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# Local detailed balance: a microscopic derivation

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## Abstract

Thermal contact is the archetype of non-equilibrium processes driven by constant non-equilibrium constraints when the latter are enforced by reservoirs exchanging conserved microscopic quantities. At a mesoscopic scale only the energies of the macroscopic bodies are accessible together with the configurations of the contact system. We consider a class of models where the contact system, as well as macroscopic bodies, have a finite number of possible configurations. The global system, with only discrete degrees of freedom, has no microscopic Hamiltonian dynamics, but it is shown that, if the microscopic dynamics is assumed to be deterministic and ergodic and to conserve energy according to some specific pattern, and if the mesoscopic evolution of the global system is approximated by a Markov process as closely as possible, then the mesoscopic transition rates obey three constraints. In the limit where macroscopic bodies can be considered as reservoirs at thermodynamic equilibrium (but with different intensive parameters), the mesoscopic transition rates turn into transition rates for the contact system and the third constraint becomes local detailed balance; the latter is generically expressed in terms of the microscopic exchange entropy variation, namely the opposite of the variation of the thermodynamic entropy of the reservoir involved in a given microscopic jump of the contact system configuration. For a finite-time evolution after contact has been switched on, we derive a fluctuation relation for the joint probability of the heat amounts received from the various reservoirs. The generalization to systems exchanging energy, volume and matter with several reservoirs, with a possible conservative external force acting on the contact system, is given explicitly.

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## 1. Introduction

An archetype of the spontaneous irreversible processes that occur when two macroscopic bodies prepared in equilibrium states with different intensive parameters are brought together is thermal contact. The simplest physical situation is when two bodies  $B_1$  and  $B_2$  initially at equilibrium at different temperatures are set into contact through a diathermal incompressible interface that can be either immaterial, the common boundary of the two solid bodies, or a very thin material wall between the two bodies that may be solids or fluids.

First we recall known results valid under the assumption that the energy of the interactions through the interface is negligible. At a macroscopic level, the laws of thermodynamics [1] predict that in the infinite time limit the isolated global system reaches an equilibrium state where the total thermodynamic entropy  $S_{\text{tot}}^{\text{TH}} = S_1^{\text{TH}} + S_2^{\text{TH}}$  is maximum with respect to any variation of the internal energies  $U_a$  ( $a = 1, 2$ ) at fixed total internal energy<sup>4</sup>  $U_{\text{tot}} = U_1 + U_2$ . The maximization condition upon  $S_{\text{tot}}^{\text{TH}}$  entails that the final inverse thermodynamic temperatures, defined<sup>5</sup> as  $\beta_a \equiv \partial S_a^{\text{TH}} / \partial U_a$ , are equal, and that the heat capacity of every macroscopic body at constant volume is positive. As a consequence, the net heat transfer that leads to equilibrium flows from the hotter body to the colder one. Recently the fluctuations of the heat transfer  $Q_2$  from body  $B_2$  towards body  $B_1$  when thermal contact is set on during a finite time  $t$  have been shown to obey a fluctuation relation [2]: under the assumption that only values of heat amounts  $Q_2$  that are far larger than the interaction energy through the interface are considered, the probabilities of measuring either a value  $Q_2$  or its opposite are linked by  $P(Q_2; t) = \exp[(\beta_1 - \beta_2)Q_2]P(-Q_2; t)$ . The latter relation implies that  $(\beta_1 - \beta_2)\langle Q_2 \rangle \geq 0$ , in agreement with the laws of thermodynamics.

In the present paper we consider the fluctuations of heat exchanges when the interaction energy  $\mathcal{E}$  through the interface between the two macroscopic bodies is taken into account. We begin by stating our *basic assumptions*.

- (i) The contact system  $S$  has a finite number of configurations  $C$ , so that its energies  $\mathcal{E}(C)$  are discretized and bounded.
- (ii) The system  $S$  has no internal dynamics (an expression of its thinness) and its configurations can change only thanks to interactions with the macroscopic bodies  $B_a$ s, which also have discrete degrees of freedom and which make the populations in energy levels of  $S$  vary<sup>6</sup>.
- (iii) We take it as the definition of the interface that  $B_a$ s do not interact directly with one another and we add the physically motivated assumption that no degree of freedom in the interface interacts directly with several  $B_a$ s.

<sup>4</sup> This property can be retrieved in the framework of equilibrium statistical mechanics, where the thermodynamic entropy  $S_{\text{tot}}^{\text{TH}}$  corresponds to the thermodynamic limit of the Boltzmann entropy  $S_{\text{tot}}^B$  and the equilibrium fluctuations of the energies in the two bodies are described by the microcanonical probability distribution.

<sup>5</sup> In the whole paper the Boltzmann constant  $k_B$  is set equal to 1, the inverse temperature reads  $1/T \equiv \beta$  and  $S$  denotes a dimensionless entropy.

<sup>6</sup> This is not the case for models that are aimed at studying how Fourier law arises when the system that settles thermal contact has a macroscopic width or length and when the degrees of freedom that are not in contact with the heat sources evolve under a deterministic energy-conserving microscopic dynamics.

- (iv) Discrete degrees of freedom cannot have Hamiltonian evolution but we assume that the dynamics of the global system is ergodic and energy preserving. In a given energy level all ergodic microscopic dynamics have the same period.

We call coarse graining the procedure that goes from a microscopic description of all the degrees of freedom of the global system to a description only of the energies  $E_a$  of the macroscopic bodies  $B_a$  and the configuration  $C$  of the system  $S$ . We call  $(C, E_1, E_2)$  a mesoscopic configuration. An immediate consequence of (iv) is that in a coarse grained description the ‘probability’ of a mesoscopic configuration  $(C, E_1, E_2)$  calculated as a time average over a period of microscopic dynamics coincides with the microcanonical probability distribution  $P_{\text{mc}}(C, E_1, E_2)$ .

The main results of the paper are the following.

–*First*, using our assumptions, in particular (iv), we show that, during a period of microscopic dynamics, the number of deterministic jumps that occur from one mesoscopic configuration of the global system to another one is equal to the number of jumps in the opposite sense.

–*Second*, we show that if the mesoscopic dynamics is replaced by the effective Markov process with the same one- and two-body ergodic averages, its transition rates between mesoscopic configurations  $(C, E_1, E_2)$  satisfy

- (1) *irreducibility* (i.e. the graph associated with the Markov process is connected)
- (2) *microreversibility* (i.e. a transition and its inverse are either both allowed or both forbidden)
- (3) the *microcanonical detailed balance* with the extra restriction that a single macroscopic body is involved in the transition and its inverse (see (2.11)).

We notice that the three properties ensure that in the infinite-time limit the stochastic evolution does lead to a unique stationary state, which coincides with the microcanonical probability distribution  $P_{\text{mc}}(C, E_1, E_2)$ .

As larger and larger macroscopic bodies are considered, one can identify longer and longer time windows during which they can be considered as being in an equilibrium state, i.e. their thermodynamic entropies are well defined and their temperatures are constant (but different in general) over the whole time window. In this regime, a Markov dynamics for the system  $S$  emerges, the irreducibility and microreversibility conditions are preserved and the mesoscopic microcanonical detailed balance for transitions among  $(C, E_1, E_2)$  turns into the so-called ‘local’ detailed balance<sup>7</sup> for transitions among  $C$ ’s (see (2.19)). The latter has been often used in the literature as a basic assumption in the description of the stochastic evolution of a system under energy exchanges with several thermostats at different temperatures (see the comments below).

–*Third*, we use the local detailed balance to exhibit an exact finite time fluctuation relation for the joint probability distribution of the heat amounts received by the interface system  $S$  from both macroscopic bodies in a protocol where thermal contact is set on at the initial time (see the text before (1.1)).

–*Fourth*, we show how the above considerations generalize to cases when not only energy but also particles and/or volume are exchanged among macroscopic bodies via an interface. The number of states of the interface (and in particular, the energies and/or particle

<sup>7</sup> Nowadays the denomination ‘local’ detailed balance seems to be the standard one used in the literature for discrete state systems driven out of equilibrium under various kinds of external constant conditions (see below). In the present thermal contact setting, the term ‘local’ may be viewed as referring to the local interaction between the contact system and each energy reservoir, but the denomination ‘generalized’ detailed balance is also to be found in [3].

contents and/or volumes it can have) are still assumed to be finite. The case where a conservative external force acts on some global coordinate of the contact system is included in the description.

A slightly extended description will allow us to situate our work in the already available literature.

