then, for y close to $y_{\alpha,\gamma}$, we have that $(J,\rho)\in\mathcal{F}^*_{\alpha,\gamma,y}$ and therefore we can apply (9.26) to (J,ρ). The thesis then follows by a Taylor's expansion of the rhs of (9.26) for y close to $y_{\alpha,\gamma}$, since

$$J_{ij}(t)-G_{ij}(t)=\frac{y-y_{\alpha,\gamma}}{y_{\alpha,\gamma}}\left(Z_{ij}(t)-[m_i(t)w_{ij}(t)-m_j(t)w_{ji}(t)]\right), \tag{9.27}$$

$$G_{ij}(t)=\mathcal{J}_{ij}(t)+o(1), \tag{9.28}$$

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$$\frac{\rho_i(t)w_{ij}(t)}{\rho_j(t)w_{ji}(t)} = \frac{\mathcal{Q}_{ij}(t)}{\mathcal{Q}_{ji}(t)} + o(1). \tag{9.29}$$

Second proof. The bound (9.24) is an immediate consequence of the bound (9.9) in theorem 3 and the general inequality (see [1, equation (29)])

$$(x-y)\ln\frac{x}{y} \geqslant \frac{2(x-y)^2}{x+y}, \qquad x,y>0. \tag{9.30}$$

Indeed, from the above inequality one gets that $(\mathcal{J}_{ij})^{-1}\ln(\mathcal{Q}_{ij}/\mathcal{Q}_{ji}) \geqslant 2(\mathcal{Q}_{ij}+\mathcal{Q}_{ji})^{-1}$. Finally, (9.25) follows from (9.24) and (2.17). □

Remark 9.5. Due to (9.30), the rhs of (9.10) in theorem 3 is lower bounded by the rhs of (9.25) in theorem 4. In particular, the bounds obtained by theorem 3 are better than the corresponding bounds obtained by theorem 4.

Corollary 9.6. *Suppose that* $\mathcal{K}(t) = \big(\mathcal{K}_{ij}(t)\big)$ *is a time-periodic current with* $\operatorname{div}\mathcal{K}=0$ *and such that* $\overline{\langle\langle \alpha,\mathcal{K}\rangle\rangle} \neq 0$. *Then it holds*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4}\frac{\sigma^*}{\overline{\langle\langle \alpha,\mathcal{K}\rangle\rangle}^2}(y-y_{\gamma,\alpha})^2 \tag{9.31}$$

and

$$D_{\alpha,\gamma} \geqslant \frac{\overline{\langle\langle \alpha,\mathcal{K}\rangle\rangle}^2}{\sigma^*}, \tag{9.32}$$

where

$$\sigma^* := \sum_{(i,j)\in E: i<j} \overline{\left(\frac{\mathcal{K}_{ij}^2}{\mathcal{J}_{ij}}\ln\frac{\mathcal{Q}_{ij}}{\mathcal{Q}_{ji}}\right)}. \tag{9.33}$$

Proof. We apply theorem 4 with a slight improvement, by taking $m:=0$ and $Z := \left(y_{\alpha,\gamma}/\,\overline{\langle\langle \alpha,\mathcal{K}\rangle\rangle}\right)\mathcal{K}$. theorem 4 would imply the thesis, with the exception that the bound (9.31) would be only local. On the other hand, since $m=0$, the error terms $o(1)$ in (9.28) and (9.29) are simply zero and the first proof of theorem 4 gives that the local bound (9.24) is in this case a global bound. □

We point out that corollary 9.6 was also obtained in [1]. Moreover, we observe that (GTUR 5) follows from corollary 9.6 by taking $\mathcal{K} := \overline{\mathcal{J}}$. Finally, by remark 9.5 we also get that $\sigma^* \geqslant \widetilde{\sigma}$, where the constant $\widetilde{\sigma}$ is defined as in (9.22).

Corollary 9.7. *Suppose that the entries of* $\overline{\gamma}$ *are not all strictly positive, and not all strictly negative. Fix any time-independent probability measure* $p=(p_i)_{i\in V}$ *on* V *with* $\langle p,\overline{\gamma}\rangle = 0$. *Recall the constant* $C_{\mathrm{a}}^*(p)$ *defined in (3.6). Then we have the upper bound*

$$I_{\alpha,\gamma}(y) \leqslant \frac{1}{4}\frac{(y-y_{\alpha,\gamma})^2}{y_{\alpha,\gamma}^2} C_{\mathrm{a}}^*(p) + o\left((y-y_{\alpha,\gamma})^2\right). \tag{9.34}$$

As a consequence we have (GTUR 6).

The above corollary follows from theorem 4 by taking $Z(t) := \mathcal{J}(t)$ and $m(t) := \pi(t) - p$, as in corollary 9.3. (GTUR 6) corresponds to [29, equation (14)]. We point out that, by remark 9.5, we get that $C_{\mathrm{a}}^*(p) \geqslant C_{\mathrm{a}}(p)$, where the constant $C_{\mathrm{a}}(p)$ is defined as in (3.4).

