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Markov trajectories: Microcanonical Ensembles based on empirical observables as compared to Canonical Ensembles based on Markov generators

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Abstract. The Ensemble of trajectories $x(0 \leq t \leq T)$ produced by the Markov generator M in a discrete configuration space can be considered as ‘Canonical’ for the following reasons: (C1) the probability of the trajectory $x(0 \leq t \leq T)$ can be rewritten as the exponential of a linear combination of its relevant empirical time-averaged observables E_n , where the coefficients involving the Markov generator are their fixed conjugate parameters; (C2) the large deviations properties of these empirical observables E_n for large T are governed by the explicit rate function $I_M^{[2.5]}(E)$ at Level 2.5, while in the thermodynamic limit $T = +\infty$, they concentrate on their typical values $E_n^{typ[M]}$ determined by the Markov generator M . This concentration property in the thermodynamic limit $T = +\infty$ suggests to introduce the notion of the ‘Microcanonical Ensemble’ at Level 2.5 for stochastic trajectories $x(0 \leq t \leq T)$, where all the relevant empirical variables E_n are fixed to some values E_n^* and cannot fluctuate anymore for finite T . The goal of the present paper is to discuss its main properties: (MC1) when the long trajectory $x(0 \leq t \leq T)$ belongs to the Microcanonical Ensemble with the fixed empirical observables E_n^* , the statistics of its subtrajectory $x(0 \leq t \leq \tau)$ for $1 \ll \tau \ll T$ is governed by the Canonical Ensemble associated to the Markov generator M^* that would make the empirical observables E_n^* typical; (MC2) in the Microcanonical Ensemble, the central role is played by the number $\Omega_T^{[2.5]}(E^*)$ of stochastic trajectories of duration T with the given empirical observables E_n^* , and by the corresponding explicit Boltzmann entropy $S^{[2.5]}(E^*) = [\ln \Omega_T^{[2.5]}(E^*)]/T$. This general framework is applied to continuous-time Markov jump processes and to discrete-time Markov chains with illustrative examples.

1 Introduction

1.1 Reminder on the Microcanonical Ensemble and the Canonical Ensemble for equilibrium

The statistical physics of Equilibrium is based on the ergodic principle: the ‘time average’ of any observable $O(\mathcal{C})$ of the configuration \mathcal{C} over the dynamical trajectory $\mathcal{C}(0 \leq t \leq T)$ should become equivalent for large time $T \rightarrow +\infty$ to an ‘Ensemble average’ computed with the appropriate Ensemble probability $P_{eq}^{Ensemble}(\mathcal{C})$ of the configuration \mathcal{C}

$$\frac{1}{T} \int_0^T dt O(\mathcal{C}(t)) \underset{T \rightarrow \infty}{\simeq} \sum_{\mathcal{C}} O(\mathcal{C}) P_{eq}^{Ensemble}(\mathcal{C}) \quad (1)$$

The various Ensembles probabilities $P_{eq}^{Ensemble}(\mathcal{C})$ are adapted to the physical conditions that determine what observables are fixed and what observables can fluctuate. Let us recall two important Equilibrium Ensembles.

[MC] In the Microcanonical Ensemble for an isolated system, where the energy E is fixed and cannot fluctuate, the configurations having a different energy $E(\mathcal{C}) \neq E$ are not possible, while the configurations having the energy $E(\mathcal{C}) = E$ are equiprobable (we assume here that the configurations \mathcal{C} and the energy E are discrete, as in the Ising model for N classical spins $S_i = \pm 1$ for instance)

$$P_{eq}^{Microcanonical[E]}(\mathcal{C}) \equiv \frac{\delta_{E,E(\mathcal{C})}}{\sum_{\mathcal{C}'} \delta_{E,E(\mathcal{C}')}} \quad (2)$$

[C] In the Canonical Ensemble for a system in contact with a thermal reservoir at inverse temperature β , the energy E can fluctuate, so that all the configurations have now a finite weight given by the exponential form

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$$P_{eq}^{Canonical[\beta]}(\mathcal{C}) \equiv \frac{e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}'} e^{-\beta E(\mathcal{C}')}} \quad (3)$$

Despite these very important physical differences concerning the possible fluctuations of the energy E , the two Ensembles become nevertheless equivalent in the thermodynamic limit of the infinite size $N \rightarrow +\infty$. This mathematical equivalence can be understood from the physical point of view as follows:

From Canonical to Microcanonical: If the system is in contact with a thermal reservoir and described by the Canonical Ensemble of Eq. 3, the relative fluctuations of the energy with respect to the averaged energy E_β^{av} in the Canonical Ensemble will become negligible in the thermodynamic limit $N \rightarrow +\infty$ as a consequence of the law of large numbers. So the Canonical Ensemble at inverse temperature β becomes equivalent in the thermodynamic limit $N \rightarrow +\infty$ to the Microcanonical Ensemble at energy $E = E_\beta^{av}$.

From Microcanonical to Canonical: If the system of size N is isolated and described by the Microcanonical Ensemble of energy E , a subsystem of large size M much smaller than N will be described by the Canonical Ensemble at the inverse temperature β_E that reproduces the correct averaged intensive energy $\frac{E}{N}$. The physical interpretation is that it is the complementary system of size $(N - M) \gg M$ that plays the role of the thermal reservoir at the inverse temperature β_E for the subsystem of size M .

1.2 Analysis of non-equilibrium steady-states via time-averaging over a large-time window T

For non-equilibrium steady states, it is natural to focus also on time-averages over long dynamical trajectories as in Eq. 1. However, since the analog of the Equilibrium distribution $P_{eq}^{Ensemble}(\mathcal{C})$ is not known a priori, one introduces the time-empirical density $\rho(\mathcal{C})$ that measures the fraction of the time spent in each configuration \mathcal{C}

$$\rho_T(\mathcal{C}) \equiv \frac{1}{T} \int_0^T dt \delta_{\mathcal{C}(t), \mathcal{C}} \quad (4)$$

from which one can reconstruct the time-average of any observable $O(\mathcal{C})$ as

$$\frac{1}{T} \int_0^T dt O(\mathcal{C}(t)) = \sum_{\mathcal{C}} O(\mathcal{C}) \rho_T(\mathcal{C}) \quad (5)$$

The goal of the large deviation theory is then to analyze how the empirical density of Eq. 4 and the time-averaged observables of Eq. 5 fluctuate around their typical values for large time T as we now recall.

1.3 Large deviations for Markov trajectories over a large-time window T : standard Levels 1, 2, 3

The theory of large deviations has become the unifying language for the statistical physics of equilibrium, non-equilibrium and dynamical systems (see the reviews [1–3] and references therein). It is based on the following standard classification that involves the three nested levels [1–3]:

- (1) the Level 1 focuses on the large deviations of the time-average of Eq. 5 for a given observable $O(\mathcal{C})$.
- (2) the Level 2 concerns the large deviations of the empirical density $\rho_T(\mathcal{C})$ of Eq. 4 as a function of the configuration \mathcal{C} ; since the empirical density $\rho_T(\mathcal{C})$ allows to reconstruct the time-average of any observable $O(\mathcal{C})$ via Eq. 5, the Level 2 can be contracted to obtain the Level 1 of any observable $O(\mathcal{C})$.
- (3) the Level 3 describes the large deviations of the whole empirical dynamical process over the time-window T , and can reproduce the Level 2 via contraction.

However this initial classification that was appropriate for Equilibrium has turned out to be inappropriate for non-equilibrium steady states for the two following reasons:

- (i) in the presence of steady currents, the large deviations at Level 2 cannot be written in closed form, while the Level 3 is actually far too general.
- (ii) many interesting time-additive observables A , like the currents, the activities, the entropy production, etc... are not of the form of the observables $O(\mathcal{C})$ of the Level 1 but involve also the elementary moves between two configurations, so that they cannot be reconstructed from the empirical density $\rho_T(\mathcal{C})$ alone.

To overcome these difficulties, a new Level has been introduced between the Level 2 and the Level 3 and has been called 2.5 (even if it is actually much closer in spirit to the Level 2).

1.4 Level 2.5 for the joint probability of the empirical density $\rho_T(\mathcal{C})$ and of the empirical flows $q_T(\mathcal{C}', \mathcal{C})$

The Level 2.5 concerns the joint probability of the empirical density $\rho_T(\mathcal{C})$ and of the empirical flows $q_T(\mathcal{C}', \mathcal{C})$ that measure the frequency of jumps from one configuration \mathcal{C} to another \mathcal{C}' configuration during the time-window T

$$q_T(\mathcal{C}', \mathcal{C}) \equiv \frac{1}{T} \sum_{t \in [0, T]: \mathcal{C}(t^+) \neq \mathcal{C}(t^-)} \delta_{\mathcal{C}(t^+), \mathcal{C}'} \delta_{\mathcal{C}(t^-), \mathcal{C}} \quad (6)$$

The introduction of the Level 2.5 has solved the two issues mentioned in the previous subsection as follows.

The issue (i) is now solved because the large deviations at Level 2.5 are closed and explicit for general Markov processes, including discrete-time Markov chains [3–8], continuous-time Markov jump processes [4, 7–30] and Diffusion processes [7, 8, 12, 13, 17, 27, 28, 31–34]. The Level 2 concerning the empirical density $\rho_T(\mathcal{C})$ alone should be now obtained via the optimization of the Level 2.5 over the empirical flows, but this contraction is not always explicit.

The issue (ii) mentioned in the previous subsection is also solved because any time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ of the Markov trajectory $\mathcal{C}(0 \leq t \leq T)$ can be rewritten as a linear combination of the empirical density $\rho_T(\mathcal{C})$ and of the empirical flows $q_T(\mathcal{C}', \mathcal{C})$ with appropriate coefficients $f(\mathcal{C})$ and $g(\mathcal{C}', \mathcal{C})$

$$\begin{aligned} &\mathcal{A}[\mathcal{C}(0 \leq t \leq T)] \\ &= \sum_{\mathcal{C}} f(\mathcal{C}) \rho_T(\mathcal{C}) + \sum_{\mathcal{C}} \sum_{\mathcal{C}' \neq \mathcal{C}} g(\mathcal{C}', \mathcal{C}) q_T(\mathcal{C}', \mathcal{C}) \\ &= \frac{1}{T} \int_0^T dt f(\mathcal{C}(t)) \\ &\quad + \frac{1}{T} \sum_{t \in [0, T]: \mathcal{C}(t^+) \neq \mathcal{C}(t^-)} g(\mathcal{C}(t^+), \mathcal{C}(t^-)) \quad (7) \end{aligned}$$

As a consequence, the large deviations properties of any time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ can be derived from the Level 2.5 via the appropriate contraction.

1.5 Microcanonical and Canonical Ensembles associated to a given time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$

Since the famous Feymann–Kac formula, the standard approach to analyze the statistics of a time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ of the Markov trajectory $\mathcal{C}(0 \leq t \leq T)$ is based on the evaluation of the generating function of $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ via the introduction of the appropriate deformed Markov generator. This approach is very powerful and has been used extensively in the field of non-equilibrium [17, 33, 35–75]. The link with the large deviations at Level 2.5 described in the previous subsection can be understood via the corresponding conditioned process obtained from the generalization of Doob’s h-transform, as explained in particular in the very detailed complementary papers [56, 57] and in the Habilitation Thesis [17]. Within this framework, once the trajectories probabilities $\mathcal{P}[\mathcal{C}(0 \leq t \leq T)]$ are given by the Markov model one is interested in, one introduces for each time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ the following Microcanonical and Canonical Ensembles (see [55–57] and references therein):

[MC] the Microcanonical Ensemble associated to the fixed value A of the time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$

$$\begin{aligned} &P_{[\mathcal{A}]}^{Microcanonical[A]}(\mathcal{C}(0 \leq t \leq T)) \\ &\equiv \frac{\mathcal{P}[\mathcal{C}(0 \leq t \leq T)] \delta_{A, \mathcal{A}[\mathcal{C}(0 \leq t \leq T)]}}{\sum_{\mathcal{C}'(0 \leq t \leq T)} \mathcal{P}[\mathcal{C}'(0 \leq t \leq T)] \delta_{A, \mathcal{A}[\mathcal{C}'(0 \leq t \leq T)]}} \quad (8) \end{aligned}$$

[C] the Canonical Ensemble associated to the parameter k conjugated to the additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$

$$\begin{aligned} &P_{[\mathcal{A}]}^{Canonical[k]}(\mathcal{C}(0 \leq t \leq T)) \\ &\equiv \frac{\mathcal{P}[\mathcal{C}(0 \leq t \leq T)] e^{kT \mathcal{A}[\mathcal{C}(0 \leq t \leq T)]}}{\sum_{\mathcal{C}'(0 \leq t \leq T)} \mathcal{P}[\mathcal{C}'(0 \leq t \leq T)] e^{kT \mathcal{A}[\mathcal{C}'(0 \leq t \leq T)]}} \quad (9) \end{aligned}$$

Although the mathematical analogy with the Equilibrium Ensembles of Eqs. 2 and 3 is obvious, there are however very important differences:

- (a) Here one introduces a new Microcanonical Ensemble and a new Canonical Ensemble for each new time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$ one is interested in, while for Equilibrium, one works with the single Microcanonical Ensemble of Eq. 2 and with the single Canonical Ensemble of Eq. 3 without introducing new Ensembles for each observable.
- (b) For most additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$, the conjugated parameter k that appear in the Canonical Ensemble of Eq. 9 remains a formal parameter that has no direct physical meaning and that cannot be controlled experimentally, in contrast to the inverse temperature β that parametrizes the Equilibrium Canonical Ensemble of Eq. 3.
- (c) The Ensembles of Eqs. 8 and 9 involve the trajectories probabilities $\mathcal{P}[\mathcal{C}(0 \leq t \leq T)]$ determined by the Markov generator, while the Equilibrium Ensembles of Eqs. 2 and 3 do not contain such a priori probabilities $P(\mathcal{C})$ on their right hand-sides. In particular, in the Microcanonical ensemble of Eq. 8, the trajectories that have the correct value of the additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)] = A$ do not have the same probability, in contrast to the Equilibrium Microcanonical Ensemble of Eq. 2, where all the configurations \mathcal{C} that have the correct value of the energy $E(\mathcal{C}) = E$ are equiprobable.

1.6 Motivation and goal of the present work

The present work has been motivated by the differences (a) (b) (c) mentioned in the previous subsection. We will explain how a closer analogy to the Equilibrium Ensembles of Eqs. 2 and 3 can be obtained if, instead of working at the level of a single time-additive observable $\mathcal{A}[\mathcal{C}(0 \leq t \leq T)]$, one works at the Level 2.5 as follows.

[C2.5] The trajectories probabilities $\mathcal{P}[\mathcal{C}(0 \leq t \leq T)]$ determined by Markov generator M can actually be considered as a ‘Canonical Ensemble at Level 2.5’: indeed, the probability $\mathcal{P}[\mathcal{C}(0 \leq t \leq T)]$ of the trajectory $\mathcal{C}(0 \leq t \leq T)$ can be rewritten as the exponential of a linear combination of its relevant empirical time-averaged observables E_n (namely the empirical density and the empirical flows), where the coefficients involving the Markov generator are their fixed conjugate parameters.

[MC2.5] It is then natural to introduce also the corresponding ‘Microcanonical Ensemble at Level 2.5’, where all the relevant empirical variables E_n (namely the empirical density and the empirical flows) are fixed to some values E_n^* and cannot fluctuate anymore for finite T : the trajectories $\mathcal{C}(0 \leq t \leq T)$ that have not the correct values E_n^* have zero weight, while all the trajectories $\mathcal{C}(0 \leq t \leq T)$ that have the correct values E_n^* are equiprobable. In this Microcanonical Ensemble at Level 2.5, the central role is thus played by the number $\Omega_T^{[2.5]}(E_n^*)$ of the stochastic trajectories of duration T with the given empirical observables E_n^* , and by the corresponding explicit Boltzmann entropy $S^{[2.5]}(E_n^*) = [\ln \Omega_T^{[2.5]}(E_n^*)]/T$.