The issue of how to get a valuable model of thermal contact can also be addressed not by assuming some properties for the microscopic dynamics but by imposing some constraints directly upon the mesoscopic transition rates in order to ensure that the stochastic evolution of the global system does lead to equilibrium in the infinite-time limit<sup>8</sup>. The uniqueness of the stationary state is guaranteed if the transition rates obey the irreducibility and micro-reversibility conditions, and it coincides with a prescribed equilibrium state if the transition rates obey the detailed balance with the corresponding equilibrium probability distribution. In the case of thermal contact, the latter distribution is the microcanonical probability  $P_{\text{mc}}(C, E_1, E_2)$ , and this approach is to be found in [3]. However, we stress that, because of the interaction pattern, the microcanonical detailed balance (2.11) arising in our derivation from the properties of the microscopic dynamics involves in fact only a single macroscopic body at a time, as explicitly written in (2.13).

As for the local detailed balance (2.19) for thermal contact, valid in the regime where the macroscopic bodies remain at equilibrium, some derivations from the existence of an underlying Hamiltonian microscopic dynamics invariant under time reversal can be found in the literature. In particular there are some similarities between our microscopic approach and the derivation by Maes and Netocny [5], who use (albeit in a different order, in the context of Hamiltonian dynamics and using time reversal) coarse graining, and, after postulating that the macroscopic bodies are in steady states, a Markovian approximation. They also use a prescription analogous to the interaction pattern for our jump dynamics, since the reservoirs are assumed to be spatially separated, each being in contact only with the system. This spatial separation and local coupling to the system ensures that the variations of the reservoir variables are determined only by the variations of the system variables [6]. In fact, this fundamental property of the contact setting has also been used in an earlier derivation of the local detailed balance in [7]<sup>9</sup>.

As for the generalization of the microscopic derivation of the local detailed balance to processes where the underlying microscopic dynamics allows exchanges of various microscopically conserved quantities (energy and/or matter and/or volume), the key observation is the following. Once the mesoscopic microcanonical detailed balance (4.1), with the constraint that only one macroscopic body is involved in a given configuration jump of the interface  $S$ , has been derived then, as already pointed out in [3], its replacement by the local detailed balance in the regime where macroscopic bodies behave as reservoirs in different thermodynamical equilibrium states corresponds to the replacement of the variation of the Boltzmann entropy of the macroscopic body involved in the configuration jump by the variation of its thermodynamic entropy at fixed intensive parameters.

<sup>8</sup> The latter point of view is that used by Glauber in his investigation of the time-dependent statistics of the Ising spin chain when spin flips are supposed to be generated by energy exchanges with a thermostat at the inverse temperature  $\beta$ : he imposes that in the infinite-time limit, the corresponding stochastic dynamics leads to the canonical equilibrium probability at inverse temperature  $\beta$  with the Ising Hamiltonian [4].

<sup>9</sup> In [7], the transition rates appear in a stochastic integral term that is added to the Liouville equation for the Hamiltonian evolution of the probability distribution of the small system in its phase space. The stochastic term is intended to mimic the effect of the instantaneous elastic collisions between the small system and the degrees of freedom of reservoirs that have a canonical equilibrium probability distribution. The argument relies on the assumption of the absence of correlation before a collision and on the time reversal invariance of both the collision process and the Hamiltonian evolution of the system when it is isolated.

Therefore the local detailed balance can be expressed in a generic way (see (2.26)) in terms of the exchange entropy variation<sup>10</sup>  $\delta_{\text{exch}} S(C' \leftarrow C)$  associated with a jump of the small system from a microscopic configuration  $C$  to another one  $C'$ , which is defined as the opposite of the infinitesimal variation of the thermodynamic entropy of the reservoir  $\mathcal{B}_a$  that causes the jump of configuration from  $C$  to  $C'$  by exchanging energy and/or volume and/or matter with the system  $S$ . Its explicit expression is given in (4.6) with some comments about its physical content. It may involve a conservative force acting on the system. In fact the local detailed balance has been used in various specific forms: for instance for the description of exchanges of particles (energy quanta) with two particle (energy) reservoirs at different chemical potentials (temperatures) at the boundaries of a one-dimensional lattice where particles move stochastically according to the rules of the symmetric simple exclusion process [8], or for coupled exchanges of energy and particles in molecular motor models (see, among others, [9–11]). The present derivation allows us to describe a mobile thin diathermal wall (with a possible conservative force acting on it) separating a vessel in two parts filled with gases at different temperatures and pressures.

We notice that for another class of non-equilibrium processes driven by constant external constraints, namely particle currents driven by a constant non-conservative force acting on particles in contact with a single heat bath (for instance interacting particles moving stochastically on a ring in some uniform field), the issue of a microscopic derivation of the corresponding local detailed balance assumed in [12] has been addressed in [13]. Then the local detailed balance has the same form as a canonical detailed balance, but the stationary state is not the canonical equilibrium state because of the periodic boundary conditions.

We consider the following protocol for thermal contact: the system  $S$  is a thin piece of material prepared at inverse temperature  $\beta_0$ , and at the initial time of measurements it is inserted between two macroscopic bodies at equilibrium at different inverse temperatures  $\beta_1$  and  $\beta_2$  (and that remain in their equilibrium state during the whole protocol). Then the transition rates of the stochastic evolution of  $S$  satisfy the local detailed balance and the joint probability of the heats  $Q_1$  and  $Q_2$  received by  $S$  from both macroscopic bodies during a time  $t$  after contact has been set on is shown to obey relation (3.16). The exchange entropy variation associated with the heats  $Q_1$  and  $Q_2$  received by  $S$  from both thermostats reads  $\Delta_{\text{exch}} S(Q_1, Q_2) = \beta_1 Q_1 + \beta_2 Q_2$ , and the detailed fluctuation relation can be written more explicitly as

$$\frac{P(Q_1, Q_2; t)}{P(-Q_1, -Q_2; t)} = e^{(\beta_0 - \beta_1)Q_1 + (\beta_0 - \beta_2)Q_2}. \quad (1.1)$$

It has been checked in a solvable model for thermal contact [14]. Moreover the corresponding integral fluctuation relation,  $\langle \exp [(\beta_1 - \beta_0)Q_1 + (\beta_2 - \beta_0)Q_2] \rangle = 1$ , where  $\langle \dots \rangle$  denotes an expectation value when the experiment is repeated a large number of times, entails through Jensen's inequality that the mean heat amounts that are exchanged from the initial time where the thermal contact is set on must satisfy

$$(\beta_0 - \beta_1)\langle Q_1(t) \rangle + (\beta_0 - \beta_2)\langle Q_2(t) \rangle \geq 0. \quad (1.2)$$

In fact, by conservation of energy,  $\langle Q_1(t) \rangle + \langle Q_2(t) \rangle$  is equal to the difference between the mean energies of the system  $\langle \mathcal{E} \rangle_t - \langle \mathcal{E} \rangle_{t=0}$ , and the inequality (1.2) also reads  $(\beta_1 - \beta_2)\langle Q_2(t) \rangle \geq (\beta_1 - \beta_0)[\langle \mathcal{E} \rangle_t - \langle \mathcal{E} \rangle_{t=0}]$ . We notice that the fluctuation relation (1.1) is compatible with the relation quoted at the beginning of the introduction and derived in [2]

<sup>10</sup> Exchange entropy variation is an abbreviation for ‘variation of entropy due to exchanges’ of energy with a thermal bath, or more generally, of some measurable conserved quantities with various reservoirs.

for a similar protocol: in the latter no material contact system  $S$  is inserted between the macroscopic bodies, but the global system is assumed to have an underlying microscopic Hamiltonian dynamics (invariant under time reversal) whose Hamiltonian contains an interaction term only when the two macroscopic bodies are in contact. (The remarks in subsection 2.1 sustain the analogy between both protocols). The initial equilibrium states of the macroscopic bodies are described in the canonical ensemble, no assumption is made about the evolution of the temperatures of the macroscopic bodies, and only heat amounts that are far larger than the variation of the interaction energy through the interface between the initial and final times of contact are considered, which in our setting is equivalent to considering only values  $|Q_2| \gg |\langle \mathcal{E} \rangle_t - \langle \mathcal{E} \rangle_{t=0}|$ .