10. Proofs IV: proof of propositions 4.1, 4.3, 4.4 and remark 4.2

10.1. Proof of proposition 4.1

The universal rate in (GTUR 2) can be written as $C(p) = \sum_i p_i^2 X_i$, where $X_i = 1/A_i$, A_i is defined in (4.1), and $A_i > 0$. By (GTUR 2) we have that

$$\frac{D_{\alpha,\gamma}}{y_{\alpha,\gamma}^2} \geqslant \frac{1}{C_\star}, \tag{10.1}$$

where $C_\star$ is the infimum of $C(p)$ as $p = (p_i)_{i\in V}$ varies among the probability measures on V with $\langle \overline{\gamma}, p\rangle = 0$. Below we show that the convex function $p \mapsto C(p)$, defined on the set of probability measures with $\langle \overline{\gamma}, p\rangle = 0$, has exactly one extremal point, hence this extremal point must be the minimum point.

By the Lagrange's multipliers method, we look to the extremal points of the function

$$f(p) = \sum_i p_i^2 X_i - a\Big(\sum_i p_i - 1\Big) - b\Big(\sum_i p_i \overline{\gamma}_i\Big),$$

a, b being the multipliers. The extremal point satisfies $2p_i^\star X_i - a - b\overline{\gamma}_i = 0$ for all $i \in V$, i.e.

$$p_i^\star = \frac{a + b\overline{\gamma}_i}{2X_i} = \frac{aA_i + bA_i\overline{\gamma}_i}{2} \qquad \forall i \in V.$$

The constants a, b are fixed by imposing that $\sum_i p_i^\star = 1$ and $\langle \overline{\gamma}, p^\star\rangle = 0$. This is equivalent to the system

$$\begin{cases} aA + bB = 2 \\ aB + bC = 0 \end{cases}$$

with $A := \sum_i A_i$, $B := \sum_i A_i\overline{\gamma}_i$ and $C := \sum_i A_i\overline{\gamma}_i^2$.

We point out that by Cauchy–Schwarz inequality we have

$$B^2 = \Big(\sum_i A_i\overline{\gamma}_i\Big)^2 = \Big(\sum_i \sqrt{A_i}(\sqrt{A_i}\overline{\gamma}_i)\Big)^2 \leqslant \Big(\sum_i A_i\Big)\Big(\sum_i A_i\overline{\gamma}_i^2\Big) = AC.$$

Moreover, the above bound becomes an identity if and only if the vectors (A_i) and $(\sqrt{A_i}\overline{\gamma}_i)$ are proportional. This condition is fulfilled in the case given by Item (i) in proposition 4.1 since $\overline{\gamma} = 0$, but not in the case given by Item (ii) in proposition 4.1, since $A_i > 0$ for all i while $\overline{\gamma} \neq 0$ has neither all entries negative nor all entries positive. Hence, for Item (ii) we have $AC \neq B^2$.

If $AC \neq B^2$, then the solution of the system is given by $a = \frac{2C}{AC-B^2}$ and $b = \frac{-2B}{AC-B^2}$, thus leading to

$$\begin{aligned} C_\star = C(p^\star) = \sum_i (p_i^\star)^2 X_i &= \sum_i p_i^\star (p_i^\star X_i) = \sum_i p_i^\star \left(\frac{a + b\overline{\gamma}_i}{2}\right) \\ &= \frac{a}{2} + \frac{b}{2}\left(\sum_i p_i^\star \overline{\gamma}_i\right) = \frac{a}{2} + \frac{b}{2}\sum_i \overline{\gamma}_i \left(\frac{aA_i + bA_i\overline{\gamma}_i}{2}\right) \\ &= \frac{a}{2} + \frac{ab}{4}B + \frac{b^2}{4}C = \frac{C}{AC - B^2}. \end{aligned}$$

This concludes the proof of item (ii) in proposition 4.1 by (10.1) and by the above observation that $AC - B^2 > 0$.

For the case corresponding to item (i) of proposition 4.1 with $\overline{\gamma} = 0$, the multiplier b can be neglected and $aA = 2$. Hence $p_i^\star = A_i / \sum_j A_j$, which leads to the identity

$$C_\star = C(p^\star) = \sum_i (p_i^*)^2 X_i = [\sum_i A_i]^{-1}.$$

10.2. Proof of remark 4.2

Since π_i is time-independent, the statement in remark 4.2 is equivalent to the inequality

$$2\sum_i A_i = \sum_i \pi_i \Big[\sum_{j:(i,j)\in E} \overline{w}_{ij}\Big]^{-1} \geqslant \Big[\sum_{(i,j)\in E} (\overline{\mathcal{Q}}_{ij})^2 \overline{(1/\mathcal{Q}_{ij})}\Big]^{-1} = 2/\widehat{\sigma}. \tag{10.2}$$

Recall that, given a positive random variable Y, it holds $\mathbb{E}[1/Y] \geqslant 1/\mathbb{E}[Y]$ by Jensen's inequality. We apply this inequality twice. As a first application we get $\overline{(1/\mathcal{Q}_{ij})} \geqslant 1/\overline{\mathcal{Q}}_{ij}$. This implies that

$$\Big[\sum_{(i,j)\in E} (\overline{\mathcal{Q}}_{ij})^2 \overline{(1/\mathcal{Q}_{ij})}\Big]^{-1} \leqslant \Big[\sum_{(i,j)\in E} \overline{\mathcal{Q}}_{ij})\Big]^{-1}. \tag{10.3}$$

As a second application we get

$$\sum_i \pi_i \Big[\sum_{j:(i,j)\in E} \overline{w}_{ij}\Big]^{-1} \geqslant \Big[\sum_i \pi_i \sum_{j:(i,j)\in E} \overline{w}_{ij}\Big]^{-1} = \Big[\sum_{(i,j)\in E} \overline{\mathcal{Q}}_{ij})\Big]^{-1}. \tag{10.4}$$

(10.2) is then a byproduct of (10.3) and (10.4).