The goal of the present paper is thus to describe in detail the properties of these Canonical and Microcanonical Ensembles at Level 2.5.

1.7 Organization of the paper

The paper is organized as follows. In Sect. 2, we explain in detail the general properties of the Canonical and the Microcanonical Ensembles at Level 2.5 with their links. This framework is then applied to continuous-time Markov jump processes in Sect. 3. In Sect. 4, we focus on the special case of undirected Markov jump processes (where the jumps between two configurations are either both possible or both impossible) to describe how the entropy $S^{[2.5]}(E)$ at Level 2.5 as a function of all the relevant empirical observables E_n can be contracted to obtain the explicit entropies of many other lower levels. Our conclusions are summarized in Sect. 5. In Appendix A, the general framework of Sect. 2 is applied to discrete-time Markov chains.

2 Canonical and Microcanonical Ensembles for Markov trajectories

In this section, we outline the general principles before the specific applications to continuous-time Markov jump processes in Sect. 3 and to discrete-time Markov chains in Appendix A.

2.1 Canonical Ensemble of trajectories $x(0 \leq t \leq T)$ associated to the Markov generator M

Let us consider a Markov process in a discrete configuration space converging towards some normalizable

steady state. Since the Markov generator M defines the dynamical rules, its matrix elements can be considered as fixed ‘intensive variables’ that will govern the statistics of the trajectories $x(0 \leq t \leq T)$ with probabilities $\mathcal{P}_M[x(0 \leq t \leq T)]$ normalized to unity

$$1 = \sum_{x(0 \leq t \leq T)} \mathcal{P}_M[x(0 \leq t \leq T)] \equiv \sum_{x(\cdot)} \mathcal{P}_M[x(\cdot)] \tag{10}$$

where the last simplified notations will be used to ease the read of equations.

2.1.1 Identification of the relevant empirical observables $E_n[x(\cdot)]$ that determine the trajectories probabilities $\mathcal{P}_M[x(\cdot)]$

The information per unit time $\mathcal{I}_M[x(0 \leq t \leq T)]$ of a given trajectory $x(0 \leq t \leq T)$ of probability $\mathcal{P}_M[x(\cdot)]$

$$\mathcal{I}_M[x(\cdot)] \equiv -\frac{\ln(\mathcal{P}_M[x(\cdot)])}{T} \tag{11}$$

depends on the trajectory $x(0 \leq t \leq T)$

$$\mathcal{I}_M[x(\cdot)] = I_M(E_n[x(\cdot)]) \tag{12}$$

only via a collection of relevant empirical observables $E_n[x(\cdot)]$ labelled by n : they correspond to the time-averaged density and to the time-averaged flows during the time window T (see Eqs. 76 and 79 for continuous-time jump processes as well as Eq. A7 for discrete-time Markov chains).

2.1.2 The information $I_M(E_n)$ as a linear combination of the relevant empirical observables E_n

As a consequence of the Markov property that allows to decompose the trajectory probability via the Chapman–Kolmogorov Equation, the information $I_M(E_n)$ is actually a linear combination of these relevant empirical time-averaged observables E_n

$$I_M(E_n) = \sum_n E_n i_n(M) \tag{13}$$

while the coefficients

$$i_n(M) \equiv \frac{\partial I_M(E_n)}{\partial E_n} \tag{14}$$

involve the matrix elements of the Markov generator M in a very simple way (see Eqs. 84 and 85 for continuous-time jump processes as well as Eqs. A14 and A15 for discrete-time Markov chains).

2.1.3 Trajectory probability in terms of the relevant empirical observables E . $[x(\cdot)] = E$.

In summary, the probability $\mathcal{P}_M[x(\cdot)]$ of the trajectory $x(0 \leq t \leq T)$ can be rewritten in terms of its relevant empirical observables $E_n[x(\cdot)]$ as

$$\begin{aligned} \mathcal{P}_M[x(\cdot)] &= e^{-TI_M[x(\cdot)]} = e^{-TI_M(E, [x(\cdot)])} \\ &= \sum_E \left[\prod_n \delta(E_n - E_n[x(\cdot)]) \right] e^{-TI_M(E)} \\ &= \sum_E \left[\prod_n \delta(E_n - E_n[x(\cdot)]) \right] e^{-T \sum_n E_n i_n(M)} \end{aligned} \tag{15}$$

where the exponential involves a linear combination of the relevant empirical time-averaged observables E_n , while the coefficients $i_n(M)$ determined by the Markov generator M can be considered as their fixed conjugate parameters.

2.1.4 Number $\Omega_T^{[2.5]}(E)$ of trajectories $x(0 \leq t \leq T)$ with the same relevant empirical observables E . $[x(\cdot)] = E$.

An important consequence of Eq. 15 is that all the trajectories $x(0 \leq t \leq T)$ that have the same relevant empirical observables $E_n = E_n[x(0 \leq t \leq T)]$ have the same probability. The normalization over all possible trajectories of Eq. 10 can be thus rewritten as a sum over these relevant empirical observables E_n

$$\begin{aligned} 1 &= \sum_{x(0 \leq t \leq T)} \mathcal{P}[x(0 \leq t \leq T)] \\ &= \sum_E \Omega_T^{[2.5]}(E) e^{-TI_M(E)} \end{aligned} \tag{16}$$

where the number $\Omega_T^{[2.5]}(E)$ of trajectories of duration T associated to given values E_n of these empirical observables

$$\Omega_T^{[2.5]}(E) \equiv \sum_{x(0 \leq t \leq T)} \left[\prod_n \delta(E_n - E_n[x(\cdot)]) \right] \tag{17}$$

will grow exponentially with respect to the time-window T in the limit $T \rightarrow +\infty$

$$\Omega_T^{[2.5]}(E) \underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(E) e^{TS^{[2.5]}(E)} \tag{18}$$

The prefactor $C^{[2.5]}(E)$ denotes the appropriate constitutive constraints for the empirical observables E_n (see Eq. 83 for continuous-time jump processes as well

as Eq. A13 for discrete-time Markov chains). The function $S^{[2.5]}(E) = \frac{\ln \Omega_T^{[2.5]}(E)}{T}$ represents the Boltzmann intensive entropy of the set of trajectories of duration T with given intensive empirical observables E_n . Note that since the Boltzmann entropy is the cornerstone of the statistical physics of Equilibrium, the definition of Boltzmann entropies for non-equilibrium systems has motivated a lot of various studies (see for instance [76] and references therein).

2.1.5 Boltzmann intensive entropy $S^{[2.5]}(E)$ as a function of the relevant empirical observables E_n

The entropy $S^{[2.5]}(E)$ introduced in Eq. 18 can be evaluated without any combinatorial computation as follows. The normalization of Eq. 16 becomes for large T

$$1 \underset{T \rightarrow +\infty}{\simeq} \sum_E C^{[2.5]}(E) e^{T[S^{[2.5]}(E) - I_M(E)]} \tag{19}$$

When the empirical variables E_n take their typical values $E_n^{typ[M]}$ for the Markov generator M , the exponential behavior in T of Eq. 19 should exactly vanish, i.e. the entropy $S^{[2.5]}(E^{typ[M]})$ should exactly compensate the information $I_M(E^{typ[M]})$

$$\begin{aligned} S^{[2.5]}(E^{typ[M]}) &= I_M(E^{typ[M]}) \\ &= \sum_n E_n^{typ[M]} i_n(M) \end{aligned} \tag{20}$$

To obtain the intensive entropy $S^{[2.5]}(E)$ for other given values E_n of the empirical observables, one just needs to introduce the modified Markov generator M^E that would make the empirical values E_n typical for this modified Markov generator

$$E_n = E_n^{typ[M^E]} \tag{21}$$

and to use Eq. 20 for this modified Markov generator M^E to obtain the entropy $S^{[2.5]}(E)$ as a function of E .

$$\begin{aligned} S^{[2.5]}(E) &= S^{[2.5]}(E^{typ[M^E]}) = I_{M^E}(E^{typ[M^E]}) \\ &= I_{M^E}(E) \end{aligned} \tag{22}$$

Plugging the linear expression of Eq. 13 for the information into Eq. 22 yields that the entropy

$$S^{[2.5]}(E) = \sum_n E_n i_n(M^E) \tag{23}$$

is nonlinear with respect to the empirical observables E_n , since the empirical observables E appear in the modified Markov generator M^E involved in the coefficients $i_n(M^E)$.

However, the linearity of the information of Eq. 13 can be used to write the coefficients of Eq. 14 for the special values $E_n^{typ[M]}$ of the empirical observables to use Eq. 20

$$i_n(M) = \frac{\partial I_M(E^{typ[M]})}{\partial E_n^{typ[M]}} = \frac{\partial S^{[2.5]}(E^{typ[M]})}{\partial E_n^{typ[M]}} \quad (24)$$

that can be now rewritten for the modified Markov generator M^E . that make the empirical values $E_n = E_n^{typ[M^E]}$ typical (Eq. 21) to obtain that the derivatives of the entropy $S^{[2.5]}(E.)$ with respect to the empirical observables E_n

$$\frac{\partial S^{[2.5]}(E.)}{\partial E_n} = i_n(M^E.) \quad (25)$$

are given by the coefficients $i_n(M^E.)$ associated to the modified Markov generator M^E . The comparison with the direct derivative of Eq. 23

$$\frac{\partial S^{[2.5]}(E.)}{\partial E_n} = i_n(M^E.) + \sum_m E_m \frac{\partial i_m(M^E.)}{\partial E_n} \quad (26)$$

yields that Eq. 25 requires the vanishing of the second contribution of Eq. 26 for any n

$$\sum_m E_m \frac{\partial i_m(M^E.)}{\partial E_n} = 0 \quad (27)$$

The property of Eq. 25 can be explicitly checked in Eq. 99 for continuous-time jump processes and in Eq. A26 for discrete-time Markov chains.

2.1.6 Large deviations at Level 2.5 for the relevant empirical observables E .

Equation 16 can be interpreted as the normalization

$$1 = \sum_E P_M^{[2.5]}(E.) \quad (28)$$

for the probability $P_M^{[2.5]}(E.)$ to see the relevant empirical observables E_n over the set of trajectories of duration T generated with the Markov generator M . For large time $T \rightarrow +\infty$, the asymptotic behavior of $\Omega_T^{[2.5]}(E.)$ in Eq. 18 can be plugged into Eq. 16 to obtain the large deviation properties for all the relevant empirical observables E_n that determine the trajectories probabilities

$$\begin{aligned} P_M^{[2.5]}(E.) &\underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(E.) e^T [S^{[2.5]}(E.) - I_M(E.)] \\ &= C^{[2.5]}(E.) e^{-TI_M^{[2.5]}(E.)} \end{aligned} \quad (29)$$

where the positive rate function at Level 2.5

$$\begin{aligned} I_M^{[2.5]}(E.) &= I_M(E.) - S^{[2.5]}(E.) \\ &= I_M(E.) - I_{M^E.}(E.) \geq 0 \end{aligned} \quad (30)$$

is simply given by the difference between the information $I_M(E.)$ associated to the Markov generator M and the information $I_{M^E.}(E.)$ associated to the modified Markov generator M^E . that would make the empirical values E_n typical (see Eq. 21).

The typical values $E_n^{typ[M]}$ for the Markov generator M are the only values of the empirical observables E_n that satisfy the constitutive constraints $C^{[2.5]}(E.)$ and that make the rate function of Eq. 30 vanish

$$I_M^{[2.5]}(E^{typ[M]}) = 0 \quad (31)$$

For large T , the Level 2.5 of Eq. 29 describes how rare it is to see empirical observables E different from their typical values $E^{typ[M]}$, while in the thermodynamic limit $T = +\infty$, the Level 2.5 of Eq. 88 reduces to delta functions for all the relevant empirical observables E_n that determine the trajectories probabilities

$$P_M^{[2.5]}(E.) \underset{T \rightarrow +\infty}{\simeq} \prod_n \delta(E_n - E_n^{typ[M]}) \quad (32)$$

2.1.7 Contraction of the explicit Level 2.5 to obtain large deviations properties of all the lower Levels

As recalled in the Introduction, the explicit large deviations at Level 2.5 of Eq. 29 concerning the joint distribution of all the relevant empirical observables E_n allows to analyze via contraction all the large deviations properties of lower levels. Let us mention some important examples:

(i) The joint distribution of any subset of the relevant empirical observables E_n can be obtained via the integration of Eq. 29 over all the empirical observables that one does not wish to keep. For instance, the distribution of the empirical density ρ . alone can be obtained via the integration of Eq. 29 over all the empirical flows with their constitutive constraints to obtain the large deviations at Level 2

$$P_M^{[2]}(\rho.) \underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho.) e^{-TI_M^{[2]}(\rho.)} \quad (33)$$

where the constitutive constraint $C^{[2]}(\rho.)$ corresponds to the normalization of the empirical density ρ . However the rate function $I_M^{[2]}(\rho.)$ at Level 2 for the empirical density alone ρ . is not always explicit when the Markov generator M does not correspond to some detailed-balance equilibrium dynamics.

(ii) Any intensive time-additive observable $\mathcal{A}_M[x(\cdot)]$ of the trajectory $x(0 \leq t \leq T)$ can be rewritten as a linear combination of the empirical observables $E_n[x(\cdot)]$ with appropriate coefficients $a_n(M)$ that may depend on the Markov generator M

$$\mathcal{A}_M[x(\cdot)] = \sum_n E_n[x(\cdot)] a_n(M) \equiv A_M(E[x(\cdot)]) \quad (34)$$

Since all the trajectories $x(0 \leq t \leq T)$ that have the same empirical observables $E_n = E_n[x(0 \leq t \leq T)]$ have the same value for the time-additive observable of Eq. 34, its probability distribution can be evaluated from the Level 2.5 of Eq. 29

$$\begin{aligned} P_M^{[Add]}(A) &\equiv \sum_{x(0 \leq t \leq T)} \mathcal{P}[x(0 \leq t \leq T)] \\ &\quad \delta\left(A - \sum_n E_n[x(\cdot)] a_n(M)\right) \\ &= \sum_E P_M^{[2.5]}(E.) \delta\left(A - \sum_n E_n a_n(M)\right) \\ &\underset{T \rightarrow +\infty}{\simeq} \sum_E C^{[2.5]}(E.) e^{-TI_M^{[2.5]}(E.)} \\ &\quad \delta\left(A - \sum_n E_n a_n(M)\right) \underset{T \rightarrow +\infty}{\simeq} e^{-TI_M^{[Add]}(A)} \end{aligned} \quad (35)$$

The rate function $I_M^{[Add]}(A)$ for the time-additive observable corresponds to the minimization of the rate function $I_M^{[2.5]}(E.)$ at Level 2.5 over the empirical observables E_n satisfying the constitutive constraints $C^{[2.5]}(E.)$ and the supplementary constraint $A = \sum_n E_n a_n(M)$ reproducing the correct value A of the additive observable

$$I_M^{[Add]}(A) = \min_{\substack{E.:C^{[2.5]}(E.) \text{ and} \\ \sum_n E_n a_n(M) = A}} \left(I_M^{[2.5]}(E.) \right) \quad (36)$$

This contraction can be analyzed via the method of Lagrange multipliers to impose the constraints, but again it is not always explicit. When the additive observable is the information $\mathcal{I}_M[x(\cdot)]$ of Eqs. 12 and 13, its large deviations properties can be analyzed via the Ruelle thermodynamic formalism recently revisited in [72]. Besides this example of the information $\mathcal{I}_M[x(\cdot)]$, there are of course many other interesting time-additive observables depending on the specific models.