For the larger class of models where reservoirs exchange microscopically conserved quantities and for which the microscopic derivation of the local detailed balance can be performed, the exchange entropy variation along a history of the system,  $\Delta_{\text{exch}} S$ , is the crucial quantity at the root of the fluctuation relations (4.12) and (4.13), which are generalizations of the pure thermal contact relations (3.16) and (3.17), respectively. The protocol for setting contact is such that the latter relations, as well as the exchange entropy variation  $\Delta_{\text{exch}} S$ , are expressed only in terms of the quantities that are exchanged between the interface and every reservoir and on the intensive equilibrium parameters of the reservoirs. All these quantities are experimentally measurable quantities. On the contrary, the probability distribution of the system configurations is very hard to determine from experiments. We recall that the probability distribution of the system configurations is involved in the variation of the system Shannon–Gibbs entropy, which appeared in the seminal works by Crooks [15–17] and has led to the notion of entropy production along a stochastic trajectory of the system microscopic configurations (see [18, 19]).

Finally we point out that the action functional introduced by Lebowitz and Spohn [20] in terms of the transition rates of a Markov process satisfying only the irreducibility constraint (2.17) and the microreversibility constraints (2.18) coincides with the opposite of the exchange entropy variation when the local detailed balance condition (2.26) is also met. As a consequence, fluctuation relations in the long-time limit (which are out of the scope of the present paper) for  $\Delta_{\text{exch}} S$  and for the cumulative exchange quantities can be derived respectively from the generic results in [20] and [21] or retrieved from the present finite time fluctuation relations. A recent extended review about the larger frame of stochastic thermodynamics is to be found in [22], and its formulation in the specific class of Markov jump processes in continuous time is reviewed in [23].

The paper is organized as follows. In section 2 constraints upon the transition rates are derived from the assumptions about the microscopic dynamics of the whole system. Our first result is derived in subsection 2.1 and appendix A. The prescription to approximate the mesoscopic dynamics by a Markov process is described in appendix B and our second result about the microcanonical detailed balance is derived in subsection 2.2. Our argument involves no time reversal symmetry, and, for a comparison, the microcanonical detailed balance is rederived in the case of an underlying Hamiltonian dynamics invariant under time reversal in appendix C. Its transformation into the local detailed balance in the limit where the sizes of the macroscopic bodies go to infinity before the time evolution of the interface system is considered is described in section 2.3. In section 3 we exhibit the derivation of the fluctuation relation (1.1) and that of the corresponding fluctuation relation for the ‘excess’ exchange entropy variation. In section 4 the key ingredients used in the previous two sections are generalized to the case of exchanges involving also variations of the volume or the number of particles.

## 2. Constraints upon transitions rates

In the present section we review some of the constraints that ergodic deterministic energy-conserving microscopic dynamics puts on the statistical mesoscopic description of a finite system  $S$  that establishes thermal contact between energy reservoirs  $\mathcal{B}_a$ s with  $a = 1, \dots, A$ .

Indeed, the following situation occurs commonly: the interactions in the whole system allow us to define one small part  $S$  in contact with otherwise independent large parts  $\mathcal{B}_a$ s. The large parts, which involve a huge number of degrees of freedom, do not interact directly among each other (this gives a criterion to identify the distinct large parts), but are in contact with the small part, which involves only a few degrees of freedom. Moreover each degree of freedom in the small part is directly in contact with at most one large part and can vary only through its interaction with the latter large part. This results in a star-shaped interaction pattern. It is convenient then to forget about the microscopic description of the large parts, and turn to a statistical description of their interactions with the small part. Some general features of the statistical description can be inferred from microscopic ergodicity.

### 2.1. Ergodicity

**2.1.1. Ergodicity in classical Hamiltonian dynamics.** In classical mechanics, the time evolution of a system in phase space is described by a Hamiltonian  $H$ . If the system is made of several interacting parts, the Hamiltonian is then referred to as the total Hamiltonian,  $H \equiv H_{\text{tot}}$ , and it splits as  $H_{\text{tot}} = H_{\text{dec}} + H_{\text{int}}$ , where  $H_{\text{dec}}$  accounts for the dynamics if the different parts were decoupled and  $H_{\text{int}}$  accounts for interactions. The energy hypersurface  $H_{\text{tot}} = E$ , usually a compact set, is invariant under the time evolution, and in a generic situation, this will be the only conserved quantity.

The ergodic hypothesis states that a generic trajectory of the system will asymptotically cover the energy hypersurface uniformly. To be more precise, phase space is endowed with the Liouville measure (i.e., in most standard cases the Lebesgue measure for the product of couples made by every coordinate and its conjugate momentum), which induces a natural measure on the energy hypersurface, and ergodicity means that, in the long run, the time spent by the system in each open set of the energy hypersurface will be proportional to its Liouville measure. Ergodicity can sometimes be built into the dynamics, or proved, but this usually requires immense effort.

Ergodicity depends crucially on the fact that the different parts are coupled: if  $H_{\text{int}} = 0$ , each part will have its energy conserved, and motion will take place on a lower-dimensional surface. If  $H_{\text{int}}$  is very small, the system will spend a long time very near this lower-dimensional surface, but, at even longer time scales, ergodicity can be restored. By taking limits in a suitable order (first infinite time and then vanishing coupling among the parts) one can argue that the consequences of ergodicity can be exploited by reasoning only on  $H_{\text{dec}}$ .

Notice that in this procedure, we have in fact some kind of dichotomy:  $H_{\text{dec}}$  defines the energy hypersurface, but cannot be used to define the ergodic motion, which is obtained from  $H_{\text{tot}} = H_{\text{dec}} + H_{\text{int}}$  via a limiting procedure. So the dynamics conserves  $H_{\text{dec}}$  but is not determined by  $H_{\text{dec}}$ .

**2.1.2. Ergodicity in deterministic dynamics for discrete variables.** Our aim is to translate the above considerations in the context of a large but finite system described by discrete variables such as classical Ising spins.

In the case of discrete dynamical variables, one can still talk about the energy  $E_{\text{tot}}$  of a configuration, but there is no phase space and no Hamiltonian dynamics available. So there is



no obvious canonical time evolution. This is where we exploit the previously mentioned dichotomy: we do not define the time evolution in terms of  $E_{\text{tot}}$ , but simply impose that the deterministic time evolution preserves  $E_{\text{dec}}$  and that it respects the star-shaped interaction pattern between the small part and the large parts. Besides this, we also impose that the time evolution is ergodic.

We consider that time is discrete as well, because ergodicity is most simply expressed in discrete time. Then deterministic dynamics is given by a bijective map, denoted by  $\mathcal{T}$  in what follows, on configuration space, applied at each time step to get a new configuration from the previous one. As the configuration space is finite, the trajectories are bound to be closed. Then, for a given initial value  $E$  of  $E_{\text{dec}}$ , a specific dynamics  $\mathcal{T}$  conserving  $E_{\text{dec}}$  corresponds to a periodic evolution of the microscopic configuration of the full system inside the energy level  $E_{\text{dec}} = E$ .

Ergodicity entails that the corresponding closed trajectory covers fully the energy level  $E_{\text{dec}} = E$ , and then it must cover it exactly once during a period because the dynamics is one to one. As a consequence the period of the ergodic evolution inside a given energy level of  $E_{\text{dec}}$  is the same for all choices of ergodic dynamics  $\mathcal{T}$  that conserves  $E_{\text{dec}}$ . This period, denoted by  $N$  in time step units, depends only on the value  $E$  of  $E_{\text{dec}}$ ,

$$N = \Omega_{\text{dec}}(E), \quad (2.1)$$

where  $\Omega_{\text{dec}}(E)$  is the total number of microscopic configurations in the level  $E_{\text{dec}} = E$ . This is reminiscent of the microcanonical ensemble. Let us note that, in classical mechanics, there is a time reversal symmetry related to an involution of phase space, changing the momenta to their opposites while leaving the positions fixed. In the discrete setting, involutions  $J$  such that  $J\mathcal{T}J = \mathcal{T}^{-1}$  always exist, but there is no obvious candidate among them for representing time reversal and allowing us to draw conclusions from it.