10.3. Proof of proposition 4.3

The last statement in proposition 4.3 is an immediate consequence of the bounds $C(p) \geqslant C_a(p)$ and $C_a^*(p) \geqslant C_a(p)$, on which we focus. The bound $C_a^*(p) \geqslant C_a(p)$ follows from remark 9.5 as discussed after corollary 9.7. Let us prove that $C(p) \geqslant C_a(p)$. Given $x, y \geqslant 0$ and $X, Y > 0$, we have

$$\frac{(x-y)^2}{X+Y} \leqslant \frac{x^2+y^2}{X+Y} = \frac{x^2}{X+Y} + \frac{y^2}{X+Y} \leqslant \frac{x^2}{X} + \frac{y^2}{Y}.$$

The above bound implies

$$\sum_{(i,j)\in E} \frac{\big(p_i w_{ij}(t) - p_j w_{ji}(t)\big)^2}{\mathcal{Q}_{ij}(t) + \mathcal{Q}_{ji}(t)} \leqslant \sum_{(i,j)\in E} \Big[\frac{\big(p_i w_{ij}(t)\big)^2}{\mathcal{Q}_{ij}(t)} + \frac{\big(p_j w_{ji}(t)\big)^2}{\mathcal{Q}_{ji}(t)}\Big]$$
$$= 2\sum_{(i,j)\in E} \frac{\big(p_i w_{ij}(t)\big)^2}{\mathcal{Q}_{ij}(t)}. \tag{10.5}$$

By taking the time average on $[0,\tau]$ in (10.5), we conclude that $C_a(p) \leqslant C(p)$.

10.4. Proof of proposition 4.4

The bound $\sigma^* \geqslant \widetilde{\sigma}$ has been derived in [1] and follows also from remark 9.5. The bound $\widehat{\sigma} \geqslant \widetilde{\sigma}$ can be derived as follows:

$$\widetilde{\sigma} = \sum_{(i,j)\in E} (\overline{\mathcal{Q}}_{ij} - \overline{\mathcal{Q}}_{ji})^2 \overline{\frac{1}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}}}$$
$$\leqslant \sum_{(i,j)\in E} (\overline{\mathcal{Q}}_{ij}^2 + \overline{\mathcal{Q}}_{ji}^2) \overline{\frac{1}{\mathcal{Q}_{ij} + \mathcal{Q}_{ji}}} \leqslant \sum_{(i,j)\in E} \overline{\mathcal{Q}}_{ij}^2 \overline{\frac{1}{\mathcal{Q}_{ij}}} + \sum_{(i,j)\in E} \overline{\mathcal{Q}}_{ji}^2 \overline{\frac{1}{\mathcal{Q}_{ji}}} = \widehat{\sigma}. \tag{10.6}$$

11. Conclusion

The TUR, introduced in [3], is a universal trade-off relation connecting the precision of a current with the average dissipation at large times. For periodically driven systems this relation fails and generalizations (GTUR's) have been provided in the literature in the form of lower bounds of the ratio of the asymptotic diffusion coefficient of the current to its square asymptotic value.

In this work we give a general overview in the time periodic case, recovering previous GTUR's, providing new ones and comparing the different GTUR's. Overall, we get seven GTUR's listed in section 3. More precisely, we have considered here a time-periodic Markov chain $\big(X(t)\big)_{t\geqslant 0}$ with continuous time and a broad class of functionals of stochastic trajectories of the form (2.9), which are general linear combinations of the empirical flow and the empirical density. Our method to get GTUR's is mainly based on the level 2.5 large deviation principles obtained in [5]. Inspired by the analysis done in our previous work [1], we provide general methods (see theorems 2–4 in sections 8 and 9) to get local/global quadratic bounds for large deviations, thus leading to GTUR's via (2.17). The resulting bounds correspond to (GTUR 1),...,(GTUR 6). The last bound (GTUR 7) has been obtained differently, by extending the analysis of [44] to generic protocols, not necessarily symmetric. This extension covers also other empirical

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functionals as detailed in theorem 1 in section 5 and goes through level 2.5 large deviation principles for time-homogeneous Markov chains with discrete time.

The range of applicability of each GTUR corresponds to a suitable class of empirical functionals and when these classes intersect it is natural to investigate which GTUR provides the best bound. We have proved that some GTUR's are tighter than others, while we have shown by providing examples that some GTUR's are incomparable (see section 4). Finally, we have studied in detail two specific examples, given by a periodically driven 2-state Markov chain and a periodically driven random walk on a ring. The latter is particularly relevant for the comparison of GTUR's.