(iii) The Level 1 concerns the additive observables $\mathcal{A}_M[x(\cdot)]$ of Eq. 34 that can be reconstructed from the empirical density ρ . alone (i.e. that do not involve the empirical flows) and whose large deviations can be thus obtained from the contraction of the Level 2 of Eq. 33.

2.1.8 Relation with the Kolmogorov–Sinai entropy h_M^{KS} of Markov trajectories

The Kolmogorov–Sinai entropy h_M^{KS} is defined via the averaged value of the intensive information

$\mathcal{I}_M[x(0 \leq t \leq T)]$ of Eq. 11 over the trajectories $x(0 \leq t \leq T)$ drawn with their probabilities $\mathcal{P}_M[x(0 \leq t \leq T)]$

$$\begin{aligned} h_M^{KS} &\equiv \lim_{T \rightarrow +\infty} \left(\sum_{x(\cdot)} \mathcal{P}_M[x(\cdot)] \mathcal{I}_M[x(\cdot)] \right) \\ &= \lim_{T \rightarrow +\infty} \left(-\frac{1}{T} \sum_{x(0 \leq t \leq T)} \mathcal{P}_M[x(0 \leq t \leq T)] \right. \\ &\quad \left. \times \ln(\mathcal{P}_M[x(0 \leq t \leq T)]) \right) \end{aligned} \quad (37)$$

So it characterizes the linear growth in T of the Shannon entropy $\mathcal{S}_M^{Shannon}(T)$ associated to the probability distribution $\mathcal{P}_M[x(0 \leq t \leq T)]$ of the trajectories

$$\begin{aligned} \mathcal{S}_M^{Shannon}(T) &\equiv - \sum_{x(0 \leq t \leq T)} \mathcal{P}_M[x(0 \leq t \leq T)] \\ &\quad \times \ln(\mathcal{P}_M[x(0 \leq t \leq T)]) \underset{T \rightarrow +\infty}{\propto} T h_M^{KS} \end{aligned} \quad (38)$$

The average of $\mathcal{I}_M[x(0 \leq t \leq T)]$ over trajectories of Eq. 37 can be rewritten as an average of the information $I_M(E.)$ of Eq. 12 over the probability $P_M^{[2.5]}(E.)$ of Eq. 29 for the empirical observables E_n

$$h_M^{KS} = \lim_{T \rightarrow +\infty} \left(\sum_E P_M^{[2.5]}(E.) I_M(E.) \right) \quad (39)$$

For $T = +\infty$, only the typical values $E^{typ[M]}$ of the empirical observables survive in Eq. 32 so that the Kolmogorov–Sinai entropy h_M^{KS} reduces to the information $I_M(E^{typ[M]})$ associated to the typical values $E^{typ[M]}$ of the empirical observables

$$h_M^{KS} = I_M(E^{typ[M]}) \quad (40)$$

Equation 20 yields that the Kolmogorov–Sinai entropy h_M^{KS} also coincides with the entropy $S^{[2.5]}(E^{typ[M]})$ associated to the typical values $E^{typ[M]}$ of the empirical observables

$$h_M^{KS} = S^{[2.5]}(E^{typ[M]}) \quad (41)$$

The physical meaning is that the average over trajectories with their probabilities $\mathcal{P}[x(0 \leq t \leq T)]$ is actually dominated in the thermodynamic limit $T \rightarrow +\infty$ by the number of Eq. 18

$$\Omega_T^{[2.5]}(E^{typ[M]}) \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[2.5]}(E^{typ[M]})} = e^{Th_M^{KS}} \quad (42)$$

of trajectories corresponding to the information of Eq. 40

$$I_M(E^{typ[M]}) = h_M^{KS} \tag{43}$$

so that all these trajectories have the same probability given by $e^{-Th_M^{KS}} = \frac{1}{\Omega_T^{[2.5]}(E^{typ[M]})}$. As a consequence, it is interesting to introduce the corresponding notion of Microcanonical Ensemble described in the next subsection.

2.2 Microcanonical Ensemble at Level 2.5 based on fixed relevant empirical observables E_n^*

2.2.1 Microcanonical Ensemble at Level 2.5 where the relevant empirical observables E_n^* cannot fluctuate

The concentration property of Eq. 32 for the all the relevant empirical observables in the thermodynamic limit $T = +\infty$ and the discussion around Eqs. 42 and 43 suggests to introduce the notion of the 'Microcanonical Ensemble' at Level 2.5 where the all the relevant empirical variables E_n are fixed to some values E_n^* satisfying the constitutive constraints $C^{[2.5]}(E^*)$

$$P_{E_n^*}^{Micro[2.5]}(E) = \prod_n \delta(E_n - E_n^*) \tag{44}$$

and thus cannot fluctuate for finite T in contrast to the Canonical fluctuations at Level 2.5 of Eq. 29 associated to the Markov generator M .

Note that here the possible elementary moves of the trajectories correspond to the empirical flows that are fixed to non-vanishing values, while the empirical flows that are fixed to vanishing values correspond to impossible elementary moves.

2.2.2 Probabilities of trajectories $x(0 \leq t \leq T)$ in the Microcanonical Ensemble at Level 2.5

In the Microcanonical Ensemble of Eq. 44, only the trajectories $x(0 \leq t \leq T)$ corresponding to the given empirical values E_n^* have a non-zero weight, and all these allowed trajectories have the same weight given by the inverse of their number $\Omega_T^{[2.5]}(E^*)$ of Eq. 17

$$\begin{aligned} \mathcal{P}_{E_n^*}^{Micro[2.5]}[x(\cdot)] &= \frac{1}{\Omega_T^{[2.5]}(E^*)} \prod_n \delta(E_n - E_n^*[x(0 \leq t \leq T)]) \end{aligned} \tag{45}$$

Using the asymptotic behavior for large T of Eq. 18, the trajectory probability of Eq. 45 involves the entropy $S^{[2.5]}(E^*)$

$$\begin{aligned} \mathcal{P}_{E_n^*}^{Micro[2.5]}[x(\cdot)] &\underset{T \rightarrow +\infty}{\simeq} e^{-TS^{[2.5]}(E^*)} \prod_n \delta(E_n^* - E_n[x(0 \leq t \leq T)]) \end{aligned} \tag{46}$$

2.2.3 Statistics of the subtrajectories on $[0, \tau]$ of the Microcanonical Ensemble trajectories on $[0, T]$ for $1 \ll \tau \ll T$

In the Sect. 2.1.4, we have seen how the analysis of the Canonical Ensemble associated to the Markov generator M actually involves the Microcanonical Ensemble via the number $\Omega_T^{[2.5]}(E)$ of trajectories with given empirical observables E_n . In the present subsection, we would like to see if the Canonical Ensemble can emerge to describe the statistics of the long subtrajectory $x(0 \leq t \leq \tau)$ belonging to the much longer trajectory $x(0 \leq t \leq T)$ drawn with the Microcanonical distribution of Eq. 46, i.e. we are interested in the regime

$$1 \ll \tau \ll T \tag{47}$$

Since this property would be the direct analog of the well-known property for Equilibrium Ensembles (as recalled at the end of the Sect. 1.1 of the Introduction), it is interesting to try to translate step by step the standard derivation for Equilibrium Ensembles which is based on the Taylor expansion of the Boltzmann entropy (see your favorite textbook on the statistical physics of Equilibrium).

When the very long trajectory $x(0 \leq t \leq T)$ with the fixed empirical observables E_n^* is decomposed into the long subtrajectory $x(0 \leq t \leq \tau)$ of empirical observables E_n and its much longer complementary subtrajectory $x(\tau \leq t \leq T)$ of empirical observables \hat{E}_n , we can use the fact that the empirical observables E_n are given by time-averaged properties to write

$$TE_n^* = \tau E_n + (T - \tau)\hat{E}_n \tag{48}$$

The number $\Omega_T^{[2.5]}(E^*)$ of total trajectories can be thus computed from the numbers $\Omega_\tau^{[2.5]}(E)$ and $\Omega_{T-\tau}^{[2.5]}(\hat{E})$ of the two subtrajectories via the multidimensional convolution

$$\begin{aligned} \Omega_T^{[2.5]}(E^*) &= \sum_E \sum_{\hat{E}} \Omega_\tau^{[2.5]}(E) \Omega_{T-\tau}^{[2.5]}(\hat{E}) \\ &\quad \times \prod_n \delta\left(E_n^* - \frac{\tau}{T}E_n - \left(1 - \frac{\tau}{T}\right)\hat{E}_n\right) \\ &= \sum_E \sum_{\hat{E}} \Omega_\tau^{[2.5]}(E) \Omega_{T-\tau}^{[2.5]}(\hat{E}) \prod_n \frac{\delta\left(\hat{E}_n - \frac{E_n^* - \frac{\tau}{T}E_n}{1 - \frac{\tau}{T}}\right)}{1 - \frac{\tau}{T}} \\ &\underset{\frac{\tau}{T} \ll 1}{\simeq} \sum_E \Omega_\tau^{[2.5]}(E) \Omega_{T-\tau}^{[2.5]}\left(\frac{E^* - \frac{\tau}{T}E}{1 - \frac{\tau}{T}}\right) \end{aligned} \tag{49}$$

As a consequence, the probability $p_\tau(E.)$ to see the empirical observables E_n during the long subtrajectory $x(0 \leq t \leq \tau)$ of duration τ reads

$$p_\tau(E.) \simeq \Omega_\tau^{[2.5]}(E.) \frac{\Omega_{T-\tau}^{[2.5]} \left(\frac{E^* - \frac{\tau}{T} E.}{1 - \frac{\tau}{T}} \right)}{\Omega_T^{[2.5]}(E^*)} \tag{50}$$

Since the constraints $C^{[2.5]}(E^*)$ are satisfied from the definition of the Microcanonical Ensemble, let us assume that the constraints $C^{[2.5]}(\hat{E}.)$ are satisfied whenever the constraints $C^{[2.5]}(E.)$ are satisfied, as can be checked on explicit examples. Using the asymptotic form of Eq. 18 for large τ , for large $(T - \tau)$ and for large T , Eq. 50 becomes

$$p_\tau(E.) \simeq C^{[2.5]}(E.) \times e^{\tau S^{[2.5]}(E.) - T S^{[2.5]}(E^*) + (T - \tau) S^{[2.5]} \left(\frac{E^* - \frac{\tau}{T} E.}{1 - \frac{\tau}{T}} \right)} \tag{51}$$

Plugging the Taylor expansion at first order in the ratio $\frac{\tau}{T} \ll 1$

$$\begin{aligned} S^{[2.5]} \left(\frac{E^* - \frac{\tau}{T} E.}{1 - \frac{\tau}{T}} \right) &= S^{[2.5]} \left(E^* + \frac{\tau}{T} (E^* - E.) + o \left(\frac{\tau^2}{T^2} \right) \right) \\ &= S^{[2.5]}(E^*) + \frac{\tau}{T} \sum_n (E_n^* - E_n) \frac{\partial S^{[2.5]}(E^*)}{\partial E_n^*} + o \left(\frac{\tau^2}{T^2} \right) \end{aligned} \tag{52}$$

into Eq. 51 yields

$$\begin{aligned} p_\tau(E.) &\simeq C^{[2.5]}(E.) e^{\tau S^{[2.5]}(E.)} e^{-T S^{[2.5]}(E^*) + (T - \tau) \left[S^{[2.5]}(E^*) + \frac{\tau}{T} \sum_n (E_n^* - E_n) \frac{\partial S^{[2.5]}(E^*)}{\partial E_n^*} + o \left(\frac{\tau^2}{T^2} \right) \right]} \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(E.) e^{\tau \left[S^{[2.5]}(E.) - S^{[2.5]}(E^*) - \sum_n (E_n - E_n^*) \frac{\partial S^{[2.5]}(E^*)}{\partial E_n^*} \right]} \end{aligned} \tag{53}$$

The factor of τ in the exponential can be simplified via the introduction of the Markov model M^{E^*} that makes the empirical observables E_n^* typical (Eq. 21)

$$E_n^* = E_n^{typ[M^{E^*}]} \tag{54}$$

to use the expression of the entropy of Eq. 23

$$S^{[2.5]}(E^*) = \sum_n E_n^* i_n(M^{E^*}) \tag{55}$$

and of its derivatives with respect to empirical observables of Eq. 25

$$\frac{\partial S^{[2.5]}(E^*)}{\partial E_n^*} = i_n(M^{E^*}) \tag{56}$$

Plugging these two equations into Eq. 53 leads to the final result

$$\begin{aligned} p_\tau(E.) &\underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(E.) \times e^{\tau \left[S^{[2.5]}(E.) - \sum_n E_n^* i_n(M^{E^*}) - \sum_n (E_n - E_n^*) i_n(M^{E^*}) \right]} \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(E.) e^{\tau \left[S^{[2.5]}(E.) - \sum_n E_n i_n(M^{E^*}) \right]} \\ &= C^{[2.5]}(E.) e^{-\tau I_{M^{E^*}}^{[2.5]}(E.)} \end{aligned} \tag{57}$$

where one recognizes the Level 2.5 of Eqs. 29 and 30 for the distribution of the empirical observables E_n in the Canonical Ensemble associated to the Markov generator M^{E^*} over the time-window τ .

In conclusion, when the total trajectory $x(0 \leq t \leq T)$ belongs to the Microcanonical Ensemble of Eq. 46 corresponding to the fixed empirical observables E_n^* , the statistical properties of the subtrajectory $x(0 \leq t \leq \tau)$ over the time-window τ satisfying $1 \ll \tau \ll T$ are governed by the Canonical Ensemble associated to the Markov generator M^{E^*} .

2.2.4 Time-additive observables in the Microcanonical Ensemble at Level 2.5

In the Canonical Ensemble associated to the Markov generator M , the additive observables defined by Eq. 34

$$A_M(E.) = \sum_n E_n a_n(M) \tag{58}$$

are fluctuating with large deviations properties governed by Eq. 35.

The Markov model M^{E^*} that makes the empirical observables E_n^* typical (Eq. 54) is thus also useful to translate the definition of Eq. 58 in the Canonical Ensemble to obtain their fixed values in the Microcanonical Ensemble associated to the fixed empirical observables E_n^*

$$A_{E^*}^{Micro[2.5]}(E.) = \sum_n E_n^* a_n(M^{E^*}) \tag{59}$$

2.3 Maximization of the explicit entropy $S^{[2.5]}(E.)$ at Level 2.5 with constraints towards lower levels

For the Canonical Ensemble, we have recalled in Sect. 2.1.7 how the explicit rate function $I_M^{[2.5]}(E.)$ at Level 2.5 could be contracted to obtain the large deviations properties of all the lower levels. For the Microcanonical Ensemble, the analog idea concerns the maximization of the entropy $S^{[2.5]}(E.)$ at Level 2.5 with constraints to obtain the entropies of all the lower levels with the following physical meaning.

From Eq. 18 giving the explicit number $\Omega_T^{[2.5]}(E.)$ of trajectories of duration T associated to given values of all the relevant empirical observables E_n , one can compute:

(i) the number of trajectories of duration T associated with any subset of the relevant empirical observables E_n via the integration of $\Omega_T^{[2.5]}(E.)$ over all the empirical observables that one does not wish to keep. For instance, the number $\Omega_T^{[2]}(\rho.)$ of trajectories of duration T associated to the given empirical density $\rho.$ can be obtained via the integration of $\Omega_T^{[2.5]}(E.)$ over all the empirical flows with their constraints to obtain the Level 2

$$\Omega_T^{[2]}(\rho.) \equiv \sum_{x(0 \leq t \leq T)} \left[\prod_x \delta(\rho_x - \rho_x[x(\cdot)]) \right] \underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho.) e^{TS^{[2]}(\rho.)} \tag{60}$$

where the constitutive constraint $C^{[2]}(\rho.)$ corresponds to the normalization of the empirical density $\rho.$ as in Eq. 33, while $S^{[2]}(\rho.)$ represents the entropy as a function of the empirical density $\rho.$ alone.