In the context of discrete variables, the star-shaped interaction pattern is implemented as follows. We may naively assume that the energy conserved by the dynamics  $\mathcal{T}$  is simply  $E_{\text{dec}}$ , as if there were no energy for the interactions between the small part and the large ones, but  $\mathcal{T}$  must reflect the fact that the large parts interact only indirectly: there is an internal interaction energy  $\mathcal{E}(C)$  for every configuration  $C$  of the small part, and each change in the small part can be associated with an elementary energy exchange with one of the large parts. If the small part can jump from configuration  $C$  to configuration  $C'$  in a single time step by exchanging energy with the large part  $B_a$ , we use the notation  $C' \in \mathbb{F}_a(C)$ . In this configuration jump, the energy  $E_{\text{dec}}$  of the global system is conserved and the energy of the large part  $B_a$  is changed from  $E_a$  to  $E'_a$  according to the conservation law

$$E'_a - E_a = \begin{cases} -[\mathcal{E}(C') - \mathcal{E}(C)] & \text{if } C' \in \mathbb{F}_a(C) \\ 0 & \text{otherwise,} \end{cases} \quad (2.2)$$

while the energies of the other large parts are unchanged. Apart from these energy exchange constraints and from ergodicity, the deterministic dynamics  $\mathcal{T}$  is supposed to obey some other natural physical constraints that will be specified later (see section 2.2).

As a final remark, we mention how, in a very simple case, some kind of deterministic map  $\mathcal{T}$  that preserves  $E_{\text{dec}}$  and obeys the star-shaped interaction pattern can be associated with a deterministic map  $\tilde{\mathcal{T}}$  that conserves  $E_{\text{tot}}$ . We consider the case where the energy exchange between every large part  $B_a$  and the small part is ensured by an interaction energy  $E_{\text{int}}^{(a)}$  between a classical spin  $\sigma_a^*$  in part  $B_a$  and a classical spin  $\sigma_a$  in the small part, and we consider only maps  $\tilde{\mathcal{T}}$  that not only conserve  $E_{\text{tot}}$  but also satisfy the following rules for all large parts: (1) spins  $\sigma_a^*$  and  $\sigma_a$  are always flipped at successive time steps (in an order depending on the

precise dynamics  $\tilde{\mathcal{T}}$ ); (2) the variations of the interaction energy  $E_{\text{int}}^{(a)}$  associated with these successive two flips are opposite to each other. Then the map  $\mathcal{T}$  that conserves  $E_{\text{dec}}$  is defined from the map  $\tilde{\mathcal{T}}$  by merging every pair of time steps where  $\sigma_a^*$  and  $\sigma_a$  are successively flipped into a single time step where  $\sigma_a^*$  and  $\sigma_a$  are simultaneously flipped. Indeed, in the latter pair of time steps of  $\tilde{\mathcal{T}}$ , by virtue of hypothesis (2), the successive two variations of  $E_{\text{int}}^{(a)}$  cancel each other and the variation of  $E_{\text{tot}}$  after these two time steps coincides with the variation of  $E_{\text{dec}}$ , since by definition the latter variation is  $\Delta E_{\text{dec}} = \Delta E_{\text{tot}} - \Delta E_{\text{int}}^{(a)}$ . Therefore, if map  $\tilde{\mathcal{T}}$  conserves  $E_{\text{tot}}$  at every time step, then the corresponding map  $\mathcal{T}$  where the latter successive two flips occur in a single time step preserves  $E_{\text{dec}}$ : the conservation rule (2.2) is indeed satisfied. The suppression of time steps in the procedure that defines  $\mathcal{T}$  from  $\tilde{\mathcal{T}}$  corresponds to a modification of the accessible configuration space that reflects the fact that the energy level  $E_{\text{tot}} = E$  and  $E_{\text{dec}} = E$  do not coincide.

### 2.1.3. Constraints from ergodicity and the interaction pattern upon coarse-grained evolution.

We start from the familiar observation that keeping track of what happens in detail in the large parts is out of our abilities, and is often not very interesting anyway. Our ultimate interest is in the evolution of the configuration  $C$  of the small part in an appropriate limit. As an intermediate step, we keep track also of the energies  $E_a$ s in the large parts, but not of the detailed configurations in the large parts.

The coarse graining that keeps track only of the time evolution of the configuration  $C$  of the small part and the energies  $E_a$ s of the large parts is defined as follows. With each microscopic configuration  $\xi$  of the full system we can associate the corresponding configuration  $C = C(\xi)$  of the small part and the corresponding energy  $E_a = E_a(\xi)$  carried by part  $B_a$ . To simplify the notation, we let  $\underline{E}$  denote the collection of  $E_a$ s, so  $\underline{E}$  is a vector with as many coordinates as there are large parts.

As shown in the previous subsection, if the initial value of the energy  $E_{\text{dec}}$  is equal to  $E$ , then, over a period equal to  $N = \Omega_{\text{dec}}(E)$  in time step units, the trajectory of  $\xi$  under any microscopic ergodic dynamics  $\mathcal{T}$  corresponds to a cyclic permutation of all the microscopic configurations in the energy level  $E_{\text{dec}} = E$ . Thus ergodicity entails that at the coarse grained level, if  $N_{(C, \underline{E})}$  denotes the occurrence number of  $(C, \underline{E})$  during the period of  $N$  time steps,  $N_{(C, \underline{E})}$  is nothing but  $\Omega_{\text{dec}}(C, \underline{E})$ , the number of microscopic configurations of the full system when the small part is in configuration  $C$  and the large parts have energies  $E_a$ s in the energy level  $E = E_{\text{dec}}$ , namely

$$N(C, \underline{E}) = \Omega_{\text{dec}}(C, \underline{E}) \quad (2.3)$$

with

$$E = E_{\text{dec}} \equiv \mathcal{E}(C) + \sum_a E_a. \quad (2.4)$$

In the following we fix the value of  $E$ , and  $N$  is called the period of the dynamics, while the energy constraint  $E = \mathcal{E}(C) + \sum_a E_a$  is often implicit in the notations.

Another crucial point is that, since any specific dynamics  $\mathcal{T}$  under consideration respects both the conservation of  $E_{\text{dec}}$  and the interaction pattern specified at the end of section 2.1.2, the number of jumps from  $(C, \underline{E})$  to  $(C', \underline{E}')$  over the period of  $N$  time steps, denoted by  $N_{(C, \underline{E}), (C', \underline{E}')}$ , is equal to the number of the reversed jumps from  $(C', \underline{E}')$  to  $(C, \underline{E})$  during the same time interval, namely

$$N_{(C, \underline{E}), (C', \underline{E}')} = N_{(C', \underline{E}'), (C, \underline{E})}. \quad (2.5)$$

In appendix A we give graph-theoretic conditions, not related to ergodicity, that ensure this property, and show that they are fulfilled in one relevant example, as a consequence of the star-shaped interaction pattern.

## 2.2. Markovian approximation for the mesoscopic dynamics

**2.2.1. Definition of a Markovian approximation for the mesoscopic dynamics.** For our purpose, we first rephrase the coarse-grained evolution as follows. As already noticed, over the period of  $N = \Omega_{\text{dec}}(E)$  time steps, a trajectory under any microscopic ergodic dynamics  $\mathcal{T}$  in the energy level  $E_{\text{dec}} = E$  corresponds to a cyclic permutation of the  $N$  microscopic configurations  $\xi$ s in the energy level. Therefore, if the configuration at some initial time is denoted by  $\xi_1$ , then the trajectory is represented by the sequence  $\omega = \xi_1 \xi_2 \dots \xi_N$  where  $\xi_{i+1} = \mathcal{T}_{\xi_i}$  with  $\xi_{N+1} = \xi_1$ . By the coarse-graining procedure that retains only the mesoscopic variable  $x \equiv (C, \underline{E})$ , the succession of distinct microscopic configurations  $\omega$  is replaced by  $w = x_1 x_2 \dots x_N$ , where  $x_i = x(\xi_i) = (C(\xi_i), \underline{E}(\xi_i))$ . In  $w$  various  $x_i$ s take the same value, and a so-called transition corresponds to the case  $x_{i+1} \neq x_i$ , namely the case where the configuration  $C$  of the small system is changed in the jump of the microscopic configuration of the full system from  $\xi_i$  to  $\xi_{i+1} = \mathcal{T}_{\xi_i}$ .

Since the large parts involve many degrees of freedom, the number of times some given value  $x = (C, \underline{E})$  appears in the coarse-grained sequence  $w$  is huge, and even if  $\omega$  is given by the deterministic rule  $\xi_{i+1} = \mathcal{T}_{\xi_i}$ , there is no such rule to describe the sequence  $w$ . Moreover the microscopic configuration at the initial time,  $\xi_1$ , is not known so that the coarse-grained sequence that actually appears in the course of time is in fact a sequence deduced from  $w$  by a translation of all indices.