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Appendix A. Periodic solutions of the continuity equation

In this short appendix we illustrate two possible approaches to find good perturbations (m, R) in section 8. We present just the general ideas since a complete development would be long and model-dependent.

A.1. Time dependent Schnakenberg theory

We consider a cycle

$$C = (i_1, i_2, \dots, i_N, i_1)$$

of the transition graph (V, E) and look for pairs (R, m) satisfying properties (P1), (P2), (P3) in section 8, just restricted to this cycle. Since we have a one dimensional ring this is relatively easy. The continuity equation reduces to

$$\dot{m}_{i_k} = R_{i_{k-1}i_k} - R_{i_k i_{k+1}}, \qquad k = 1, \dots, N, \tag{A.1}$$

where the sums $k \pm 1$ are modulo N. The general solution is therefore given by

$$\begin{cases} m_{i_k}(t) = M_k + \widehat{\alpha}_{k-1}(t) - \widehat{\alpha}_k(t), \\ R_{i_k i_{k+1}}(t) = \alpha_k(t), \end{cases}$$

where α_k, $k = 1, 2, \dots, N$, are arbitrary time-periodic functions such that $\int_0^\tau \alpha_k(t)\mathrm{d}t$ does not depend on k. The functions $\widehat{\alpha}_k$ are the corresponding primitives of α_k and M_k are arbitrary numbers such that $\sum_{k=1}^N M_k = 0$.

A special degenerate case is obtained as follows. Consider two particles, performing time-periodic deterministic trajectories on the cycle C. Call m the difference of the empirical densities associated to the trajectory of the first and of the second particle, respectively. Similarly call R the difference of the empirical flows. Then the pair (m, R) satisfies properties (P1), (P2), (P3).

Once obtained solutions on elementary cycles, a trial pair (m, R) satisfying properties (P1), (P2), (P3) for the transition graph (V, E) can be obtained as a combination of them. The classic Schnakenberg theory allows to construct divergence free flows using cycles. This approach in a sense is a time-dependent version of this theory, giving solutions of the continuity equation using the cycle decomposition.

A.2. Perturbations from Markov models

Another possible approach that can be useful in specific situations is obtained by the following observation. Consider a Markov chain with periodic rates $\widetilde{w}$. If we call $\widetilde{\pi}$ its invariant time periodic distribution and $\widetilde{\mathcal{Q}}_{ij} = \widetilde{\pi}_i(t)\widetilde{w}_{ij}(t)$ the corresponding asymptotic flow we have that $\widetilde{\pi}$ and $\widetilde{\mathcal{Q}}$ are related by the continuity equation. We can therefore fix the pair (m, R) by $m_i(t) = M_i - \widetilde{\pi}_i(t)$ and $R_{ij}(t) = \widetilde{\mathcal{Q}}_{ij}(t)$, where the arbitrary numbers M_i satisfy the condition $\sum_i M_i = 1$. This special way of proceeding can be useful in specific cases where there is a simple and natural periodic chain to be introduced.

For both approaches we just discussed the constraints given by $(P1), (P2)$ and $(P3)$ in section 8. To really implement the methods it is necessary to satisfy also the additional constraint $(P4)$ in section 8. This further restriction has to be imposed on the perturbations discussed above.

Appendix B. Derivation of theorem 1

We use the same notation introduced in section 5. Recall that Θ_τ is the family of piecewise constant paths $\Gamma : [0, \tau] \to V$. $\mathcal{P}(\Theta_\tau)$ is the set of probability measures on Θ_τ. $\mathcal{R}_\tau : \Theta_\tau \to \Theta_\tau$ is the time-reflection around $\tau/2$ and P is the probability law of the random path $(X(t))_{0\leqslant t\leqslant\tau}$ induced by the τ-periodic stationary state. Note that $P \in \mathcal{P}(\Theta_\tau)$. We denote by $E[\cdot]$ the expectation w.r.t. P.

The GTUR (5.7) is an immediate consequence of (5.6) and the identity $2D_F = 1/I''_F(y_F)$. We now explain how to derive (5.6) .

We first focus on the empirical object

$$Q^{(n)} := \frac{1}{n}\sum_{j=0}^{n-1} \delta_{(X_{j\tau+s})_{0\leqslant s\leqslant\tau}}, \tag{B.1}$$

where $\delta_{(X_{j\tau+s})_{0\leqslant s\leqslant\tau}}$ is the measure on Θ_τ of unitary mass concentrated on the path $(X_{j\tau+s})_{0\leqslant s\leqslant\tau}$. $Q^{(n)}$ is a trajectory-dependent probability on the path space Θ_τ (shortly, $Q^{(n)} \in \mathcal{P}(\Theta_\tau)$). It can be described by words as follows. Given the trajectory $(X_t)_{0\leqslant t\leqslant n\tau}$ of the Markov chain up to time $n\tau$, we cut this trajectory at the intermediate times $\tau, 2\tau, \ldots, (n-1)\tau$. The resulting subpaths can be written as

$$(X_s)_{0\leqslant s\leqslant\tau}, \quad (X_{\tau+s})_{0\leqslant s\leqslant\tau}, \quad \ldots, \quad (X_{(n-1)\tau+s})_{0\leqslant s\leqslant\tau} \tag{B.2}$$

and are elements of Θ_τ. Then $Q^{(n)}$ is a linear combination of Dirac measures on the space Θ_τ and the weight assigned to each $\Gamma \in \Theta_\tau$ is given by the relative frequency of appearances of Γ in the above list (B.2).