(ii) the number $\Omega_T^{[Add]}(A)$ of trajectories of duration T corresponding to a given value A of the additive observable of Eq. 59 can be obtained from the integration of $\Omega_T^{[2.5]}(E.)$ with the appropriate constraint fixing the value of A

$$\Omega_T^{[Add]}(A) = \sum_{E.} \Omega_T^{[2.5]}(E.) \delta \left(A - \sum_n E_n a_n(M^{E.}) \right) \underset{T \rightarrow +\infty}{\simeq} \sum_{E.} C^{[2.5]}(E.) e^{TS^{[2.5]}(E.)} \delta \left(A - \sum_n E_n a_n(M^{E.}) \right) \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[Add]}(A)} \tag{61}$$

The entropy $S^{[Add]}(A)$ thus corresponds to the maximization of the entropy $S^{[2.5]}(E.)$ at Level 2.5 over the empirical observables E_n satisfying the constitutive constraints $C^{[2.5]}(E.)$ and the constraint $A = \sum_n E_n a_n(M^{E.})$ reproducing the correct value A of the additive observable

$$S^{[Add]}(A) = \max_{\substack{E.: C^{[2.5]}(E.) \text{ and} \\ \sum_n E_n a_n(M^{E.}) = A}} \left[S^{[2.5]}(E.) \right] \tag{62}$$

(iii) the Level 1 concerns the additive observables A that can be reconstructed from the empirical density $\rho.$ alone, so that their number $\Omega_T^{[1]}(A)$ can be obtained from the integration of the Level 2 of Eq. 60.

(iii) Finally, the Level 0 concerns the total number of trajectories of duration T when one integrates $\Omega_T^{[1]}(A)$ over all the empirical observables $E.$ or when one integrates $\Omega_T^{[2]}(\rho.)$ over all possible empirical densities $\rho.,$ or when one integrates $\Omega_T^{[Add]}(A)$ over all possible values A

$$\Omega_T^{[0]} \equiv \sum_{E.} C^{[2.5]}(E.) e^{TS^{[2.5]}(E.)} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[0]}} \tag{63}$$

The entropy $S^{[0]}$ already appears in Ruelle the thermodynamic formalism as discussed with simple examples in [72].

3 Application to continuous-time Markov jump processes

3.1 Canonical Ensemble of trajectories $x(0 \leq t \leq T)$ associated to the Markov jump generator w

3.1.1 Markov jump process converging towards some normalizable steady state

The continuous-time jump dynamics is defined by the Master Equation in discrete configuration space

$$\partial_t P_x(t) = \sum_y w_{x,y} P_y(t) \tag{64}$$

where the off-diagonal $x \neq y$ positive matrix elements $w_{x,y} \geq 0$ represent the jump rates per unit time from y towards $x \neq y$, while the corresponding diagonal elements are negative and are fixed by the conservation of probability to be

$$w_{y,y} = - \sum_{x \neq y} w_{x,y} \tag{65}$$

The steady-state P_x^* of Eq. 64

$$0 = \sum_y w_{x,y} P_y^* \tag{66}$$

is assumed to be normalizable

$$1 = \sum_y P_y^* \tag{67}$$

Here the elementary jump from y towards x is possible if the corresponding off-diagonal element is positive $w_{x,y} > 0$, while it is impossible if $w_{x,y} = 0$. In particular, it is important to mention the following special cases:

- (i) Directed dynamics: for any pair $x \neq y$, the two elementary jumps between them are never both possible

$$\text{Directed: } w_{x,y}w_{y,x} = 0 \tag{68}$$

- (ii) Undirected dynamics: for any pair $x \neq y$, the two jumps between them are either both possible $w_{x,y}w_{y,x} > 0$ or both impossible $w_{x,y} = w_{y,x} = 0$

$$\text{Undirected: } w_{x,y}w_{y,x} > 0 \text{ or } w_{x,y} = w_{y,x} = 0 \tag{69}$$

- (iii) Equilibrium dynamics: special case of undirected dynamics where on each link $x \neq y$ with possible moves $w_{x,y}w_{y,x} > 0$, there is no steady current in the steady state, i.e. the two steady flows on each link satisfy the Detailed-Balance condition

$$\text{Detailed Balance: } w_{x,y}P_y^* = w_{y,x}P_x^* \tag{70}$$

3.1.2 Trajectories probabilities and their normalization

A trajectory $x(t)$ on the time interval $0 \leq t \leq T$ can be decomposed into a certain number $K \geq 0$ of jumps $k = 1, \dots, K$ occurring at times $0 < t_1 < \dots < t_K < T$ between the successive configurations $(x_0 \rightarrow x_1 \rightarrow x_2 \dots \rightarrow x_K)$ that are visited between these jumps. The probability density of this trajectory for fixed initial condition x_0

$$x(0 \leq t \leq T) = (x_0; t_1; x_1; t_2; \dots; x_{K-1}; t_K; x_K) \tag{71}$$

reads in terms of the matrix elements of the Markov generator $w_{..}$,

$$\begin{aligned} \mathcal{P}[x(0 \leq t \leq T) = (x_0; t_1; x_1; t_2; \dots; x_{K-1}; t_K; x_K)] \\ = e^{(T-t_K)w_{x_K, x_K}} w_{x_K, x_{K-1}} \\ \times e^{(t_K-t_{K-1})w_{x_{K-1}, x_{K-1}}} \dots w_{x_2, x_1} \\ \times e^{(t_2-t_1)w_{x_1, x_1}} w_{x_1, x_0} e^{t_1 w_{x_0, x_0}} \\ = e^{(T-t_K)w_{x_K, x_K}} \prod_{k=1}^K \left[w_{x_k, x_{k-1}} e^{(t_k-t_{k-1})w_{x_{k-1}, x_{k-1}}} \right] \end{aligned} \tag{72}$$

The normalization of over all possible trajectories on $[0, T]$ involves the sum over the number K of jumps, the sum over the K configurations (x_1, \dots, x_K) where x_k has to be different from x_{k-1} , and the integration

over the jump times with the measure $dt_1 \dots dt_K$ and the constraint $0 < t_1 < \dots < t_K < T$

$$\begin{aligned} 1 &= \sum_{K=0}^{+\infty} \int_0^T dt_K \int_0^{t_K} dt_{K-1} \dots \int_0^{t_2} dt_1 \sum_{x_K \neq x_{K-1}} \\ &\times \sum_{x_{K-1} \neq x_{K-2}} \dots \sum_{x_2 \neq x_1} \sum_{x_1 \neq x_0} \\ &= \mathcal{P}[x(0 \leq t \leq T) (x_0; t_1; x_1; t_2; \dots; x_{K-1}; t_K; x_K)] \end{aligned} \tag{73}$$

3.1.3 Identification of the relevant empirical observables that determine the trajectories probabilities

The trajectory probability of Eq. 72 can be rewritten more compactly without the explicit enumeration of all the jumps as

$$\begin{aligned} \mathcal{P}_w [x(0 \leq t \leq T)] \\ = \exp \left[\sum_{t \in [0, T]: x(t^+) \neq x(t^-)} \ln(w_{x(t^+), x(t^-)}) \right. \\ \left. + \int_0^T dt w_{x(t), x(t)} \right] \end{aligned} \tag{74}$$

The corresponding information per unit time $\mathcal{I}_w [x(0 \leq t \leq T)]$ of Eq. 11

$$\begin{aligned} \mathcal{I}_w [x(\cdot)] &\equiv - \frac{\ln(\mathcal{P}_{[w_{..}]} [x(\cdot)])}{T} \\ &= - \frac{1}{T} \sum_{t \in [0, T]: x(t^+) \neq x(t^-)} \ln(w_{x(t^+), x(t^-)}) \\ &\quad - \frac{1}{T} \int_0^T dt w_{x(t), x(t)} \end{aligned} \tag{75}$$

involves only the following empirical time-averaged observables:

- (a) the empirical density

$$\rho_x \equiv \frac{1}{T} \int_0^T dt \delta_{x(t), x} \tag{76}$$

measures the fraction of the time spent by the trajectory $x(0 \leq t \leq T)$ in each configuration x and is normalized to unity

$$\sum_x \rho_x = 1 \tag{77}$$

Its typical value is the steady state P^* of Eq. 66

$$\rho_x^{typ[w]} = P_x^* \tag{78}$$

(b) the empirical flows

$$q_{x,y} \equiv \frac{1}{T} \sum_{t \in [0,T]: x(t^+) \neq x(t^-)} \delta_{x(t^+),x} \delta_{x(t^-),y} \quad (79)$$

represent the density of jumps from y towards $x \neq y$ seen in the trajectory $x(0 \leq t \leq T)$. For large T , these empirical flows satisfy the following stationarity constraints: for any configuration x , the total incoming flow into x is equal to the total outgoing flow out of x (up to boundary terms of order $1/T$ that involve only the initial configuration at $t = 0$ and the final configuration at time $t = T$)

$$\sum_{y \neq x} q_{x,y} = \sum_{y \neq x} q_{y,x} \quad (80)$$

The typical values of the empirical flows are the steady state flows of the master Eq. 66

$$q_{x,y}^{typ[w]} = w_{x,y} P_y^* = w_{x,y} \rho_x^{typ[w]} \quad (81)$$

With respect to the general formalism of Sect. 2, this means that

- (i) the relevant empirical observables E , that determine the trajectories probabilities are the empirical density ρ , and the empirical flows $q_{..}$,

$$E = (\rho; q_{..}) \quad (82)$$

- (ii) their constitutive constraints $C^{[2.5]}(E)$ are given by Eqs. 77 and 80

$$C^{[2.5]}(\rho; q_{..}) = \delta \left(\sum_x \rho_x - 1 \right) \times \prod_x \delta \left(\sum_{y \neq x} q_{x,y} - \sum_{y \neq x} q_{y,x} \right) \quad (83)$$

- (iii) Eq. 75 yields that the information $I_w(E)$ is given by the following linear combination of the empirical observables $E = (\rho; q_{..})$

$$\begin{aligned} I_w(\rho; q_{..}) &= \sum_y \sum_{x \neq y} \left(w_{x,y} \rho_y - q_{x,y} \ln(w_{x,y}) \right) \\ &\equiv \sum_y \rho_y i_y(w) + \sum_y \sum_{x \neq y} q_{x,y} i_{x,y}(w) \end{aligned} \quad (84)$$

The corresponding coefficients that represent their intensive conjugate parameters

$$i_y(w) \equiv \sum_{x \neq y} w_{x,y} = -w_{y,y}$$

$$i_{x,y}(w) \equiv -\ln(w_{x,y}) \quad (85)$$

are very simple in terms of the matrix elements $w_{..}$ of the Markov generator.

3.1.4 Boltzmann intensive entropy $S^{[2.5]}(\rho; q_{..})$ as a function of the empirical observables $E = (\rho; q_{..})$

Eq. 81 yields that the modified Markov generator w^E that would make the empirical observables $E = (\rho; q_{..})$ typical is given by the jump rates for $x \neq y$

$$w_{x,y}^E \equiv \frac{q_{x,y}}{\rho_y} \quad (86)$$

As a consequence, Eq. 20 yields the entropy $S^{[2.5]}(\rho; q_{..})$ as a function of the empirical observables $E = (\rho; q_{..})$ reads using Eqs. 84 and 86

$$\begin{aligned} S^{[2.5]}(\rho; q_{..}) &= I_{w^E}(\rho; q_{..}) \\ &= \sum_y \sum_{x \neq y} \left[q_{x,y} - q_{x,y} \ln \left(\frac{q_{x,y}}{\rho_y} \right) \right] \end{aligned} \quad (87)$$

As stressed after Eq. 23, it is nonlinear with respect to the empirical observables $E = (\rho; q_{..})$.

3.1.5 Rate function at level 2.5 for the empirical observables $E = (\rho; q_{..})$

The joint probability distribution of the empirical density ρ , and the empirical flows $q_{..}$ follows the large deviation form [4, 7–30]

$$P_w^{[2.5]}(\rho; q_{..}) \underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(\rho; q_{..}) e^{-T I_w^{[2.5]}(\rho; q_{..})} \quad (88)$$

where the constitutive constraints $C^{[2.5]}(\rho; q_{..})$ have been written in Eq. 83, while the rate function at Level 2.5 is given by the difference between the information of Eq. 84 and the entropy from Eq. 87

$$\begin{aligned} I_w^{[2.5]}(\rho; q_{..}) &= I_w(\rho; q_{..}) - S^{[2.5]}(\rho; q_{..}) \\ &= \sum_y \sum_{x \neq y} \left[q_{x,y} \ln \left(\frac{q_{x,y}}{w_{x,y} \rho_y} \right) - q_{x,y} + w_{x,y} \rho_y \right] \end{aligned} \quad (89)$$

3.1.6 Kolmogorov–Sinai entropy h_w^{KS}

The Kolmogorov–Sinai entropy h_w^{KS} of Eqs. 40 and 41 reads using the typical values of Eqs. 78 and 81

$$h_w^{KS} = \sum_y P_y^* \sum_{x \neq y} w_{x,y} \left(1 - \ln(w_{x,y}) \right) \quad (90)$$

so that it can be computed whenever the steady state $P^*(y)$ associated to the generator w is known (see [72] for more discussions with examples).

3.2 Microcanonical Ensemble at Level 2.5 with fixed empirical density and flows

3.2.1 Microcanonical Ensemble at Level 2.5 where the empirical density and flows cannot fluctuate for finite T

In the Microcanonical Ensemble of Eq. 44

$$P_{(\rho^*;q_{.,.}^*)}^{Micro[2.5]}(\rho.;q_{.,.}) = \left[\prod_x \delta(\rho_x - \rho_x^*) \right] \left[\prod_y \prod_{x \neq y} \delta(q_{x,y} - q_{x,y}^*) \right] \quad (91)$$

the empirical observables $(\rho.;q_{.,.})$ are fixed to given values $(\rho^*;q_{.,.}^*)$ satisfying the constitutive constraints of Eq. 83

$$C^{[2.5]}(\rho^*;q_{.,.}^*) = \delta\left(\sum_x \rho_x^* - 1\right) \prod_x \delta\left(\sum_{y \neq x} q_{x,y}^* - \sum_{y \neq x} q_{y,x}^*\right) \quad (92)$$

and cannot fluctuate for finite T , in contrast to Eq. 88 in the Canonical Ensemble associated to the Markov generator w .

Here the jump from y towards $x \neq y$ is possible if the corresponding fixed empirical flow is positive $q_{x,y}^* > 0$, while it is impossible if $q_{x,y}^* = 0$.