As explained in appendix B.1, one may associate to the sequence  $w$  a (discrete time) Markov chain such that the mean occurrence frequencies of the patterns  $x$  and  $xx'$  in a stationary stochastic sample are equal to the corresponding values,  $N_x/N$  and  $N_{xx'}/N$ , in the sequence  $w$  determined by the dynamics  $\mathcal{T}$  (up to a translation of all indices corresponding to a different value of the initial microscopic configuration). Whether this Markovian effective description is accurate depends on several things: the choice of  $\mathcal{T}$ , the kind of statistical properties of  $w$  one wants to check, etc.

We may also argue (see appendix B.2) that a continuous time description is enough if we restrict our attention to microscopic dynamical maps  $\mathcal{T}$ s such that transitions, namely the patterns  $xx'$  with  $x' \neq x$ , are rare and of comparable mean occurrence frequencies over the period of  $N$  time steps. In other words, most of the steps in the dynamics amount to reshuffling the configurations of the large parts without changing their energies, leaving the configuration of the small part untouched. The latter physical constraint and the hypothesis of the validity of the Markovian approximation select a particular class of dynamics  $\mathcal{T}$ .

With these assumptions, we associate to the sequence  $w$  of coarse grained variables  $(C, \underline{E})$  a Markov process whose stationary measure shares some of the statistical properties of  $w$ , namely the values of the mean occurrence frequencies of length 1 and length 2 patterns. The transition rate from  $(C, \underline{E})$  to  $(C', \underline{E}')$  with  $(C, \underline{E}) \neq (C', \underline{E}')$  in the approximated Markov process is given by (B.4), where we just have to make the substitutions  $N_x = N_{(C, \underline{E})}$  and  $N_{xx'} = N_{(C, \underline{E}), (C', \underline{E}')}$ , with the result

$$W(C', \underline{E}' \leftarrow C, \underline{E}) = \frac{N_{(C, \underline{E}), (C', \underline{E}')}}{\tau N_{(C, \underline{E})}} \quad \text{for } (C, \underline{E}) \neq (C', \underline{E}'), \quad (2.6)$$

where  $\tau$  is a time scale such that  $W(C', \underline{E}' \leftarrow C, \underline{E})$  is of order unity. The corresponding stationary distribution is given by (B.2),

$$P_{\text{st}}^W(C, \underline{E}) = \frac{N_{(C, \underline{E})}}{N}. \quad (2.7)$$

We recall that  $N = \sum_{(C, \underline{E})} N_{(C, \underline{E})}$  and  $N_{(C, \underline{E})} = \sum_{(C', \underline{E}')} N_{(C, \underline{E}), (C', \underline{E}')}.$

**2.2.2. Microcanonical detailed balance and other properties.** By virtue of the ergodicity property (2.3) at the coarse-grained level, the transition rate in the approximated Markov process reads

$$W(C', \underline{E}' \leftarrow C, \underline{E}) = \frac{N_{(C, \underline{E}), (C', \underline{E}')}}{\tau \Omega_{\text{dec}}(C, \underline{E})} \quad \text{for } (C, \underline{E}) \neq (C', \underline{E}'). \quad (2.8)$$

Meanwhile, by virtue of the ergodicity properties (2.1) and (2.3), the corresponding stationary distribution (2.7) is merely the microcanonical distribution

$$P_{\text{st}}^W(C, \underline{E}) = \frac{\Omega_{\text{dec}}(C, \underline{E})}{\Omega_{\text{dec}}(E)} \equiv P_{\text{mc}}(C, \underline{E}). \quad (2.9)$$

Ergodicity also entails that all microscopic configurations  $\xi$ s in the energy level appear in the sequence  $\omega$ , and therefore all possible values of  $x$  also appear in the coarse-grained sequence  $w$ : so any mesoscopic state  $(C, \underline{E})$  can be reached from any other mesoscopic state  $(C', \underline{E}')$  by a succession of elementary transitions, even if they are not involved in an elementary transition (i.e. if  $N_{(C, \underline{E}), (C', \underline{E}')} = 0$ ); in other words the graph associated with the transition rates  $W(C', \underline{E}' \leftarrow C, \underline{E})$  is connected, or, equivalently, the Markov matrix defined from the transition rates is *irreducible*.

The constraint (2.5) imposed by the interaction pattern upon the coarse-grained evolution over a period of  $N$  time steps entails that the transition rates of the approximated Markov process given by (2.8) obey two properties. First,

$$W(C', \underline{E}' \leftarrow C, \underline{E}) \quad \text{and} \quad W(C, \underline{E} \leftarrow C', \underline{E}') \quad (2.10)$$

are either both  $=0$  or both  $\neq 0$ . This property may be called *microreversibility*. Second, if the transition rates do not vanish, they obey the equality

$$\frac{W(C', \underline{E}' \leftarrow C, \underline{E})}{W(C, \underline{E} \leftarrow C', \underline{E}')} = \frac{\Omega_{\text{dec}}(C', \underline{E}')}{\Omega_{\text{dec}}(C, \underline{E})} = \frac{P_{\text{mc}}(C', \underline{E}')}{P_{\text{mc}}(C, \underline{E})}. \quad (2.11)$$

Observe that the arbitrary time scale  $\tau$  has disappeared in this equation. The equality between the ratio of transition rates and the ratio of probabilities in the corresponding stationary distribution is the so-called detailed balance relation. Here the stationary distribution is that of the microcanonical ensemble, and we will refer to relation (2.11) as the *microcanonical detailed balance*.

In appendix C, we rederive a microcanonical detailed balance similar to (2.11) when the underlying microscopic dynamics is Hamiltonian and invariant under time reversal. (Similar arguments can be found in derivations that rely on different assumptions in [24, 25].) The evolution of the probability distribution of the mesoscopic variables is approximated by a Markov process according to the same scheme as that introduced in section 2.2.1. Eventually the comparison between the ways in which the microcanonical detailed balance arises in that case and in our previous argument is the following.

- When the microscopic variables are continuous coordinates in phase space and evolve according to a Hamiltonian dynamics, in the framework of statistical ensemble theory the stationary measure for the mesoscopic variables is the measure that is preserved under the microscopic dynamics; the fact that it coincides with the microcanonical distribution is

enforced by the invariance of the Liouville measure in phase space under the Hamiltonian evolution; the microcanonical detailed balance for mesoscopic variables that are even functions of microscopic momenta mainly arises from the invariance under time reversal of the trajectories in phase space (see (C.1)).

- When the microscopic dynamical variables are discrete and evolve under an energy-conserving map, the stationary measure for mesoscopic variables is defined as the average over a period of the microscopic dynamics; the fact that it is equal to the microcanonical distribution arises from the ergodicity imposed on the microscopic map  $\mathcal{T}$  (see (2.1) and (2.3)); the microcanonical detailed balance emerges from the equality between the frequencies of a given transition and the reversed one (over the period needed for the microscopic map to cover the energy level), equality that is enforced by the star-shaped interaction pattern (see (2.5)).

**2.2.3. Further consequence of the interaction pattern.** In the interaction pattern, large parts do not interact directly with one another and  $\Omega_{\text{dec}}(C, \underline{E}) = \prod_a \Omega_a(E_a)$ , where  $\Omega_a(E_a)$  denotes the number of configurations in large part  $\mathcal{B}_a$  with energy  $E_a$  when it is isolated. Moreover, the energy of a single large part is changed in a given transition, so if  $(C', \underline{E}')$  is obtained from  $(C, \underline{E})$  by an energy exchange with part  $\mathcal{B}_a$  that makes  $C$  jump to  $C'$  we have the result, with the notation introduced in (2.2),

$$\text{if } C' \in \mathbb{F}_a(C) \quad \frac{\Omega_{\text{dec}}(C', \underline{E}')}{\Omega_{\text{dec}}(C, \underline{E})} = \frac{\prod_b \Omega_b(E'_b)}{\prod_b \Omega_b(E_b)} = \frac{\Omega_a(E'_a)}{\Omega_a(E_a)}. \quad (2.12)$$

We have used the energy conservation rule  $E'_b = E_b - \delta_{a,b}[\mathcal{E}(C') - \mathcal{E}(C)]$ , so that for  $b \neq a$  the multiplicity factors are unchanged in the transition.