Note that $Q^{(n)}$ is also the empirical measure of the Markov chain $(W_k)_{k\geqslant0}$ on Θ_τ, where $W_k := (X_{k\tau+s})_{0\leqslant s\leqslant\tau}$. We point out that in this appendix $Q^{(n)}$ is defined as in (B.1) in order to make the notation closer to the one in [44], in particular $Q^{(n)}$ is not the empirical flow as in the rest of the file (see section 2.15).

The link with the empirical functional (5.4) is given by the identity

$$Y_n^{(F)} = \int_{\Theta_\tau} \mathrm{d}Q^{(n)}(\Gamma)F(\Gamma). \tag{B.3}$$

As discussed in appendix B.1 $Q^{(n)}$ fulfills an LDP with speed n and the associated LD rate functional I (which has not to be confused with the function I in (2.14)) satisfies the inequality

$$I(Q) \leqslant H(Q|P) \tag{B.4}$$

for any $Q \in \mathcal{P}(\Theta_\tau)$ satisfying (B.5). To have $I(Q) < +\infty$ we need that

$$Q(\Gamma_0 = i) = Q(\Gamma_\tau = i) \qquad \forall i \in V. \tag{B.5}$$

This follows from the fact that $Q^{(n)}(\Gamma_0 = i) = Q^{(n)}(\Gamma_\tau = i) + O(1/n)$ (simply, the final value of $(X_{j\tau+s})_{0\leqslant s\leqslant\tau}$ equals the initial value of $(X_{(j+1)\tau+s})_{0\leqslant s\leqslant\tau}$). By the contraction principle we get that $Y_n^{(F)}$ satisfies an LDP with speed n, whose LD rate functional I_F is given by

$$I_F(y) = \inf\Big\{ I(Q)\ :\ Q \in \mathcal{P}(\Theta_\tau),\ \int_{\Theta_\tau} \mathrm{d}Q(\Gamma)F(\Gamma) = y \Big\}. \tag{B.6}$$

By combining (B.4) and (B.6) we have

$$I_F(y) \leqslant H(Q|P) \qquad \forall Q \in \mathcal{P}(\Theta_\tau) \text{ fulfilling (B.5) and } \int_{\Theta_\tau} \mathrm{d}Q(\Gamma)F(\Gamma) = y. \tag{B.7}$$

We apply (B.7) with some special $Q = Q^y$ that we take absolutely continuous w.r.t. P. Since $y_F \neq 0$, for some function G we can write Q^y as

$$\frac{\mathrm{d}Q^y}{\mathrm{d}P} = 1 + \frac{y - y_F}{y_F}(1 - G). \tag{B.8}$$

Due to (B.8), the properties $Q^y \in \mathcal{P}(\Theta_\tau)$, $\int_{\Theta_\tau} \mathrm{d}Q^y(\Gamma)F(\Gamma) = y$ and (B.5) are satisfied if and only if

$$E[G] = 1, \qquad E[FG] = 0 \quad \text{and} \quad E[G 1_{\Gamma_0 = i}] = E[G 1_{\Gamma_\tau = i}] \ \ \forall i \in V. \tag{B.9}$$

We claim that, using that $F \circ \mathcal{R}_\tau = -F$, the last two conditions on (B.9) are always satisfied if

$$\frac{G}{G \circ \mathcal{R}_\tau} = \frac{\mathrm{d}P \circ \mathcal{R}_\tau}{\mathrm{d}P}, \tag{B.10}$$

where $P \circ \mathcal{R}_\tau$ is the probability on Θ_τ defined as $P \circ \mathcal{R}_\tau(A) := P(\mathcal{R}_\tau(A))$ for $A \subset \Theta_\tau$ measurable.

Let us derive the claim. Assuming (B.10), we can write

$$\begin{aligned} E\big[GF\big] &= -E\big[G(F \circ \mathcal{R}_\tau)\big] = -\int_{\Theta_\tau} \mathrm{d}(P \circ \mathcal{R}_\tau)(\Gamma)(G \circ \mathcal{R}_\tau)(\Gamma)F(\Gamma) \\ &= -E\Big[\frac{\mathrm{d}P \circ \mathcal{R}_\tau}{\mathrm{d}P}(G \circ \mathcal{R}_\tau)F\Big] = -E[GF], \end{aligned} \tag{B.11}$$

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thus implying that $E[GF] = 0$ (note that (B.10) has been used to get the last identity). Similarly one can derive the last condition of (B.9) from (B.10).