In particular, the two special cases of Eqs. 68 and 69 mentioned at the end of Sect. 3.1.1 translate into:

- (i) Directed dynamics: for any pair $x \neq y$, the two jumps between them are never both possible

$$\text{Directed: } q_{x,y}^* q_{y,x}^* = 0 \quad (93)$$

- (ii) Undirected dynamics: for any pair $x \neq y$, the two jumps between them are either both possible $q_{x,y}^* q_{y,x}^* > 0$ or both impossible $q_{x,y}^* = q_{y,x}^* = 0$

$$\text{Undirected: } q_{x,y}^* q_{y,x}^* > 0 \quad \text{or} \quad q_{x,y}^* = q_{y,x}^* = 0 \quad (94)$$

- (iii) Equilibrium dynamics: special case of undirected dynamics where on each link $x \neq y$ with possible flows $q_{x,y}^* q_{y,x}^* > 0$, these two empirical flows on each link satisfy the Detailed-Balance condition

$$\text{Detailed Balance: } q_{x,y}^* = q_{y,x}^* \quad (95)$$

3.2.2 Probabilities of trajectories $x(0 \leq t \leq T)$ in the Microcanonical Ensemble

In the Microcanonical Ensemble of Eq. 45, only the trajectories $[x(0 \leq t \leq T)]$ corresponding to the empirical values $(\rho^*;q_{.,.}^*)$ have a non-zero weight, and all these allowed trajectories have the same weight given by the inverse of their number $\Omega_T^{[2.5]}(\rho^*;q_{.,.}^*)$ of Eq. 17

$$\begin{aligned} \mathcal{P}_{(\rho^*;q_{.,.}^*)}^{Micro[2.5]}[x(\cdot)] &= \frac{1}{\Omega_T^{[2.5]}(\rho^*;q_{.,.}^*)} \left[\prod_x \delta(\rho_x^* - \rho_x[x(\cdot)]) \right] \\ &\quad \left[\prod_y \prod_{x \neq y} \delta(q_{x,y}^* - q_{x,y}[x(\cdot)]) \right] \end{aligned} \quad (96)$$

For large T , Eq. 45 reads

$$\begin{aligned} \mathcal{P}_{(\rho^*;q_{.,.}^*)}^{Micro[2.5]}[x(\cdot)]_{T \rightarrow +\infty} &\simeq e^{-T S^{[2.5]}(\rho^*;q_{.,.}^*)} \\ &\quad \left[\prod_x \delta\left(\rho_x^* - \rho_x[x(\cdot)]\right) \right] \left[\prod_y \prod_{x \neq y} \delta\left(q_{x,y}^* - q_{x,y}[x(\cdot)]\right) \right] \end{aligned} \quad (97)$$

with the entropy $S^{[2.5]}(\rho^*;q_{.,.}^*)$ of Eq. 87

$$S^{[2.5]}(\rho^*;q_{.,.}^*) = \sum_y \sum_{x \neq y} \left[q_{x,y}^* - q_{x,y}^* \ln\left(\frac{q_{x,y}^*}{\rho_y^*}\right) \right] \quad (98)$$

3.2.3 Statistics of the subtrajectories on $[0, \tau]$ of the Microcanonical Ensemble trajectories on $[0, T]$ for $1 \ll \tau \ll T$

As explained in details in Sect. 2.2.3, the fact that the Canonical Ensemble emerges to describe the statistics of the subtrajectories is based on the property of Eq. 25 concerning the derivatives of the entropy $S^{[2.5]}(E_n)$ with respect to the empirical observables E_n . For Markov jump processes, the derivatives of the entropy $S^{[2.5]}(\rho.;q_{.,.})$ of Eq. 87 with respect to the empirical density ρ_y and with respect to the empirical flows $q_{x,y}$ can be indeed rewritten in terms of the modified generator w^E of Eq. 86 and correspond to the coefficients of Eq. 85

$$\begin{aligned} \frac{\partial S^{[2.5]}(\rho.;q_{.,.})}{\partial \rho_y} &= \frac{1}{\rho_y} \sum_{x \neq y} q_{x,y} \\ &= \sum_{x \neq y} w_{x,y}^E = -w_{y,y}^E = i_y(w^E) \\ \frac{\partial S^{[2.5]}(\rho.;q_{.,.})}{\partial q_{x,y}} &= -\ln\left(\frac{q_{x,y}}{\rho_y}\right) \end{aligned}$$

$$= -\ln(w_{x,y}^E) = i_{x,y}(w^E) \tag{99}$$

in agreement with the general property of Eq. 25.

3.3 Simple example of continuous-time directed trajectories on a ring: entropies at various levels

The simplest example of continuous-time directed trajectories is based on a ring of L sites with periodic boundary conditions $x + L \equiv x$: the empirical flow $q_{x,y}$ is non-vanishing only for $x = y + 1$

$$q_{x,y} = \delta_{x,y+1} q_{y+1,y} \tag{100}$$

and the stationarity constraints of Eq. 80 yields that the L elements $q_{x+1,x}$ take the same value j along the ring $x = 1, 2, \dots, L$, that represents the current j flowing through each link of the ring

$$q_{x+1,x} = j \tag{101}$$

3.3.1 Number $\Omega_T^{[2.5]}(\rho., j)$ of trajectories with the empirical density $\rho.$ and the current j

Since the empirical flows $q_{..}$ of Eqs. 100 and 101 involve a single positive parameter $j \in [0, +\infty[$, the entropy of Eq. 87 reduces to

$$S^{[2.5]}(\rho.; j) = \sum_{y=1}^L \left[j - j \ln\left(\frac{j}{\rho_y}\right) \right] + j \sum_{y=1}^L \ln(\rho_y) = L[j - j \ln(j)] + j \sum_{y=1}^L \ln(\rho_y) \tag{102}$$

and the number $\Omega_T^{[2.5]}(\rho., j)$ of trajectories reads

$$\Omega_T^{[2.5]}(\rho., j) \underset{T \rightarrow +\infty}{\simeq} \delta\left(\sum_{x=1}^L \rho_x - 1\right) \theta(j) e^{TS^{[2.5]}(\rho., j)} \tag{103}$$

3.3.2 Number $\Omega_T^{[2]}(\rho.)$ of trajectories with the empirical density $\rho.$

The number of trajectories $\Omega_T^{[2]}(\rho.)$ with the empirical density $\rho.$ can be computed via the integration of Eq. 103 over the current j

$$\begin{aligned} \Omega_T^{[2]}(\rho.) &= \int dj \Omega_T^{[2.5]}(\rho., j) \underset{T \rightarrow +\infty}{\simeq} \delta\left(\sum_{x=1}^L \rho_x - 1\right) \\ &\times \int_0^{+\infty} dj e^{TS^{[2.5]}(\rho., j)} \\ &\underset{T \rightarrow +\infty}{\simeq} \delta\left(\sum_{x=1}^L \rho_x - 1\right) e^{TS^{[2]}(\rho.)} \end{aligned} \tag{104}$$

The optimization of the entropy $S^{[2.5]}(\rho., j)$ of Eq. 102 over the current j

$$0 = \frac{\partial S^{[2.5]}(\rho., j)}{\partial j} = -L \ln(j) + \sum_{y=1}^L \ln(\rho_y) \tag{105}$$

leads to the optimal current

$$j^{opt} = e^{\frac{1}{L} \sum_{y=1}^L \ln(\rho_y)} = \left[\prod_{y=1}^L \rho_y \right]^{\frac{1}{L}} \tag{106}$$

that can be plugged into Eq. 102 to obtain the entropy at Level 2 that governs Eq. 104

$$S^{[2]}(\rho.) = S^{[2.5]}(\rho., j^{opt}) = L j^{opt} = L \left[\prod_{y=1}^L \rho_y \right]^{\frac{1}{L}} \tag{107}$$

3.3.3 Number $\Omega_T^{[Current]}(j)$ of trajectories with the empirical current j

The number of trajectories $\Omega_T^{[Current]}(j)$ with the empirical current j can be computed via the integration of Eq. 103 over the empirical density $\rho.$

$$\begin{aligned} \Omega_T^{[Current]}(j) &= \int d\rho. \Omega_T^{[2.5]}(\rho., j) \underset{T \rightarrow +\infty}{\simeq} \theta(j) \\ &\times \int d\rho. \delta\left(\sum_{x=1}^L \rho_x - 1\right) e^{TS^{[2.5]}(\rho., j)} \\ &\underset{T \rightarrow +\infty}{\simeq} \theta(j) e^{TS^{[Current]}(j)} \end{aligned} \tag{108}$$

To optimize the entropy $S^{[2.5]}(\rho., J)$ of Eq. 102 over the empirical density $\rho.$ satisfying the normalization constraint, one introduces the following Lagrangian containing the Lagrange multiplier μ

$$\begin{aligned} \mathcal{L}_j(\rho.) &\equiv S^{[2.5]}(\rho., j) - \mu \left(\sum_{y=1}^L \rho_y - 1 \right) \\ &= L[j - j \ln(j)] + j \sum_{y=1}^L \ln(\rho_y) - \mu \left(\sum_{y=1}^L \rho_y - 1 \right) \end{aligned} \tag{109}$$

The optimization over ρ_y

$$0 = \frac{\partial \mathcal{L}_j(\rho.)}{\partial \rho_y} = \frac{j}{\rho_y} - \mu \tag{110}$$

yields that the optimal density $\rho_y^{opt} = \frac{j}{\mu}$ does not depend on the position y , so that its value is actually

fixed by the normalization constraint

$$\rho_y^{opt} = \frac{1}{L} \tag{111}$$

Plugging this uniform optimal solution into Eq. 102 leads to the entropy $S^{[Current]}(j)$ that governs Eq. 108

$$S^{[Current]}(j) = S^{[2.5]}(\rho_y^{opt}, j) = jL [1 - \ln(jL)] \tag{112}$$

3.3.4 Total number $\Omega_T^{[0]}$ of trajectories

The total number $\Omega_T^{[0]}$ of trajectories can be computed from the integration of Eq. 108 over the current j

$$\Omega_T^{[0]} = \int dj \Omega_T^{[Current]}(j) \underset{T \rightarrow +\infty}{\simeq} \int_0^{+\infty} dj e^{TS^{[Current]}(j)} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[0]}} \tag{113}$$

The optimization of Eq. 112 over the current j

$$0 = \frac{\partial S^{[Current]}(j)}{\partial j} = -L \ln(jL) \tag{114}$$

yields the optimal value

$$j^{opt} = \frac{1}{L} \tag{115}$$

that can be plugged into Eq. 112 to obtain the entropy at Level 0

$$S^{[0]} = S^{[Current]}(j^{opt}) = Lj^{opt} = 1 \tag{116}$$

This simple value can be understood from the integration of the measure on the first line of Eq. 73, where the sums over the positions disappear as a consequence of the one-dimensional directed character of the present model

$$\begin{aligned} \sum_{K=0}^{+\infty} \int_0^T dt_K \int_0^{t_K} dt_{K-1} \dots \int_0^{t_2} dt_1 &= \sum_{K=0}^{+\infty} \frac{1}{K!} \prod_{k=1}^K \left[\int_0^T dt_k \right] \\ &= \sum_{K=0}^{+\infty} \frac{T^K}{K!} = e^T = e^{TS^{[0]}} \end{aligned} \tag{117}$$

in agreement with the entropy found in Eq. 116.

4 Undirected Markov jump processes: explicit entropies at various levels

In this section, we focus on the case of undirected jump processes satisfying Eq. 94, where the contraction of

the entropy at Level 2.5 can be implemented to obtain explicit expressions for many entropies of lower levels.

4.1 Replacing the empirical flows $q_{..}$ by the empirical currents $j_{..}$ and the empirical activities $a_{..}$

On each link $x \neq y$ where the two flows are possible $q_{x,y}q_{y,x} > 0$, it is convenient to choose an order $x > y$ and to introduce the corresponding neighborhood notations N_x^\pm

$$\begin{aligned} \text{Order on each link } q_{x,y}q_{y,x} > 0: \\ x \in N_y^+ \text{ and } y \in N_x^- \end{aligned} \tag{118}$$

while the total neighborhood N_y of y is the reunion of N_y^+ and N_y^- .

The two non-vanishing empirical flows $q_{x,y}$ and $q_{y,x}$ can be replaced by their antisymmetric and symmetric parts called respectively the empirical current $j_{x,y}$ and the empirical activity $a_{x,y}$

$$\begin{aligned} j_{x,y} &= q_{x,y} - q_{y,x} = -j_{y,x} \\ a_{x,y} &= q_{x,y} + q_{y,x} = a_{y,x} \end{aligned} \tag{119}$$

The constitutive constraints of Eq. 83 do not contain the activities $a_{..}$ and are factorized

$$C^{[2.5]}(\rho.; j_{..}) = C^{[2]}(\rho.) C^{statio}(j_{..}) \tag{120}$$

into the normalization constraint for the empirical density ρ .

$$C^{[2]}(\rho.) = \delta \left(\sum_x \rho_x - 1 \right) \tag{121}$$

and into the stationarity constraints for the empirical currents $j_{..}$

$$\begin{aligned} C^{statio}(j_{..}) &= \prod_x \delta \left(\sum_{y \in N_x} j_{x,y} \right) \\ &= \prod_x \delta \left(\sum_{y \in N_x^+} j_{x,y} + \sum_{y \in N_x^-} j_{x,y} \right) \end{aligned} \tag{122}$$

4.2 Number $\Omega_T^{[2.5]}(\rho.; j_{..}; a_{..})$ of trajectories $x(\cdot)$ with the empirical density ρ , currents $j_{..}$ and activities $a_{..}$

Via the change of variables of Eq. 119, the number $\Omega_T^{[2.5]}(\rho.; j_{..}; a_{..})$ of trajectories $x(0 \leq t \leq T)$ with the empirical density ρ , the empirical currents $j_{..}$ and the empirical activities $a_{..}$ is given by

$$\Omega_T^{[2.5]}(\rho; j_{\dots}; a_{\dots}) \underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) C^{statio}(j_{\dots}) e^{TS^{[2.5]}(\rho; j_{\dots}; a_{\dots})} \tag{123}$$

where the constraints have been written in Eqs. 121 and 122, while the entropy $S^{[2.5]}(\rho; j_{\dots}; a_{\dots})$ at Level 2.5 of Eq. 98 becomes using the choice of some ordering $x > y$ on each link (Eq. 118)

$$\begin{aligned} S^{[2.5]}(\rho; j_{\dots}; a_{\dots}) &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y} + j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{2\rho_y} \right) - \frac{a_{x,y} - j_{x,y}}{2} \ln \left(\frac{a_{x,y} - j_{x,y}}{2\rho_x} \right) \right] \\ &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4\rho_x\rho_y} \right) - \frac{j_{x,y}}{2} \ln \left(\frac{(a_{x,y} + j_{x,y})\rho_x}{(a_{x,y} - j_{x,y})\rho_y} \right) \right] \end{aligned} \tag{124}$$

To see more clearly how the entropy $S^{[2.5]}(\rho; j_{\dots}; a_{\dots})$ depends on the empirical currents j_{\dots} , let us rewrite Eq. 124 as a sum

$$S^{[2.5]}(\rho; j_{\dots}; a_{\dots}) = \sum_y \sum_{x \in N_y^+} S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) \tag{125}$$

of the contributions associated to the links $[x, y]$

$$\begin{aligned} S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) &\equiv a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4\rho_x\rho_y} \right) - \frac{j_{x,y}}{2} \ln \left(\frac{(a_{x,y} + j_{x,y})\rho_x}{(a_{x,y} - j_{x,y})\rho_y} \right) \end{aligned} \tag{126}$$

The contribution of the link $[x, y]$ can be decomposed into its even and its odd parts with respect to the link current $j_{x,y}$

$$\begin{aligned} S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) &= S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) + S_{[x,y]odd}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) \end{aligned} \tag{127}$$

The even contribution reads

$$S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y})$$

$$\begin{aligned} &= \frac{S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) + S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; -j_{x,y}; a_{x,y})}{2} \\ &= a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4\rho_x\rho_y} \right) - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \end{aligned} \tag{128}$$

while the odd contribution

$$\begin{aligned} &S_{[x,y]odd}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) \\ &= \frac{S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) - S_{[x,y]}^{[2.5]}(\rho_x; \rho_y; -j_{x,y}; a_{x,y})}{2} \\ &= \frac{j_{x,y}}{2} \ln \left(\frac{\rho_y}{\rho_x} \right) \end{aligned} \tag{129}$$

is simply linear in the current $j_{x,y}$. The sum of all these odd links contributions vanishes as a consequence of the antisymmetry of the current $j_{x,y} = -j_{y,x}$ of Eq. 119 and of the stationarity constraint $C^{statio}(j_{\dots})$ of Eq. 122

$$\begin{aligned} &\sum_y \sum_{x \in N_y^+} S_{[x,y]odd}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) \\ &= \sum_y \sum_{x \in N_y^+} \frac{j_{x,y}}{2} \ln(\rho_y) - \sum_y \sum_{x \in N_y^+} \frac{j_{x,y}}{2} \ln(\rho_x) \\ &= - \sum_x \frac{\ln(\rho_x)}{2} \left[\sum_{y \in N_x^+} j_{x,y} + \sum_{y \in N_x^-} j_{x,y} \right] \\ &= - \sum_x \frac{\ln(\rho_x)}{2} \left[\sum_{y \in N_x} j_{x,y} \right] = 0 \end{aligned} \tag{130}$$

As a consequence, the entropy of Eq. 125 reduces to the sum of the even contributions of the links

$$\begin{aligned} S^{[2.5]}(\rho; j_{\dots}; a_{\dots}) &= \sum_y \sum_{x \in N_y^+} S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y}) \\ &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4\rho_x\rho_y} \right) - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{+} \right) \right] \end{aligned} \tag{131}$$

The physical meaning is that once the empirical density ρ and the empirical activity a_{\dots} are given, any realization of the empirical links currents $j_{x,y}$ that satisfies the stationary constraints of Eq. 122 has the same entropy as the configuration with the reversed empirical link currents $(-j_{x,y})$ that also satisfies the stationary con-

straints

$$S^{[2.5]}(\rho; j_{..}; a_{..}) = S^{[2.5]}(\rho; -j_{..}; a_{..}) \tag{132}$$

4.3 Number $\Omega_T^{[2.25]}(\rho; a_{..})$ of trajectories $x(\cdot)$ with the empirical density ρ , and the empirical activities $a_{..}$.