The latter ratio of microstate numbers can be expressed in terms of the Boltzmann entropies when each part  $\mathcal{B}_a$  is isolated. The dimensionless Boltzmann entropy (see footnote 5)  $S_a^B(E_a)$  for the isolated part  $\mathcal{B}_a$  when its energy is equal to  $E_a$  is defined by  $\Omega_a(E_a) \equiv \exp S_a^B(E_a)$ . With these notations, if the transition rate  $W(C', \underline{E}' \xleftarrow{\mathbb{F}_a} C, \underline{E})$ , where  $C' \in \mathbb{F}_a(C)$ , is nonzero, then the transition rate for the reversed jump  $W(C, \underline{E} \xleftarrow{\mathbb{F}_a} C', \underline{E}')$ , where  $C \in \mathbb{F}_a(C')$ , is also nonzero (see (2.10)) and, by virtue of (2.12), the relation (2.11) is reduced to

$$\frac{W(C', \underline{E}' \xleftarrow{\mathbb{F}_a} C, \underline{E})}{W(C, \underline{E} \xleftarrow{\mathbb{F}_a} C', \underline{E}')} = \frac{\Omega_a(E'_a)}{\Omega_a(E_a)} \equiv e^{S_a^B(E'_a) - S_a^B(E_a)}. \quad (2.13)$$

The latter formula is the first important stage of the argument.

We stress that the present argument does not involve any kind of underlying time reversal. Here the time reversal symmetry arises only at the statistical level of description represented by the Markov evolution ruled by the transition rates.

Notice also that, as only certain ratios are fixed, different ergodic deterministic microscopic dynamics can lead to very different transition rates, a remnant of the fact that the coupling between a large part and the small part can take any value *a priori*.

Formula (2.13) is also a clue to understand *a contrario* what kind of physical input is needed for the homogeneous Markov approximation to be valid. Indeed, why didn't we do the homogeneous Markov approximation directly on the small part? We could certainly imagine dynamics making this a valid choice. However, it is in general incompatible with the pattern of interactions (see the end of section 2.1.2) that is the basis of our argument. For

instance, if in the coarse-graining procedure we had retained only the configurations  $C$ s of the small part, then the corresponding graph introduced in appendix A would have been a cycle instead of a tree in the case of a small part made of two spins (see [14]), and the crucial property (2.5) would have been lost: over the period of  $N$  time steps of the microscopic dynamics  $N_{C,C'} \neq N_{C',C}$ . In fact, we may expect, or impose on physical grounds, that  $\Omega_a$  will be exponentially large in the size of large part  $B_a$  (i.e. its number of degrees of freedom  $\mathcal{N}_a$ ), so that even the ratio  $\Omega_a(E'_a)/\Omega_a(E_a) = \Omega_a(E_a - [\mathcal{E}(C') - \mathcal{E}(C)])/\Omega_a(E_a)$  will vary significantly over the trajectory, meaning that transition probabilities involving only the small part cannot be taken to be constant along the trajectory: the energies of the large parts are relevant variables.

### 2.3. The transient regime when large parts are described in the thermodynamic limit

**2.3.1. Large parts in the thermodynamic limit.** We now assume that the large parts are large enough that they are accurately described by a thermodynamic limit, which we take at the most naive level. To recall what we mean by that, we concentrate on one large part for a while, and suppress the index used to label it. Suppose this large part has  $\mathcal{N}$  degrees of freedom, and suppose that energies are close to an energy  $E$  for which the Boltzmann entropy is  $S^B(E)$ . That the thermodynamic limit exists means that if one lets  $\mathcal{N} \rightarrow +\infty$  while the ratio  $E/\mathcal{N}$  goes to a finite limit  $\epsilon$ , there is a differentiable function  $s^B(\epsilon)$  such that the ratio  $S^B(E)/\mathcal{N}$  goes to  $s^B(\epsilon)$ . The quantity

$$\frac{ds^B}{d\epsilon} \equiv \beta \quad (2.14)$$

is nothing but the inverse temperature. In that case, as long as  $\Delta E \ll E$  (where  $E$  scales as  $\mathcal{N}\Delta\epsilon$  with  $\Delta\epsilon$  some finite energy scale),  $S^B(E + \Delta E) - S^B(E) \rightarrow \beta\Delta E$  when  $\mathcal{N} \rightarrow +\infty$ . For  $\mathcal{N}$  large enough, the relation  $S^B(E + \Delta E) - S^B(E) \sim \beta\Delta E$  is a good approximation.

**2.3.2. Transient regime and local detailed balance (LDB).** Notice that when transitions occur, which, by the definition of  $\tau$  in (2.6), happens typically once on the macroscopic time scale, the changes in the energies of the large parts are finite, so that over long windows of time evolution, involving many changes in the small part, the relation

$$S_a^B(E'_a) - S_a^B(E_a) \sim \beta_a [E'_a - E_a] \quad (2.15)$$

is not spoiled, where  $E'_a$  and  $E_a$  are the energies in large part  $B_a$  at any moment within the window.

In fact the larger the large parts, the longer the time window for which (2.15) remains valid. The relation between the sizes  $\mathcal{N}_a$ s of the large parts and of the length of the time window depends on the details of  $\mathcal{T}$  (which still has to fulfil the imposed physical conditions). This relation also depends on the values of the energy per degree of freedom in every large part,  $E_a/\mathcal{N}_a$ , which are essentially constant in such a window.

Because of the ergodicity hypothesis, the largest window (of size comparable to the period of  $\mathcal{T}$  to logarithmic precision) has the property that the energies  $E_a$ s in the large parts will be such that all  $\beta_a$ s are close to each other and the system will be at equilibrium. Indeed, inside the largest time window, the system remains in the region of the energy level where the energies  $E_a$ s are the most probable, and in the thermodynamic limit the most probable values for the  $E_a$ s in the microcanonical ensemble are the values  $E_a^*$ s that maximize the product  $\prod_a \Omega_a(E_a)$  under the constraint  $E = \sum_a E_a$  (since the system energies are negligible with

respect to those of the large parts). The latter maximization condition is equivalent to the equalities  $ds^B/de_a(\epsilon_a^*) = ds^B/de_b(\epsilon_b^*)$  for all pairs of large parts.

However, if the system starts in a configuration such that the  $\beta_a$ s are distinct, the time window over which  $E_a/\mathcal{N}_a$  and  $\beta_a$  are constant (to a good approximation) will be short with respect to the period of the microscopic dynamics, but long enough that (2.15) still holds for a long time interval. Then by putting together the information on the ratio of transition rates in terms of Boltzmann entropies (2.13), the transient regime approximation (2.15) and the energy conservation (2.2), we get

$$\frac{W\left(C', \underline{E}' \xleftarrow{\mathbb{F}_a} C, \underline{E}\right)}{W\left(C, \underline{E} \xleftarrow{\mathbb{F}_a} C', \underline{E}'\right)} \sim e^{-\beta_a[\mathcal{E}(C') - \mathcal{E}(C)]}. \quad (2.16)$$

Now the right-hand side depends only on the configurations of the small system, and the parameters  $\beta_a$ s are constants. Letting the large parts get larger and larger while adjusting the physical properties adequately, we can ensure that the time over which (2.16) remains valid gets longer and longer, so, in the thermodynamic limit for the large parts, the transient regime lasts forever. This situation is our main interest in what follows.

In the transient regime the transition rate from configuration  $C$  to configuration  $C'$  is denoted as  $(C'|W|C)$ . As well as the transition rates  $W(C', \underline{E}' \xleftarrow{\mathbb{F}_a} C, \underline{E})$ , the rates  $(C'|W|C)$  must satisfy the three consequences derived from the properties of the underlying microscopic deterministic dynamics pointed out in section 2.1.2, namely ergodicity, energy conservation and specific interaction pattern. First, as shown in section 2.2.2 for the mesoscopic configurations  $(C, \underline{E})$ , any configuration  $C$  can be reached by a succession of jumps with non-zero transition rates from any configuration  $C'$ , namely in the network representation of the stochastic evolution

$$\text{the graph associated with the transition rates is connected.} \quad (2.17)$$

In other words, the Markov matrix defined from the transition rates must be irreducible and the property (2.17) is referred to as the *irreducibility* condition. Second, from (2.10), the transition rates must obey the *microscopic reversibility* condition for any couple of configurations  $(C, C')$ , namely

$$(C'|W|C) \neq 0 \quad \Leftrightarrow \quad (C|W|C') \neq 0. \quad (2.18)$$

Third, from (2.16) one gets a constraint obeyed by the ratio of transition rates in the transient regime,

$$\text{for } C' \in \mathbb{F}_a(C) \quad \frac{(C'|W|C)}{(C|W|C')} = e^{-\beta_a[\mathcal{E}(C') - \mathcal{E}(C)]}. \quad (2.19)$$

The latter relation is the so-called local detailed balance (LDB), which is also referred to in the literature as the ‘generalized detailed balance’.