One possible choice for (B.10) satisfying the constrain $E[G] = 1$ is

$$G = \frac{(1+\mathrm{e}^{Z})^{-1}}{E\left[(1+\mathrm{e}^{Z})^{-1}\right]}, \qquad \mathrm{e}^{-Z} = \frac{d(P\circ\mathcal{R}_\tau)}{\mathrm{d}P}. \tag{B.12}$$

Note that $E[Z] = \tau\sigma_{\mathrm{naive}}$ (see (5.2) and (5.3)).

Remark B.1. Let us naively think of the path space as countable. Writing G_Γ for $G(\Gamma)$, $\widetilde{\Gamma} := \mathcal{R}_\tau(\Gamma)$ and setting $C_\Gamma := P_\Gamma G_\Gamma$, (B.10) is equivalent to $C_\Gamma = C_{\widetilde{\Gamma}}$, while (B.8) reads

$$Q^y_\Gamma = P_\Gamma + \frac{y-y_F}{y_F}(P_\Gamma - C_\Gamma). \tag{B.13}$$

The identity $E(G) = 1$ would read $\sum_\Gamma C_\Gamma = 1$. The choice $C_\Gamma = \frac{1}{\mathcal{N}}\frac{P_\Gamma P_{\widetilde{\Gamma}}}{P_\Gamma + P_{\widetilde{\Gamma}}}$ as in [44] ($\mathcal{N}$ being the normalization constant) would correspond to

$$G_\Gamma = \frac{C_\Gamma}{P_\Gamma} = \frac{1}{\mathcal{N}}\frac{P_{\widetilde{\Gamma}}}{P_\Gamma + P_{\widetilde{\Gamma}}},$$

which is equivalent to

$$\frac{1}{G_\Gamma} = \mathrm{const}\left(1 + \frac{\mathrm{d}P}{\mathrm{d}P\circ\mathcal{R}}\right) = \mathrm{const}\left(1+\mathrm{e}^{Z}\right).$$

The above form of G is exactly the choice (B.12).

From now on G is as in (B.12). For simplicity we write

$$G = \frac{1}{\mathcal{N}}\frac{1}{1+e^{Z}}, \qquad \mathcal{N} = E\left[(1+e^{Z})^{-1}\right]. \tag{B.14}$$

By (B.7) we have

$$I_F(y) \leqslant H(Q^y|P) = E\Big[\frac{\mathrm{d}Q^y}{\mathrm{d}P}\ln\frac{\mathrm{d}Q^y}{\mathrm{d}P}\Big]. \tag{B.15}$$

Using that $x\ln x = x - 1 + \frac{1}{2}(x-1)^2 + o((x-1)^2)$, we obtain (recall that $E(G) = 1$)

$$\begin{aligned} I_F(y) &\leqslant \frac{1}{2}\frac{(y-y_F)^2}{y_F^2}E\big[(1-G)^2\big] + o\big((y-y_F)^2\big) \\ &= \frac{1}{2}\frac{(y-y_F)^2}{y_F^2}\big(E\big[G^2\big]-1\big) + o\big((y-y_F)^2\big). \end{aligned} \tag{B.16}$$

Now observe that

$$E[G^2] = \int d(P\circ\mathcal{R}_\tau)(\Gamma)(G\circ\mathcal{R}_\tau)^2 = E\Big[\frac{\mathrm{d}P\circ\mathcal{R}_\tau}{\mathrm{d}P}(G\circ\mathcal{R}_\tau)^2\Big]. \tag{B.17}$$

Using (B.10) we get that

$$E\Big[\frac{\mathrm{d}P\circ\mathcal{R}_\tau}{\mathrm{d}P}(G\circ\mathcal{R}_\tau)^2\Big] = E\Big[\frac{\mathrm{d}P\circ\mathcal{R}_\tau}{\mathrm{d}P}G^2\cdot\Big(\frac{\mathrm{d}P}{\mathrm{d}P\circ\mathcal{R}_\tau}\Big)^2\Big] = E\Big[G^2\frac{\mathrm{d}P}{\mathrm{d}P\circ\mathcal{R}_\tau}\Big] = E[G^2e^Z]. \tag{B.18}$$

As a byproduct of (B.17) and (B.18) we conclude that $E[G^2]=E[G^2e^Z]$ and therefore

$$E[G^2] = \frac{1}{2}E[G^2(1+e^Z)] = \frac{1}{2\mathcal{N}^2}E[(1+e^Z)^{-2}(1+e^Z)] = \frac{1}{2\mathcal{N}} = \frac{1}{2E\left[(1+e^Z)^{-1}\right]}. \tag{B.19}$$

Inserting the above identity in (B.16) we get

$$I_F(y) \leqslant \frac{1}{2}\frac{(y-y_F)^2}{y_F^2}\left(\frac{1}{2E\left[(1+e^Z)^{-1}\right]}-1\right)+o\big((y-y_F)^2\big). \tag{B.20}$$

We now claim that

$$\frac{1}{\mathcal{N}} = \frac{1}{E\left[(1+e^Z)^{-1}\right]} \leqslant 1+\mathrm{e}^{E[Z]} = 1+\mathrm{e}^{\tau\sigma_{\text{naive}}} \tag{B.21}$$

(note that the identities in (B.21) follow from the definitions). By plugging (B.21) into (B.20) we get that

$$I_F(y) \leqslant \frac{1}{4}\frac{(y-y_F)^2}{y_F^2}\left(\mathrm{e}^{\tau\sigma_{\text{naive}}}-1\right)+o\big((y-y_F)^2\big), \tag{B.22}$$

which implies (5.6).