The number $\Omega_T^{[2.25]}(\rho; a_{..})$ of trajectories $x(0 \leq t \leq T)$ with given empirical density ρ , and given empirical activities $a_{..}$ can be obtained via the integration of Eq. 123 over the currents $j_{..}$.

$$\begin{aligned} \Omega_T^{[2.25]}(\rho; a_{..}) &\equiv \int dj_{..} \Omega_T^{[2.5]}(\rho; j_{..}; a_{..}) \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) \int dj_{..} C^{statio}(j_{..}) \\ &\quad e^{TS^{[2.5]}(\rho; j_{..}; a_{..})} \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) e^{TS^{[2.25]}(\rho; a_{..})} \end{aligned} \tag{133}$$

The behavior of the even link contribution of Eq. 128 with respect to the link current $j_{x,y} \in] - a_{x,y}, + a_{x,y}[$ can be analyzed as follows: the first partial derivative with respect to the current $j_{x,y}$

$$\frac{\partial S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y})}{\partial j_{x,y}} = -\frac{1}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \tag{134}$$

is of the opposite sign of the current $j_{x,y}$, while the second partial derivative remains negative

$$\frac{\partial^2 S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y})}{\partial^2 j_{x,y}} = -\frac{2a_{x,y}}{a_{x,y}^2 - j_{x,y}^2} < 0 \tag{135}$$

Since the link entropy $S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}; a_{x,y})$ is maximal for vanishing current

$$j_{x,y}^{opt} = 0 \tag{136}$$

the conclusion is that, for any given empirical density ρ , and any given empirical activities $a_{..}$, the vanishing of the empirical currents $j_{x,y}^{opt} = 0$ on all the links $[x, y]$ allows to maximize the entropy $S^{[2.5]}(\rho; j_{..}; a_{..})$ of Eq. 131 over the currents, while the stationary constraints of Eq. 122 are trivially satisfied. So the entropy $S^{[2.25]}(\rho; a_{..})$ governing Eq. 133 is given by Eq. 131 with Eq. 128 for vanishing currents $j_{..}^{opt} = 0$

$$\begin{aligned} S^{[2.25]}(\rho; a_{..}) &= S^{[2.5]}(\rho; j_{..}^{opt} = 0; a_{..}) \\ &= \sum_y \sum_{x \in N_y^+} S_{[x,y]even}^{[2.5]}(\rho_x; \rho_y; j_{x,y}^{opt} = 0; a_{x,y}) \end{aligned}$$

$$= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2}{4\rho_x \rho_y} \right) \right] \tag{137}$$

4.4 Number $\Omega_T^{[2.25'] }(\rho; j_{..})$ of trajectories $x(\cdot)$ with the empirical density ρ , and the empirical currents $j_{..}$.

The number $\Omega_T^{[2.25'] }(\rho; j_{..})$ of trajectories $x(0 \leq t \leq T)$ with the given empirical density ρ , and the given empirical currents $j_{..}$ can be obtained from the integration of Eq. 123 over the activities $a_{..}$.

$$\begin{aligned} \Omega_T^{[2.25'] }(\rho; j_{..}) &\equiv \int da_{..} \Omega_T^{[2.5]}(\rho; j_{..}; a_{..}) \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) C^{statio}(j_{..}) \\ &\quad \int da_{..} e^{TS^{[2.5]}(\rho; j_{..}; a_{..})} \\ &\underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) C^{statio}(j_{..}) \\ &\quad e^{TS^{[2.25'] }(\rho; j_{..})} \end{aligned} \tag{138}$$

The maximization of the entropy $S^{[2.5]}(\rho; j_{..}; a_{..})$ of Eq. 131 over $a_{x,y}$

$$0 = \frac{\partial S^{[2.5]}(\rho; j_{..}; a_{..})}{\partial a_{x,y}} = -\frac{1}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4\rho_x \rho_y} \right) \tag{139}$$

leads to the optimal values

$$a_{x,y}^{opt} = \sqrt{j_{x,y}^2 + 4\rho_x \rho_y} \tag{140}$$

that can be plugged into the entropy $S^{[2.5]}(\rho; j_{..}; a_{..})$ of Eq. 131 to obtain the entropy $S^{[2.25'] }(\rho; j_{..})$ at Level 2.25' governing Eq. 138

$$\begin{aligned} S^{[2.25'] }(\rho; j_{..}) &= S^{[2.5]}(\rho; j_{..}; a_{..}^{opt}) \\ &= \sum_y \sum_{x \in N_y^+} \left[\sqrt{j_{x,y}^2 + 4\rho_x \rho_y} \right. \\ &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{\sqrt{j_{x,y}^2 + 4\rho_x \rho_y} + j_{x,y}}{\sqrt{j_{x,y}^2 + 4\rho_x \rho_y} - j_{x,y}} \right) \right] \end{aligned} \tag{141}$$

4.5 Number $\Omega_T^{[2]}(\rho)$ of trajectories $x(\cdot)$ with the empirical density ρ .

The number $\Omega_T^{[2]}(\rho)$ of trajectories $x(\cdot)$ with the empirical density ρ , of Eq. 60 can be computed via the integration of Eq. 133 over the empirical activities a_{\dots} ,

$$\Omega_T^{[2]}(\rho) = \int da_{\dots} \Omega_T^{[2.25]}(\rho; a_{\dots}) \underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) \int da_{\dots} e^{TS^{[2.25]}(\rho; a_{\dots})} \underset{T \rightarrow +\infty}{\simeq} C^{[2]}(\rho) e^{TS^{[2]}(\rho)} \tag{142}$$

The optimization of the entropy $S^{[2.25]}(\rho; a_{\dots})$ of Eq. 137 over the activity $a_{x,y}$

$$0 = \frac{\partial S^{[2.25]}(\rho; a_{\dots})}{\partial a_{x,y}} = -\frac{1}{2} \ln \left(\frac{a_{x,y}^2}{4\rho_x \rho_y} \right) \tag{143}$$

leads to the optimal values

$$a_{x,y}^{opt} = \sqrt{4\rho_x \rho_y} \tag{144}$$

can be plugged into the entropy $S^{[2.25]}(\rho; a_{\dots})$ of Eq. 137 to obtain the explicit entropy $S^{[2]}(\rho)$ at Level 2 governing Eq. 142

$$S^{[2]}(\rho) = S^{[2.25']}(\rho; a_{\dots}^{opt}) = 2 \sum_y \sum_{x \in N_y^+} \sqrt{\rho_x \rho_y} = \sum_y \sum_{x \in N_y} \sqrt{\rho_x \rho_y} \tag{145}$$

This entropy $S^{[2]}(\rho)$ can be also recovered as the optimal value of the entropy $S^{[2.25']}(\rho; j_{\dots})$ of Eq. 141 for the optimal vanishing currents $j_{x,y}^{opt} = 0$

$$S^{[2]}(\rho) = S^{[2.25']}(\rho; j_{\dots}^{opt} = 0) = 2 \sum_y \sum_{x \in N_y^+} [\sqrt{\rho_x \rho_y}] = \sum_y \sum_{x \in N_y} \sqrt{\rho_x \rho_y} \tag{146}$$

4.6 Total number $\Omega_T^{[0]}$ of trajectories $x(\cdot)$

Let us now consider the Level 0 of Eq. 63 via the integration of the explicit Level 2 of Eq. 142 over the empirical density ρ .

$$\Omega_T^{[0]} \equiv \int d\rho C^{[2]}(\rho) e^{TS^{[2]}(\rho)} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[0]}} \tag{147}$$

To optimize the entropy $S^{[2]}(\rho)$ at Level 2 over the empirical density ρ , in the presence of the normalization

constraint $C^{[2]}(\rho)$ of Eq. 121, let us introduce the following Lagrangian containing the Lagrange multiplier μ

$$\mathcal{L}_2(\rho) = S^{[2]}(\rho) - \mu \left(\sum_x \rho_x - 1 \right) = \sum_y \sum_{x \in N_y} \sqrt{\rho_x \rho_y} - \mu \left(\sum_x \rho_x - 1 \right) \tag{148}$$

The optimization over ρ_x

$$0 = \frac{\partial \mathcal{L}_2(\rho)}{\partial \rho_x} = \sum_{y \in N_x} \frac{\sqrt{\rho_y}}{\sqrt{\rho_x}} - \mu \tag{149}$$

can be rewritten as the following eigenvalue equation for the positive eigenvector $\sqrt{\rho}$, of the symmetric neighborhood matrix satisfying $N_{x,y} = 1$ if x and y are neighbors

$$\mu \sqrt{\rho_x} = \sum_{y \in N_x} \sqrt{\rho_y} = \sum_y N_{x,y} \sqrt{\rho_y} \tag{150}$$

while μ is the corresponding highest Perron–Frobenius eigenvalue. The entropy $S^{[0]}$ corresponds to the optimal value of the Lagrangian obtained for the optimal density ρ , satisfying the eigenvalue Eq. 150 and the normalization constraint

$$S^{[0]} = \mathcal{L}_2^{opt} = \sum_y \sqrt{\rho_y} \left[\sum_{x \in N_y} \sqrt{\rho_x} \right] = \sum_y \sqrt{\rho_y} [\mu \sqrt{\rho_y}] = \mu \sum_y \rho_y = \mu \tag{151}$$

The conclusion is that the entropy $S^{[0]}$ reduces to the eigenvalue μ of Eq. 150, so that it will be explicit only when the eigenvalue equation of Eq. 150 can be solved for the symmetric neighborhood matrix N_{\dots} , one is interested in.

Simplest example of the finite regular lattice in dimension d with periodic boundary conditions

The simplest example is the case of a finite regular lattice in dimension d with periodic boundary conditions, where each site has $(2d)$ neighbors: then the eigenvector of Eq. 150 takes the same value on each site, so that the eigenvalue reduces to $\mu = 2d$ and leads to the entropy

$$S^{[0]} = \mu = 2d \tag{152}$$

This simple value can be understood from the integration of the measure on the first line of Eq. 73, where the sums over the K positions x_k simply produce the factor $(2d)^K$

$$\begin{aligned} & \sum_{K=0}^{+\infty} \int_0^T dt_K \int_0^{t_K} dt_{K-1} \dots \int_0^{t_2} dt_1 (2d)^K \\ &= \sum_{K=0}^{+\infty} \frac{(2d)^K}{K!} \prod_{k=1}^K \left[\int_0^T dt_k \right] \\ &= \sum_{K=0}^{+\infty} \frac{(2dT)^K}{K!} = e^{2dT} \end{aligned} \tag{153}$$

in agreement with the entropy of Eq. 152.

4.7 Number $\Omega_T^{[TotalActivity]}(A)$ of trajectories $x(\cdot)$ with a given total activity A

As a simple example of additive observable, let us now consider the total activity

$$A \equiv \sum_y \sum_{x \in N_y^+} a_{x,y} = \sum_y \sum_{x \in N_y} \frac{a_{x,y}}{2} \tag{154}$$

The number $\Omega_T^{[TotalActivity]}(A)$ of trajectories $x(\cdot)$ with a given total activity A can be obtained via the integration of $\Omega_T^{[2.25]}(\rho; a_{\dots})$ of Eq. 133 over the empirical density and the empirical activities with the constraint imposing the value A of Eq. 154

$$\begin{aligned} \Omega_T^{[TotalActivity]}(A) &= \int d\rho. \int da_{\dots} \delta \left(A - \sum_y \sum_{x \in N_y} \frac{a_{x,y}}{2} \right) \\ & \Omega_T^{[2.25]}(\rho; a_{\dots}) \\ & \underset{T \rightarrow +\infty}{\simeq} \int d\rho. \int da_{\dots} \delta \left(\sum_x \rho_x - 1 \right) \delta \left(A - \sum_y \sum_{x \in N_y^+} a_{x,y} \right) \\ & e^{TS^{[2.25]}(\rho; a_{\dots})} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[TotalActivity]}(A)} \end{aligned} \tag{155}$$

To optimize the entropy $S^{[2.25]}(\rho; a_{\dots})$ over the empirical density and the empirical activities in the presence of the two constraints, let us introduce the following Lagrangian with the two Lagrange multipliers (λ, ν)

$$\begin{aligned} \mathcal{L}_A(\rho; a_{\dots}) &= S^{[2.25]}(\rho; a_{\dots}) - \lambda \left(\sum_x \rho_x - 1 \right) \\ & - \nu \left(\sum_y \sum_{x \in N_y^+} a_{x,y} - A \right) \\ &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2}{4\rho_x \rho_y} \right) \right] \\ & - \lambda \left(\sum_x \rho_x - 1 \right) - \nu \left(\sum_y \sum_{x \in N_y^+} a_{x,y} - A \right) \end{aligned} \tag{156}$$

The optimization over ρ_y

$$0 = \frac{\partial \mathcal{L}_A(\rho; a_{\dots})}{\partial \rho_y} = \frac{1}{\rho_y} \sum_{x \in N_y} \frac{a_{x,y}}{2} - \lambda \tag{157}$$

gives

$$\sum_{x \in N_y} \frac{a_{x,y}}{2} = \lambda \rho_y \tag{158}$$

The summation over y yields using the two constraints

$$A = \sum_y \sum_{x \in N_y} \frac{a_{x,y}}{2} = \lambda \sum_y \rho_y = \lambda \tag{159}$$

so that the Lagrange multiplier λ is simply given by the value A of the total activity. The optimization over $a_{x,y}$

$$0 = \frac{\partial \mathcal{L}_A(\rho; a_{\dots})}{\partial a_{x,y}} = -\frac{1}{2} \ln \left(\frac{a_{x,y}^2}{4\rho_x \rho_y} \right) - \nu \tag{160}$$

yields

$$a_{x,y} = 2e^{-\nu} \sqrt{\rho_x \rho_y} \tag{161}$$

that can be plugged into Eq. 158 using $\lambda = A$ of Eq. 159

$$A\rho_y = \sum_{x \in N_y^+} 2e^{-\nu} \sqrt{\rho_x \rho_y} = e^{-\nu} \sqrt{\rho_y} \sum_{x \in N_y} \sqrt{\rho_x} \tag{162}$$

to obtain that the optimal density should satisfy

$$(Ae^\nu) \sqrt{\rho_y} = \sum_{x \in N_y} \sqrt{\rho_x} \tag{163}$$

where one recognizes the eigenvalue problem already discussed in Eq. 150, so that the Lagrange multiplier ν can be rewritten in terms of A and in terms of the eigenvalue $\mu = S^{[0]}$ of Eq. 150

$$\nu = \ln \left(\frac{S^{[0]}}{A} \right) \tag{164}$$

The entropy $S^{[TotalActivity]}(A)$ of Eq. 155 corresponds to the optimal value of the entropy $S^{[2.25]}(\rho; a_{\dots})$

$$\begin{aligned} S^{[TotalActivity]}(A) &= S^{[2.25]}(\rho^{opt}; a_{\dots}^{opt}) = A(1 + \nu) \\ &= A \left[1 + \ln \left(\frac{S^{[0]}}{A} \right) \right] \end{aligned} \tag{165}$$

Simplest example of the finite regular lattice in dimension d with periodic boundary conditions

Let us consider again the simplest case of a finite regular lattice in dimension d with periodic boundary conditions discussed around Eq. 152, so that Eq. 165 becomes

$$S^{[TotalActivity]}(A) = A \left[1 + \ln \left(\frac{2d}{A} \right) \right] \tag{166}$$

This simple entropy function can be understood the number of trajectories $\frac{(2dT)^K}{K!}$ with the total number of jumps $K = TA$ in Eq. 153 using the Stirling formula for the factorial $K! = (TA)!$ for large T

$$\begin{aligned} \frac{(2dT)^{TA}}{(TA)!} &\underset{T \rightarrow +\infty}{\approx} \frac{(2dT)^{TA}}{\left(\frac{TA}{e}\right)^{TA}} = \left(\frac{2de}{A}\right)^{TA} \\ &= e^{TA[1+\ln(\frac{2d}{A})]} = e^{TS^{[TotalActivity]}(A)} \end{aligned} \tag{167}$$

in agreement with the entropy of Eq. 166.