We stress that, by selecting a time window while taking the thermodynamic limit for the large parts, the microcanonical detailed balance (2.11) is replaced by the local detailed balance (2.13), except in the case of the largest time window where all  $\beta_a$ s are equal. In the latter case, the microcanonical detailed balance (2.11) is replaced by the canonical detailed balance and the statistical time reversal symmetry is preserved. Indeed, the equilibrium thermodynamic regime is reached either if we start from a situation in which  $\prod_a \Omega_a(E_a)$  is close to its maximum along the trajectory in the energy level  $E_{\text{dec}} = E$ , or if we wait long enough so that  $\prod_a \Omega_a(E_a)$  becomes close to this maximum. As recalled above, this is true



for most of the period of the microscopic dynamics, but reaching this situation may take a huge number of time steps if the starting point was far from the maximum. By an argument similar to that used in the derivation of (2.15), when  $\prod_a \Omega_a(E_a)$  is closed to its maximum and the large parts are considered in the thermodynamic limit, all  $\beta_a$ s are equal to the same value  $\beta$  and the relative weight of two configurations in the microcanonical ensemble,  $P_{\text{mc}}(C', \underline{E}')/P_{\text{mc}}(C, \underline{E})$  given by (2.9), tends to  $\exp(-\beta[\mathcal{E}(C') - \mathcal{E}(C)])$ . Then the equilibrium microcanonical distribution  $P_{\text{mc}}(C, \underline{E})$  tends to the canonical distribution

$$P_{\text{can}}^\beta(C) \equiv \frac{e^{-\beta\mathcal{E}(C)}}{Z(\beta)}, \quad (2.20)$$

where  $Z(\beta)$  is the canonical partition function at the inverse temperature  $\beta$ . Meanwhile, the detailed balance relation (2.11) in the microcanonical equilibrium ensemble for the transition rates  $W(C', \underline{E}' \leftarrow C, \underline{E})$  becomes a detailed balance relation in the canonical ensemble at the inverse temperature  $\beta$  of the whole system for the transition rates  $(C'|W|C)$ , namely

$$\frac{(C'|W|C)}{(C|W|C')} = e^{-\beta[\mathcal{E}(C') - \mathcal{E}(C)]} = \frac{P_{\text{can}}^\beta(C')}{P_{\text{can}}^\beta(C)}. \quad (2.21)$$

The local detailed balance (2.19), valid in transient regimes, differs from the latter detailed balance in the canonical ensemble by two features: the various  $\beta_a$ s of the distinct large parts appear in place of the common equilibrium inverse temperature  $\beta$ , and the stationary distribution for the transition rates is not known *a priori*.

We conclude this discussion with the following remarks. We have not tried to exhibit explicit physical descriptions of the large parts or explicit formulæ for the dynamical map  $\mathcal{T}$ . Though it is not too difficult to give examples for fixed sizes of the large parts, it is harder to get a family of such descriptions sharing identical physical properties for varying large part sizes, a feature which is crucial to really make sense of the limits we took blindly in our derivation. It is certainly doable, but cumbersome, and we have not tried to pursue this idea. Let us note also that in principle, taking large parts of increasing sizes can be used to enhance the validity of the approximation of the (discrete-time) Markov chain by a (continuous-time) Markov process. As the physics of the continuous time limit does not seem to be related to the physics of convergence towards a heat bath description we have preferred to keep the discussion separate, taking a continuous-time description as starting point.

**2.3.3. Expression of LDB in terms of exchange entropy variation.** Observe that though we have given no detailed analysis of the dynamics or the statistical properties of the large parts, their influence on the effective Markov dynamics of the small system enters only through the inverse temperatures  $\beta_a$  defined in (2.14). So we can consistently assume that each large part becomes a thermal bath with its own temperature. The leading term in  $S_a^B(E'_a) - S_a^B(E_a)$  is the variation  $\delta S_a^{TH}(C' \leftarrow C)$  of the thermodynamic entropy of bath  $B_a$  when it flips the small system from configuration  $C$  to configuration  $C'$ ,

$$\delta S_a^{TH}(C' \leftarrow C) = \begin{cases} \beta_a[E'_a - E_a] & \text{if } C' \in \mathbb{F}_a(C) \\ 0 & \text{otherwise.} \end{cases} \quad (2.22)$$

Then we have an idealized description of a thermal contact between heat baths. This is the situation on which we concentrate in this paper.

By definition of a heat source, the variation  $\delta S_a^{TH}(C' \leftarrow C)$  of the thermodynamic entropy of bath  $B_a$  when it flips the system from configuration  $C$  to configuration  $C'$  reads



$$\delta S_a^{TH}(C' \leftarrow C) = -\beta_a \delta q_a(C' \leftarrow C), \quad (2.23)$$

where  $\delta q_a(C' \leftarrow C)$  is the heat received by the small system from part  $B_a$ . According to the expression (2.22) and to the energy conservation relation (2.2),

$$\begin{cases} \delta q_a(C' \leftarrow C) = \mathcal{E}(C') - \mathcal{E}(C) & \text{if } C' \in \mathbb{F}_a(C) \\ \delta q_a(C' \leftarrow C) = 0 & \text{otherwise.} \end{cases} \quad (2.24)$$

Let us introduce  $\delta_{\text{exch}} S(C' \leftarrow C)$  the exchange entropy variation of the small system (see footnote 10) that is associated with the heat exchanges with the thermostats when the small system goes from configuration  $C$  to configuration  $C'$ . Thanks to the definition (2.22)

$$\delta_{\text{exch}} S(C' \leftarrow C) \equiv -\sum_a \delta S_a^{TH}(C' \leftarrow C). \quad (2.25)$$

Then the local detailed balance (2.19) can be rewritten in a form that does not involve explicitly the heat bath responsible for the transition from  $C$  to  $C'$ ,

$$\frac{(C'|W|C)}{(C|W|C')} = e^{-\delta_{\text{exch}} S(C' \leftarrow C)}. \quad (2.26)$$

### 3. Exchange entropy variation and symmetries at finite time under LDB

#### 3.1. LDB and symmetry between time-reversed histories

For a history  $\mathcal{H}ist$  where the system starts in configuration  $C_0$  at time  $t_0 = 0$  and ends in configuration  $C_f$  at time  $t$  after going through successive configurations  $C_0, C_1, \dots, C_N = C_f$ , the exchange entropy variation  $\Delta_{\text{exch}} S[\mathcal{H}ist]$  corresponding to the history is defined from the heat amounts  $Q_1[\mathcal{H}ist]$  and  $Q_2[\mathcal{H}ist]$  received from two thermal baths as

$$\Delta_{\text{exch}} S[\mathcal{H}ist] \equiv \beta_1 Q_1[\mathcal{H}ist] + \beta_2 Q_2[\mathcal{H}ist] \quad \text{with} \quad Q_a[\mathcal{H}ist] \equiv \sum_{i=0}^{N-1} \delta q_a(C_{i+1} \leftarrow C_i). \quad (3.1)$$

The  $N$  instantaneous jumps from one configuration to another occur at  $N$  successive intermediate times  $T_i$ , which are continuous stochastic variables: the system jumps from  $C_{i-1}$  to  $C_i$  at time  $T_i$  ( $i=1, \dots, N$ ) in the time interval  $[t_i, t_i + dt_i[$ , with  $t_0 < t_1 < t_2 < \dots < t_N < t$ . The probability measure for such a history is related to the probability density  $\Pi_{C_f, C_0}[\mathcal{H}ist]$  by

$$dP_{C_f, C_0}[\mathcal{H}ist] \equiv dt_1 \dots dt_N \Pi_{C_f, C_0}[\mathcal{H}ist] \quad (3.2)$$

where, for a time-translational invariant process,

$$\begin{aligned} \Pi_{C_f, C_0}[\mathcal{H}ist] &= e^{-(t-t_N)\Lambda(C_N)} (C_N | W | C_{N-1}) e^{-(t_N-t_{N-1})\Lambda(C_{N-1})} \\ &\times \dots e^{-(t_2-t_1)\Lambda(C_1)} (C_1 | W | C_0) e^{-(t_1-t_0)\Lambda(C_0)} \end{aligned} \quad (3.3)$$

and  $\Lambda(C)$  is the total exit rate (also called escape rate) from configuration  $C$ ,  $\Lambda(C) \equiv \sum_{C' \neq C} (C'|W|C)$ . The average of a functional  $F[\mathcal{H}ist]$  over the histories that start in configuration  $C_0$  and end in configuration  $C_f$  is computed as  $\langle F \rangle_{C_f, C_0} = \int dP_{C_f, C_0}[\mathcal{H}ist] F[\mathcal{H}ist]$  with

$$\int dP_{C_f, C_0}[\mathcal{H}ist] = \sum_{N=0}^{+\infty} \sum_{C_1} \dots \sum_{C_{N-1}} \int_{t_0 < t_1 < \dots < t_N} dP_{C_f, C_0}[\mathcal{H}ist]. \quad (3.4)$$