Inequality (B.21) corresponds to [44, equation (17)] and follows from a very tricky algebra in [44, Appendix A] that we adapt to our terminology. Since $E[\mathrm{e}^{-Z}]=1$ (by the definition of Z), P' defined as $\mathrm{d}P'=\frac{1+\mathrm{e}^{-Z}}{2}\mathrm{d}P$ is a probability measure on Θ_τ. By applying Jensen's inequality w.r.t. this probability P' we have

$$\ln\mathcal{N} = \ln E\big[(1+e^Z)^{-1}\big] = \ln E\Big[\frac{1+\mathrm{e}^{-Z}}{2}\frac{2\mathrm{e}^{-Z}}{(1+\mathrm{e}^{-Z})^2}\Big] \geqslant E\Big[\frac{1+\mathrm{e}^{-Z}}{2}\ln\frac{2\mathrm{e}^{-Z}}{(1+\mathrm{e}^{-Z})^2}\Big].$$

Since $E[\mathrm{e}^{-Z}Z]=-E[Z]$ (by the definition of Z), we have

$$E[Z] = -E\Big[\frac{\mathrm{e}^{-Z}-1}{2}Z\Big].$$

Hence, setting $u:=\mathrm{e}^{-Z}$, one gets a bound corresponding to [44, equation (A.1)]:

$$\ln\mathcal{N}+E[Z] \geqslant E\Big[\frac{1+u}{2}\ln\frac{2u}{(1+u)^2}+\frac{u-1}{2}\ln u\Big]. \tag{B.23}$$

Since $\frac{1+a}{2}\ln\frac{2a}{(1+a)^2}+\frac{a-1}{2}\ln a \geqslant (1-\ln 2)\frac{1+a}{2}-\frac{2a}{a+1}$ for $a>0$ and since $\mathrm{d}P'=\frac{1+u}{2}\mathrm{d}P$ is a probability, we can lower bound the rhs of (B.23) by

$$E\Big[(1-\ln 2)\frac{1+u}{2}-\frac{2u}{u+1}\Big] = (1-\ln 2)-2E\Big[\frac{\mathrm{e}^{-Z}}{\mathrm{e}^{-Z}+1}\Big] = (1-\ln 2)-2\mathcal{N}. \tag{B.24}$$

Since $1-\ln 2-2a \geqslant \ln(1-a)$ for all $a\geqslant 0$, one concludes from (B.23) and (B.24) that $\ln\mathcal{N}+E[Z]\geqslant\ln(1-\mathcal{N})$. This last estimate trivially implies (B.21).

B.1. Large deviations of $Q^{(n)}$

Given $Q \in \mathcal{P}(\Theta_\tau)$ we define, for $k, l \in V$,

$$\begin{cases} q_k = Q(\Gamma_0 = k) \\ q_{k,l} = Q(\Gamma_0 = k, \Gamma_\tau = \ell). \end{cases}$$

We let $\overline{q} = \left(q_{k,l}\right)_{(k,l)\in V\times V}$. When we want to stress the dependence on Q, we write $q_k[Q]$, $q_{k,l}[Q]$, $\overline{q}[Q]$. Recall that P is the law on Θ_τ of the random trajectory $\left(X_s\right)_{0\leqslant s\leqslant\tau}$ when X_0 has initial distribution π_0. We then set $p_{k,l} := q_{k,l}[P]$ and $p_k := q_k[P]$.

We consider the pair empirical measure

$$\overline{q}^{(n)} := \frac{1}{n}\sum_{j=0}^{n-1} \delta_{(X_{j\tau}, X_{(j+1)\tau})}, \tag{B.25}$$

and observe that $\overline{q}^{(n)} := \overline{q}[Q^{(n)}]$. By [27, theorem IV.3], $\overline{q}^{(n)}$ satisfies a LD principle with speed n and rate functional I_2 defined as follows. Let $\widetilde{\mathfrak{M}}_1(V\times V)$ be given by the families

$$\overline{c} = (c_{kl})_{(k,l)\in V\times V}$$

with

$$c_{kl} \geqslant 0, \qquad \sum_k\sum_l c_{k,l} = 1, \qquad \sum_k c_{kl} = \sum_k c_{lk}.$$

If $\overline{q} \in \widetilde{\mathfrak{M}}_1(V\times V)$, then

$$I_2\left(\overline{q}\right) := \sum_{k,l} q_{k,l}\ln\frac{q_{kl}}{q_k P(X_\tau = l\,|\,X_0 = k)} = \sum_{k,l} q_{k,l}\ln\frac{q_{kl}}{p_{kl}} - \sum_{q_k} q_k \ln\frac{q_k}{p_k}, \tag{B.26}$$

otherwise $I_2\left(\overline{q}\right) := +\infty$.