4.8 Number $\Omega_T^{[Flows]}(j_{..}, a_{..})$ of trajectories $x(\cdot)$ with the empirical currents $j_{..}$ and the empirical activities $a_{..}$

The number $\Omega_T^{[Flows]}(j_{..}, a_{..})$ of trajectories $x(\cdot)$ with the empirical currents $j_{..}$ and the empirical activities $a_{..}$ can be obtained via the integration of Eq. 123 over the empirical density ρ .

$$\begin{aligned} \Omega_T^{[Flows]}(j_{..}, a_{..}) &= \int d\rho \Omega_T^{[2.5]}(\rho; j_{..}, a_{..}) \underset{T \rightarrow +\infty}{\approx} \\ &C^{statio}(j_{..}) \int d\rho \delta \left(\sum_x \rho_x - 1 \right) \\ &e^{TS^{[2.5]}(\rho; j_{..}, a_{..})} \\ &\underset{T \rightarrow +\infty}{\approx} C^{statio}(j_{..}) e^{TS^{[Flows]}(j_{..}, a_{..})} \end{aligned} \tag{168}$$

where the entropy of Eq. 131 can be rewritten as

$$\begin{aligned} S^{[2.5]}(\rho; j_{..}, a_{..}) &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4} \right) \right. \\ &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \right] \\ &+ \sum_y \sum_{x \in N_y^+} \frac{a_{x,y}}{2} [\ln(\rho_x) + \ln(\rho_y)] \\ &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4} \right) \right. \\ &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \right] \end{aligned}$$

$$+ \sum_x A_x \ln(\rho_x) \tag{169}$$

where we have introduced the notation

$$A_x \equiv \sum_{y \in N_x} \frac{a_{x,y}}{2} \tag{170}$$

for the activity related to the point x , while the total activity of Eq. 154 studied in the previous subsection corresponds to

$$A = \sum_x \sum_{y \in N_x} \frac{a_{x,y}}{2} = \sum_x A_x \tag{171}$$

To optimize the entropy $S^{[2.5]}(\rho; j_{..}, a_{..})$ over the empirical density ρ , satisfying the normalization constraint, one introduces the following Lagrangian containing the Lagrange multiplier η

$$\begin{aligned} \mathcal{L}_{[j_{..}, a_{..}]}(\rho) &= S^{[2.5]}(\rho; j_{..}, a_{..}) - \eta \left(\sum_x \rho_x - 1 \right) \\ &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4} \right) \right. \\ &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \right] \\ &+ \sum_x A_x \ln(\rho_x) - \eta \left(\sum_x \rho_x - 1 \right) \end{aligned} \tag{172}$$

The optimization over ρ_x

$$0 = \frac{\partial \mathcal{L}_{[j_{..}, a_{..}]}(\rho)}{\partial \rho_x} = \frac{A_x}{\rho_x} - \eta \tag{173}$$

leads to the optimal value

$$\rho_x = \frac{A_x}{\eta} \tag{174}$$

The summation over x yields using the normalization

$$1 = \sum_x \rho_x = \frac{1}{\eta} \sum_x A_x = \frac{A}{\eta} \tag{175}$$

so that the Lagrange multiplier η is simply given by the total activity A .

Plugging the optimal solution

$$\rho_x = \frac{A_x}{A} \tag{176}$$

into $S^{[2.5]}(\rho; j_{..}, a_{..})$ of Eq. 169 yields the entropy $S^{[Flows]}(j_{..}, a_{..})$ governing Eq. 123

$$S^{[Flows]}(j_{..}, a_{..}) = S^{[2.5]}(\rho^{opt}; j_{..}, a_{..})$$

$$\begin{aligned}
 &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4} \right) \right. \\
 &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \right] \\
 &\quad + \sum_y A_y \ln \left(\frac{A_y}{A} \right) \\
 &= \sum_y \sum_{x \in N_y^+} \left[a_{x,y} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}^2 - j_{x,y}^2}{4} \right) \right. \\
 &\quad \left. - \frac{j_{x,y}}{2} \ln \left(\frac{a_{x,y} + j_{x,y}}{a_{x,y} - j_{x,y}} \right) \right] \\
 &\quad + \sum_y \sum_{x \in N_y} \frac{a_{x,y}}{2} \ln \left(\frac{\sum_{z \in N_y} \frac{a_{z,y}}{2}}{\sum_{z'} \sum_{z'' \in N_{z'}} \frac{a_{z',z''}}{2}} \right) \tag{177}
 \end{aligned}$$

where we have replaced A_y and A by their expressions of Eqs. 170 and 171 in terms of the link activities $a_{,..}$.

4.9 Number $\Omega_T^{[Activities]}(a_{,..})$ of trajectories $x(\cdot)$ with the empirical activities $a_{,..}$

The number $\Omega_T^{[Activities]}(a_{,..})$ of trajectories $x(\cdot)$ with the empirical activities $a_{,..}$ can be obtained via the integration of Eq. 168 over the empirical currents $j_{,..}$

$$\begin{aligned}
 \Omega_T^{[Activities]}(a_{,..}) &= \int dj_{,..} \Omega_T^{[Flows]}(j_{,..}, a_{,..}) \Big|_{T \rightarrow +\infty} \simeq \\
 &\int dj_{,..} C^{statio}(j_{,..}) e^{TS^{[Flows]}(j_{,..}; a_{,..})} \\
 &\Big|_{T \rightarrow +\infty} \simeq e^{TS^{[Activities]}(a_{,..})} \tag{178}
 \end{aligned}$$

As in Eq. 136, one obtains that the optimal currents vanish

$$j_{x,y}^{opt} = 0 \tag{179}$$

so that the entropy $S^{[Activities]}(a_{,..})$ is directly obtained from the entropy of Eq. 177

$$\begin{aligned}
 S^{[Activities]}(a_{,..}) &= S^{[Flows]}(j_{,..}^{opt} = 0; a_{,..}) \\
 &= \sum_y \sum_{x \in N_y} \left[\frac{a_{x,y}}{2} - \frac{a_{x,y}}{2} \ln \left(\frac{a_{x,y}}{2} \right) \right] \\
 &\quad + \sum_y \sum_{x \in N_y} \frac{a_{x,y}}{2} \ln \left(\frac{\sum_{z \in N_y} \frac{a_{z,y}}{2}}{\sum_{z'} \sum_{z'' \in N_{z'}} \frac{a_{z',z''}}{2}} \right) \tag{180}
 \end{aligned}$$

5 Conclusions

In this paper, we have revisited the statistical physics of Markov trajectories $x(0 \leq t \leq T)$ via the notion of the Canonical Ensemble at Level 2.5 associated to the Markov generator M and the notion of the Microcanonical Ensemble at Level 2.5 associated to fixed values of all the relevant empirical observables E_n .

We have first explained why the Ensemble of trajectories $x(0 \leq t \leq T)$ produced by the Markov generator M can be considered as 'Canonical':

(C1) The probability of the trajectory $x(0 \leq t \leq T)$ can be rewritten as the exponential of a linear combination of its relevant empirical observables E_n , where the coefficients involving the Markov generator are their fixed conjugate parameters.

(C2) The large deviations properties of these relevant empirical observables E_n for large T are governed by the explicit rate function $I_M^{[2.5]}(E_.)$ at Level 2.5, while in the thermodynamic limit $T = +\infty$, they concentrate on their typical values $E_n^{typ[M]}$ determined by the Markov generator M .

We have then analyzed the properties of the 'Microcanonical Ensemble' at Level 2.5 for stochastic trajectories $x(0 \leq t \leq T)$, where all the relevant empirical variables E_n are fixed to some values E_n^* and cannot fluctuate anymore for finite T :

(MC1) When the long trajectory $x(0 \leq t \leq T)$ belongs to the Microcanonical Ensemble at Level 2.5 with the fixed empirical observables E_n^* , the statistics of its subtrajectory $x(0 \leq t \leq \tau)$ for $1 \ll \tau \ll T$ is governed by the Canonical Ensemble at Level 2.5 associated to the Markov generator M^* that would make the empirical observables E_n^* typical.

(MC2) In the Microcanonical Ensemble at Level 2.5, the central role is played by the number $\Omega_T^{[2.5]}(E^*)$ of stochastic trajectories of duration T with the given empirical observables E_n^* , and by the corresponding explicit Boltzmann entropy $S^{[2.5]}(E^*) = [\ln \Omega_T^{[2.5]}(E^*)] / T$ at Level 2.5.

We have described in detail how this general framework can be applied to continuous-time Markov jump processes and to discrete-time Markov chains, with the simple examples of directed trajectories on a ring. Finally for the special case of undirected Markov jump processes (where the jumps between two configurations are either both possible or both impossible), we have shown how the entropy $S^{[2.5]}(\rho, j_{,..}, a_{,..})$ at Level 2.5 as a function of the empirical density ρ , the empirical currents $j_{,..}$ and the empirical activities $a_{,..}$ can be contracted to obtain the explicit entropies of many other lower levels.

Data availability statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: This manuscript has no associated data (theoretical work).]

Appendix A: application to discrete-time Markov chains

In this Appendix, we describe how the general framework of section 2 can be applied to discrete-time Markov chains in a discrete configuration space.

A.1 Canonical Ensemble of trajectories $x(0 \leq t \leq T)$ associated to a Markov chain generator W

A.1.1 Discrete-time Markov chain converging towards some normalizable steady state

Let us now consider the discrete-time Markov chain dynamics for the probability $P_y(t)$ to be in configuration y at time t

$$P_x(t + 1) = \sum_y W_{x,y} P_y(t) \tag{A1}$$

where the Markov Matrix elements are positive $W_{x,y} \geq 0$ and satisfy the normalization

$$\sum_x W_{x,y} = 1 \tag{A2}$$

The steady-state solution P_x^* of Eq. A1

$$P_x^* = \sum_y W_{x,y} P_y^* \tag{A3}$$

is assumed to be normalizable

$$1 = \sum_y P_y^* \tag{A4}$$

A.1.2 Identification of the relevant empirical observables that determine the trajectories probabilities

The probability of the whole trajectory $x(0 \leq t \leq T)$ starting at the fixed configuration x_0 at time $t = 0$ reads

$$\mathcal{P}[x(0 \leq t \leq T)] = \delta_{x(0),x_0} \left[\prod_{t=1}^T W_{x(t),x(t-1)} \right] \tag{A5}$$

The corresponding information per unit time $\mathcal{I}_W [x(0 \leq t \leq T)]$ of Eq. 11 reads

$$\mathcal{I}_W [x(\cdot)] \equiv -\frac{\mathcal{P}_{[W_{\cdot,\cdot}]} [x(\cdot)]}{T} = -\frac{1}{T} \sum_{t=1}^T \ln (W_{x(t),x(t-1)}) \tag{A6}$$

so that it depends only the empirical time-averaged 2-point density

$$\rho_{x,y} \equiv \frac{1}{T} \sum_{t=1}^T \delta_{x(t),x} \delta_{x(t-1),y} \tag{A7}$$

The empirical 2-point density allows to reconstruct the empirical 1-point density via the summation over the first

or the second index (up to a boundary term of order $1/T$ that is negligible for large time $T \rightarrow +\infty$)

$$\rho_x \equiv \frac{1}{T} \sum_{t=1}^T \delta_{x(t),x} = \sum_y \rho_{x,y} = \sum_y \rho_{y,x} \tag{A8}$$

with the normalization

$$\sum_x \rho_x = 1 \tag{A9}$$

The typical value of the empirical 1-point density is the steady state of Eq. A3

$$\rho_x^{typ[W]} = P_x^* \tag{A10}$$

while the typical value of the empirical 2-point density is given by the steady-state flows of Eq. A3

$$\rho_{x,y}^{typ[W]} = W_{x,y} P_y^* = W_{x,y} \rho_y^{typ[W]} = W_{x,y} \sum_z \rho_{z,y}^{typ[W]} \tag{A11}$$

With respect to the general formalism of Sect. 2, this means that

- (i) the relevant empirical observables E_n that determine the trajectories probabilities are given by the empirical 2-point density $\rho_{x,y}$

$$E. = (\rho_{\cdot,\cdot}) \tag{A12}$$

- (ii) their constitutive constraints $C^{[2.5]}(E.)$ are given by Eqs. A8 and A9

$$C^{[2.5]}(\rho_{\cdot,\cdot}) = \delta \left(\sum_{x,y} \rho_{x,y} - 1 \right) \prod_x \left[\delta \left(\sum_y \rho_{x,y} - \sum_y \rho_{y,x} \right) \right] \tag{A13}$$

- (iii) the information $I_W(E.)$ obtained from Eq. A6 corresponds to the following linear combination of the empirical observables $E. = (\rho_{\cdot,\cdot})$

$$I_W(\rho_{\cdot,\cdot}) = -\sum_{x,y} \rho_{x,y} \ln (W_{x,y}) \equiv \sum_{x,y} \rho_{x,y} i_{x,y}(W) \tag{A14}$$

where the coefficients representing their intensive conjugate parameters

$$i_{x,y}(W) \equiv -\ln (W_{x,y}) \tag{A15}$$

are very simple in terms of the Markov matrix elements $W_{x,y}$.

A.1.3 Boltzmann intensive entropy $S^{[2.5]}(\rho_{\cdot,\cdot})$ as a function of the empirical 2-point density $\rho_{\cdot,\cdot}$.