Proposition B.2. *$Q^{(n)}$ satisfies a LDP with speed n and rate function*

$$I(Q) = I_2\left(\overline{q}\right) + \sum_{k,l} q_{k,l} H[Q_{kl}|P_{kl}] \qquad \forall Q \in \mathcal{P}(\Theta_\tau), \tag{B.27}$$

where

- $\overline{q} = \overline{q}[Q]$, $q_{k,l} = q_{k,l}[Q]$;
- *I_2 is the pair empirical measure LD functional for the discrete time homogeneous Markov chain $(X_{n\tau})_{n\geqslant 0}$, which has invariant distribution π_0;*
- $Q_{k,l} := Q(\cdot|X_0 = k, X_\tau = l)$;
- $P_{k,l} := P(\cdot|X_0 = k, X_\tau = l)$;
- *$H[Q_{kl}|P_{kl}]$ is the relative entropy of the probability Q_{kl} w.r.t. the probability P_{kl}.*

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Proof. We only sketch the main idea which can be easily formalized. We will make some abuse of notation for the sake of intuition. Recall that $\overline{q} = \overline{q}[Q]$. Given $Q \in \mathcal{P}(\Theta_\tau)$ we have

$$P\big(Q^{(n)} = Q\big) = P\big(Q^{(n)} = Q,\ \overline{q}^{(n)} = \overline{q}\big) = P\big(Q^{(n)} = Q,\ |\,\overline{q}^{(n)} = \overline{q}\big)P\big(\overline{q}^{(n)} = \overline{q}\big). \tag{B.28}$$

By [27, theorem IV.3] we have

$$P\big(\overline{q}^{(n)} = \overline{q}\big) = \mathrm{e}^{-nI_2(\overline{q})}. \tag{B.29}$$

Consider the time interval $[0, n\tau]$ as the union $\cup_{j=0}^{n-1} A_j$, where $A_j = [\,j\tau, (\,j+1)\tau]$. If we know that $\overline{q}^{(n)} = \overline{q}$, then for each pair (k, l) we know that there are $q_{kl}n$ intervals A_j's where the trajectory starts at k and ends at l (we call such a random set of intervals $\mathcal{A}_{kl}$). If we further condition on these intervals, then the random trajectories on A_j, with $A_j \in \mathcal{A}_{kl}$, behave as nq_{kl} i.i.d. random variables with value in Θ_τ and with distribution $P_{k,l}$. Moreover, the random objects involved are independent when varying (k, l). By applying Cramér's theorem and the independence we conclude that

$$P\big(Q^{(n)} = Q,\ |\,\overline{q}^{(n)} = \overline{q}\big) = \prod_{(k,l)} \mathrm{e}^{-q_{kl}nH[Q_{k,l}|P_{k,l}]}. \tag{B.30}$$

The thesis then follows as a byproduct of (B.28)–(B.30). □

Note that, since in (B.27), $\overline{q} = \overline{q}[Q]$ and $Q \in \mathcal{P}(\Theta_\tau)$, we get that $\overline{q} \in \widetilde{\mathfrak{M}}_1(V \times V)$ if and only if $\sum_k q_{kl} = \sum_k q_{lk}$ for each $l \in V$, which is equivalent to (B.5). As a consequence, if $Q \in \mathcal{P}(\Theta_\tau)$ fulfills (B.5) then

$$I_2\left(\overline{q}\right) = \sum_{k,l} q_{k,l} \ln \frac{q_{kl}}{p_{kl}} - \sum_{q_k} q_k \ln \frac{q_k}{p_k} \text{ where } \overline{q} = \overline{q}[Q]. \tag{B.31}$$

By combining (B.27) and (B.31) one easily gets that the LD rate functional $I(Q)$, for $Q \in \mathcal{P}(\Theta_\tau)$ fulfilling (B.5), can be written as

$$I(Q) = H(Q|P) - \sum_k q_k \ln \frac{q_k}{p_k}. \tag{B.32}$$

We derive (B.32) for completeness. Given $k, l \in V$ we set $\Theta_\tau(k, l) := \{\Gamma \in \Theta_\tau : \Gamma_0 = k,\ \Gamma_\tau = l\}$. Then, when $Q_{k,l} \ll P_{k,l}$ (the case $Q_{k,l} \not\ll P_{k,l}$ can be treated easily)

$$\begin{aligned} H[Q_{k,l}|P_{k,l}] &= \int_{\Theta_\tau(k,l)} \mathrm{d}Q_{k,l}(\Gamma) \ln \frac{\mathrm{d}Q_{k,l}}{\mathrm{d}P_{k,l}}(\Gamma) \\ &= \frac{1}{q_{k,l}} \int_{\Theta_\tau(k,l)} \mathrm{d}Q(\Gamma) \ln \frac{\mathrm{d}Q}{\mathrm{d}P}(\Gamma) - \ln \frac{q_{k,l}}{p_{k,l}}. \end{aligned} \tag{B.33}$$

By combining the above equation with (B.26) and (B.27) we get the (B.32).

As a consequence we have

$$I(Q) \leqslant H(Q|P) \tag{B.34}$$

for any $Q \in \mathcal{P}(\Theta_\tau)$ fulfilling (B.5).

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