Eq. A11 yields that the modified Markov matrix W^E that would make the empirical observables $E. = (\rho_{\cdot,\cdot})$ typical is given by

$$W_{x,y}^E \equiv \frac{\rho_{x,y}}{\rho_y} = \frac{\rho_{x,y}}{\sum_z \rho_{z,y}} \tag{A16}$$

As a consequence, Eq. 20 yields that the entropy $S^{[2.5]}(\rho_{\cdot,\cdot})$ as a function of the empirical observables $E_{\cdot} = (\rho_{\cdot,\cdot})$ reads using Eqs. A14 and A16

$$S^{[2.5]}(\rho_{\cdot,\cdot}) = I_{WE}(\rho_{\cdot,\cdot}) = - \sum_{x,y} \rho_{x,y} \ln \left(\frac{\rho_{x,y}}{\rho_y} \right) = - \sum_{x,y} \rho_{x,y} \ln \left(\frac{\rho_{x,y}}{\sum_z \rho_{z,y}} \right) \tag{A17}$$

As stressed after Eq. 23, it is non-linear with respect to the empirical observables $E_{\cdot} = (\rho_{\cdot,\cdot})$.

A.1.4 Rate function $I_W^{[2.5]}(\rho_{\cdot,\cdot})$ at level 2.5 for the empirical observables $E_{\cdot} = (\rho_{\cdot,\cdot})$

For large T , the probability to see the empirical 2-point density $\rho_{\cdot,\cdot}$ follows the large deviation form at Level 2.5 [3–8]

$$P_W^{[2.5]}(\rho_{\cdot,\cdot}) \underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(\rho_{\cdot,\cdot}) e^{-TI_W^{[2.5]}(\rho_{\cdot,\cdot})} \tag{A18}$$

where the constitutive constraints $C(\rho_{\cdot,\cdot})$ have been written in Eq. A13, while the rate function is given by the difference between the information of Eq. A14 and the entropy from Eq. A17

$$I_W^{[2.5]}(\rho_{\cdot,\cdot}; \rho_{\cdot}) = I_W(\rho_{\cdot,\cdot}) - S^{[2.5]}(\rho_{\cdot,\cdot}) = \sum_x \sum_y \rho_{x,y} \ln \left(\frac{\rho_{x,y}}{W_{x,y} \sum_z \rho_{z,y}} \right) \tag{A19}$$

A.1.5 Kolmogorov–Sinai entropy h_W^{KS}

The Kolmogorov–Sinai entropy h_w^{KS} of Eqs. 40 and 41 reads using the typical values of Eq. A11

$$h_W^{KS} = - \sum_{x,y} \rho_{x,y}^{typ[W]} \ln(W_{x,y}) = - \sum_{x,y} W_{x,y} P_y^* \ln(W_{x,y}) \tag{A20}$$

so that it can be thus evaluated whenever the steady state $P^*(y)$ associated to the Markov matrix W is known (see [72] for simple examples in relation with the Ruelle thermodynamic formalism).

A.2 Microcanonical Ensemble at Level 2.5 with fixed empirical 2-point density $\rho_{\cdot,\cdot}^*$

A.2.1 Microcanonical Ensemble at Level 2.5 where the empirical 2-point density $\rho_{\cdot,\cdot}^*$ cannot fluctuate for finite T

In the Microcanonical Ensemble of Eq. 44

$$P_{(\rho_{\cdot,\cdot}^*)}^{Micro[2.5]}(\rho_{\cdot,\cdot}) = \prod_{x,y} \delta(\rho_{x,y} - \rho_{x,y}^*) \tag{A21}$$

the empirical 2-point density $\rho_{\cdot,\cdot}$ is fixed to $\rho_{\cdot,\cdot}^*$ satisfying the constitutive constraints of Eq. A13

$$C^{[2.5]}(\rho_{\cdot,\cdot}^*) = \delta \left(\sum_{x,y} \rho_{x,y}^* - 1 \right) \prod_x \left[\delta \left(\sum_y \rho_{x,y}^* - \sum_y \rho_{y,x}^* \right) \right] \tag{A22}$$

and cannot fluctuate for finite T , in contrast to Eq. A18 concerning the Level 2.5 in the Canonical Ensemble associated to the Markov matrix W .

A.2.2 Probabilities of trajectories $x(0 \leq t \leq T)$ in the Microcanonical Ensemble

In the Microcanonical Ensemble of Eq. 45, only the trajectories $[x(0 \leq t \leq T)]$ corresponding to the empirical 2-point density $\rho_{\cdot,\cdot}^*$ have a non-zero weight, and all these allowed trajectories have the same weight given by the inverse of their number $\Omega_T^{[2.5]}(\rho_{\cdot,\cdot}^*)$ of Eq. 17

$$\mathcal{P}_{(\rho_{\cdot,\cdot}^*)}^{Micro[2.5]}[x(\cdot)] = \frac{1}{\Omega_T^{[2.5]}(\rho_{\cdot,\cdot}^*)} \prod_{x,y} \delta(\rho_{x,y}^* - \rho_{x,y}[x(\cdot)]) \tag{A23}$$

For large T , Eq. 45 reads

$$\mathcal{P}_{(\rho_{\cdot,\cdot}^*)}^{Micro[2.5]}[x(\cdot)] \underset{T \rightarrow +\infty}{\simeq} e^{-TS^{[2.5]}(\rho_{\cdot,\cdot}^*)} \prod_{x,y} \delta(\rho_{x,y}^* - \rho_{x,y}[x(\cdot)]) \tag{A24}$$

with the entropy $S^{[2.5]}(\rho_{\cdot,\cdot}^*)$ of Eq. A17

$$S^{[2.5]}(\rho_{\cdot,\cdot}^*) = - \sum_{x,y} \rho_{x,y}^* \ln \left(\frac{\rho_{x,y}^*}{\sum_z \rho_{z,y}^*} \right) \tag{A25}$$

A.2.3 Statistics of the subtrajectories on $[0, \tau]$ of the Microcanonical Ensemble trajectories on $[0, T]$ for $1 \ll \tau \ll T$

As explained in details in Sect. 2.2.3, the fact that the Canonical Ensemble emerges to describe the statistics of the subtrajectories is based on the property of Eq. 25 concerning the derivatives of the entropy $S^{[2.5]}(E_{\cdot})$ with respect to the empirical observables E_n .

For Markov chains, the derivative of the entropy $S^{[2.5]}(\rho_{\cdot,\cdot})$ of Eq. A17 with respect to the empirical 2-point density $\rho_{x,y}$ indeed involves the coefficients $i_{x,y}(W^E)$ of Eq. A15 associated to the modified Markov matrix $W_{x,y}^E$ of Eq. A16

$$\frac{\partial S^{[2.5]}(\rho_{\cdot,\cdot})}{\partial \rho_{x,y}} = - \ln \left(\frac{\rho_{x,y}}{\sum_z \rho_{z,y}} \right) - 1 + 1 = - \ln \left(\frac{\rho_{x,y}}{\sum_z \rho_{z,y}} \right) = - \ln(W_{x,y}^E) = i_{x,y}(W^E) \tag{A26}$$

in agreement with the general property of Eq. 25.

A.3 Simple example of discrete-time directed trajectories on a ring: entropies at various levels

The simplest example of directed trajectories is based on a ring of L sites with periodic boundary conditions $x + L \equiv x$: when the particle is on site y at time t , it can either jump to the right neighbor ($y + 1$) or it remains on site y , so that

the empirical 2-point density $\rho_{x,y}$ is non-vanishing only for $x = y$ and $x = y + 1$

$$\rho_{x,y} = \delta_{x,y}\rho_{y,y} + \delta_{x,y+1}\rho_{y+1,y} \tag{A27}$$

A.3.1 Parametrization of the 2-point empirical density ρ_{\dots} in terms of the 1-point density ρ_x and of the global current J

The empirical 1-point density ρ_x can be computed from the empirical 2-point density $\rho_{x,y}$ of Eq. A27 via the two possible sums of Eq. A8

$$\begin{aligned} \rho_x &= \sum_y \rho_{x,y} = \rho_{x,x} + \rho_{x,x-1} \\ \rho_x &= \sum_y \rho_{y,x} = \rho_{x,x} + \rho_{x+1,x} \end{aligned} \tag{A28}$$

The compatibility between the two equations yields that the L elements $\rho_{x+1,x}$ take the same value J along the ring $x = 1, 2, \dots, L$, that represents the current J flowing through each link of the ring

$$\rho_{x+1,x} = J \tag{A29}$$

The remaining diagonal elements $\rho_{x,x}$ can be then computed from the 1-point density ρ_x and the current J via Eq. A28

$$\rho_{x,x} = \rho_x - J \tag{A30}$$

In summary, the 2-point empirical density of Eq. A27 is now parametrized by

$$\rho_{x,y} = \delta_{x,y}(\rho_x - J) + \delta_{x,y+1}J \tag{A31}$$

where the current J should be positive $J \geq 0$ and smaller $J \leq \rho_x$ than the empirical density ρ_x for any $x = 1, \dots, L$. In summary, the remaining constitutive constraints read

$$C^{[2.5]}(\rho, J) = \delta\left(\sum_{x=1}^L \rho_x - 1\right) \theta(J) \left[\prod_{x=1}^L \theta(\rho_x - J)\right] \tag{A32}$$

A.3.2 Number of Trajectories $\Omega_T^{[2.5]}(\rho, J)$ with the empirical density ρ_x and the current J

Via the parametrization of Eq. A31, the entropy of Eq. A17 reduces to

$$\begin{aligned} S^{[2.5]}(\rho, J) &= \sum_{x=1}^L \left[-(\rho_x - J) \ln\left(\frac{\rho_x - J}{\rho_x}\right) - J \ln\left(\frac{J}{\rho_x}\right) \right] \\ &= \sum_{x=1}^L \left[-\rho_x \ln\left(\frac{\rho_x - J}{\rho_x}\right) + J \ln\left(\frac{\rho_x - J}{J}\right) \right] \end{aligned} \tag{A33}$$

and the number of trajectories $\Omega_T^{[2.5]}(\rho, J)$ reads

$$\Omega_T^{[2.5]}(\rho, J) \underset{T \rightarrow +\infty}{\simeq} C^{[2.5]}(\rho, J) e^{TS^{[2.5]}(\rho, J)} \tag{A34}$$

A.3.3 Number of Trajectories $\Omega_T^{[2]}(\rho)$ with the empirical density ρ .

The number of trajectories $\Omega_T^{[2]}(\rho)$ with the empirical density ρ can be obtained via the integration of Eq. A34 over the current J

$$\begin{aligned} \Omega_T^{[2]}(\rho) &= \int dJ \Omega_T^{[2.5]}(\rho, J) \underset{T \rightarrow +\infty}{\simeq} \delta\left(\sum_{x=1}^L \rho_x - 1\right) \\ &\int_0^{+\infty} dJ \left[\prod_{x=1}^L \theta(\rho_x - J) \right] e^{TS^{[2.5]}(\rho, J)} \\ &\underset{T \rightarrow +\infty}{\simeq} \delta\left(\sum_{x=1}^L \rho_x - 1\right) e^{TS^{[2]}(\rho)} \end{aligned} \tag{A35}$$

The optimization of the entropy $S^{[2.5]}(\rho, J)$ at Level 2.5 over the current J

$$0 = \frac{\partial S^{[2.5]}(\rho, J)}{\partial J} = \sum_{x=1}^L \ln\left(\frac{\rho_x - J}{J}\right) = \ln\left[\prod_{x=1}^L \left(\frac{\rho_x - J}{J}\right)\right] \tag{A36}$$

yields that the optimal current $J^{opt} = J^{opt}[\rho]$ as a function of the given empirical density ρ is given by the solution of

$$1 = \prod_{x=1}^L \left(\frac{\rho_x - J^{opt}}{J^{opt}}\right) \tag{A37}$$

It should be plugged into the entropy at Level 2.5 to obtain the entropy at Level 2

$$S^{[2]}(\rho) = S^{[2.5]}(\rho, J^{opt}[\rho]) = -\sum_{x=1}^L \rho_x \ln\left(\frac{\rho_x - J^{opt}[\rho]}{\rho_x}\right) \tag{A38}$$

A.3.4 Number of Trajectories $\Omega_T^{[Current]}(J)$ with the empirical current J

The number of trajectories $\Omega_T^{[Current]}(J)$ with the empirical current J can be obtained via the integration of Eq. A34 over the empirical density ρ .

$$\begin{aligned} \Omega_T^{[Current]}(J) &= \int d\rho \Omega_T^{[2.5]}(\rho, J) \underset{T \rightarrow +\infty}{\simeq} \theta(J) \\ &\int d\rho \delta\left(\sum_{x=1}^L \rho_x - 1\right) \left[\prod_{x=1}^L \theta(\rho_x - J)\right] \\ &e^{TS^{[2.5]}(\rho, J)} \end{aligned} \tag{A39}$$

To optimize the entropy $S^{[2.5]}(\rho, J)$ over the empirical density ρ satisfying the normalization constraint, one introduces the following Lagrangian containing the Lagrange multiplier μ

$$\begin{aligned} \mathcal{L}_J(\rho) &\equiv S^{[2.5]}(\rho, J) - \mu \left(\sum_{x=1}^L \rho_x - 1\right) \\ &= \sum_{x=1}^L \left[-\rho_x \ln\left(\frac{\rho_x - J}{\rho_x}\right) + J \ln\left(\frac{\rho_x - J}{J}\right) \right] \end{aligned}$$

$$-\mu \left(\sum_{x=1}^L \rho_x - 1 \right) \tag{A40}$$

The optimization over ρ_x

$$0 = \frac{\partial \mathcal{L}_J(\rho.)}{\partial \rho_x} = -\ln \left(\frac{\rho_x - J}{\rho_x} \right) - \mu \tag{A41}$$

yields that the optimal density ρ_x^{opt} is a function of J and μ , so that it does not depend on the position x , and its value is thus fixed by the normalization constraint

$$\rho_x^{opt} = \frac{1}{L} \tag{A42}$$

that can be plugged into the entropy at Level 2.5 to obtain the entropy $S^{[Current]}(J)$ for the current alone

$$\begin{aligned} S^{[Current]}(J) &= S^{[2.5]}(\rho^{opt}, J) \\ &= -(1 - LJ) \ln(1 - LJ) - LJ \ln(LJ) \end{aligned} \tag{A43}$$

that governs Eq. A39

$$\begin{aligned} \Omega_T^{[Current]}(J) &= \int d\rho \Omega_T^{[2.5]}(\rho., J) \underset{T \rightarrow +\infty}{\simeq} \theta(J)\theta\left(\frac{1}{L} - J\right) \\ &e^{TS^{[Current]}(J)} \end{aligned} \tag{A44}$$

A.3.5 Total number of Trajectories $\Omega_T^{[0]}$ at Level 0

The total number $\Omega_T^{[0]}$ of trajectories can be obtained from the integration of Eq. A44 over the current J

$$\begin{aligned} \Omega_T^{[0]} &= \int dJ \Omega_T^{[Current]}(J) \underset{T \rightarrow +\infty}{\simeq} \\ &\int_0^{\frac{1}{L}} dJ e^{TS^{[Current]}(J)} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[0]}} \end{aligned} \tag{A45}$$

The optimization of the entropy $S^{[Current]}(J)$ of Eq. A43 over the current J

$$0 = \frac{\partial S^{[Current]}(J)}{\partial J} = L \ln \left(\frac{1 - LJ}{LJ} \right) \tag{A46}$$

yields the optimal value

$$J^{opt} = \frac{1}{2L} \tag{A47}$$

that can be plugged into the entropy $S^{[Current]}(J)$ of Eq. A43 to obtain the entropy at Level 0

$$S^{[0]} = S^{[Current]}(J^{opt}) = \ln 2 \tag{A48}$$

i.e. one recovers that the number of trajectories of Eq. A45 is simply

$$\Omega_T^{[0]} \underset{T \rightarrow +\infty}{\simeq} e^{TS^{[0]}} = e^{T \ln 2} = 2^T \tag{A49}$$

as it should.

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