Then the average of a functional when the initial distribution of configurations is  $P_0$  reads

$$\langle F \rangle_{P_0} = \sum_{C_f} \sum_{C_0} P_0(C_0) \int dP_{C_f, C_0}[\mathcal{H}ist] F[\mathcal{H}ist]. \quad (3.5)$$

Let  $\mathbb{T}$  be the time reversal operator for histories. If  $\mathcal{H}ist$  is a history that starts at time  $t_0 = 0$  in  $C_0$  and ends at time  $t$  in  $C_f$  after  $N$  jumps from  $C_{i-1}$  to  $C_i$  at time  $T_i$ ,  $\mathbb{T}\mathcal{H}ist$  is a history that starts at time  $t_0 = 0$  in  $C_f$  and ends at  $C_0$  at time  $t$  after  $N$  jumps from  $C'_{i-1}$  to  $C'_i$  at time  $T'_i$  with  $C'_i = C_{N-i}$  and  $T'_i = t - T_{N-i+1}$ , namely

$$\begin{aligned} \mathcal{H}ist: & \quad C_0 \text{ at } t_0 = 0 \quad C_0 \xrightarrow{T_1} C_1 \dots C_{N-1} \xrightarrow{T_N} C_f \\ \mathbb{T}\mathcal{H}ist: & \quad C_f \text{ at } t_0 = 0 \quad C_f \xrightarrow{T'_1} C_{N-1} \dots C_1 \xrightarrow{T'_N} C_0. \end{aligned} \quad (3.6)$$

From the definition (3.2) of the measure  $dP_{C_0, C_f}$  over histories starting in configuration  $C_0$  and ending in configuration  $C_f$ ,

$$\frac{dP_{C_f, C_0}[\mathcal{H}ist]}{dP_{C_0, C_f}[\mathbb{T}\mathcal{H}ist]} = \prod_{i=0}^{N-1} \frac{(C_{i+1} | \mathbb{W} | C_i)}{(C_i | \mathbb{W} | C_{i+1})}. \quad (3.7)$$

When the transition rates obey the local detailed balance (2.26) written in terms of  $\delta_{\text{exch}} S(C' \leftarrow C)$ , the exchange entropy variation for the history, defined in (3.1), can be rewritten as

$$\Delta_{\text{exch}} S[\mathcal{H}ist] \stackrel{\text{LDB}}{=} -\ln \prod_{i=0}^{N-1} \frac{(C_{i+1} | \mathbb{W} | C_i)}{(C_i | \mathbb{W} | C_{i+1})}, \quad (3.8)$$

and equation (3.7) can be rewritten as

$$\frac{dP_{C_f, C_0}[\mathcal{H}ist]}{dP_{C_0, C_f}[\mathbb{T}\mathcal{H}ist]} \stackrel{\text{LDB}}{=} e^{-\Delta_{\text{exch}} S[\mathcal{H}ist]}. \quad (3.9)$$

We stress that, according to (3.8), when the LDB is satisfied the expression of the exchange entropy variation for a history defined in (3.1) coincides with the opposite of the ‘action functional’ introduced by Lebowitz and Spohn in [20] in the generic case where the LDB does not necessarily hold.

### 3.2. Symmetry between time-reversed evolutions with fixed heat amounts

The probability  $P(C_f | Q_1, Q_2, t | C_0)$  that the system has evolved from configuration  $C_0$  at  $t_0 = 0$  to configuration  $C_f$  at  $t$  while receiving the heat amounts  $Q_1$  and  $Q_2$  from the thermostats 1 and 2 reads

$$P(C_f | Q_1, Q_2; t | C_0) \equiv \int dP_{C_f, C_0}[\mathcal{H}ist] \delta(Q_1[\mathcal{H}ist] - Q_1) \delta(Q_2[\mathcal{H}ist] - Q_2), \quad (3.10)$$

where  $\int dP_{C_f, C_0}$  denotes the ‘summation’ over the histories from  $C_0$  to  $C_f$  defined in (3.4). The time-reversal symmetry property (3.9) for the history measure  $dP_{C_f, C_0}[\mathcal{H}ist]$  implies the following relation between probabilities of forward and backward evolutions where initial and final configurations are exchanged (and heat amounts are changed into their opposite values),

$$\frac{P(C_f | Q_1, Q_2; t | C_0)}{P(C_0 | -Q_1, -Q_2; t | C_f)} = e^{-\Delta_{\text{exch}} S(Q_1, Q_2)}, \quad (3.11)$$

with the definition

$$\Delta_{\text{exch}} S(Q_1, Q_2) \equiv \beta_1 Q_1 + \beta_2 Q_2. \quad (3.12)$$

An analogous relation for  $\Delta_{\text{exch}} S$  in place of  $(Q_1, Q_2)$  is derived in [26] in the case where the microscopic dynamics of the heat baths is assumed to be Hamiltonian.

### 3.3. Symmetries in protocols starting from an equilibrium state

We consider a protocol where the system is prepared in an equilibrium state at the inverse temperature  $\beta_0$  and suddenly put at time  $t_0 = 0$  in thermal contact with the two thermostats at the inverse temperatures  $\beta_1$  and  $\beta_2$  respectively. Then the system evolution is a relaxation from an equilibrium state to a stationary non-equilibrium state.

The initial equilibrium distribution at the inverse temperature  $\beta_0$  is the canonical distribution (2.20).  $Z(\beta_0)$  cancels in the ratio  $P_{\text{can}}^{\beta_0}(C_0)/P_{\text{can}}^{\beta_0}(C_f)$  and

$$\ln \frac{P_{\text{can}}^{\beta_0}(C_0)}{P_{\text{can}}^{\beta_0}(C_f)} = \beta_0 [\mathcal{E}(C_f) - \mathcal{E}(C_0)] = \beta_0 (Q_1 + Q_2), \quad (3.13)$$

where the last equality is enforced by energy conservation. Then the time-reversal symmetry (3.11) and the specific form (3.13) for  $\ln [P_{\text{can}}^{\beta_0}(C_0)/P_{\text{can}}^{\beta_0}(C_f)]$  imply that

$$\frac{P(C_f | Q_1, Q_2; t | C_0) P_{\text{can}}^{\beta_0}(C_0)}{P(C_0 | -Q_1, -Q_2; t | C_f) P_{\text{can}}^{\beta_0}(C_f)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2)}, \quad (3.14)$$

where the excess exchange entropy variation  $\Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2)$  is defined as the difference between the exchange entropy variation in an evolution under the non-equilibrium constraint  $\beta_1 \neq \beta_2$  where the system receives heat amounts  $Q_1$  and  $Q_2$  and that in an evolution under the equilibrium condition  $\beta_1 = \beta_2 = \beta_0$  where the system would received the same heat amounts. It reads

$$\begin{aligned} \Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2) &= \Delta_{\text{exch}} S(Q_1, Q_2) - \beta_0 (Q_1 + Q_2) \\ &= (\beta_1 - \beta_0) Q_1 + (\beta_2 - \beta_0) Q_2. \end{aligned} \quad (3.15)$$

A crucial point is that  $\Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2)$  does not depend explicitly on the initial and final configurations and is only a function of the heat amounts received from the thermal baths.

As a consequence, the measurable joint distribution  $P_{P_{\text{can}}^{\beta_0}}(Q_1, Q_2; t)$  for the heat amounts  $Q_1$  and  $Q_2$  received between  $t_0 = 0$  and  $t$  when the initial configuration of the system is distributed according to  $P_{\text{can}}^{\beta_0}$ , namely  $P_{P_{\text{can}}^{\beta_0}}(Q_1, Q_2; t) = \sum_{C_0, C_f} P(C_f | Q_1, Q_2, t | C_0) P_{P_{\text{can}}^{\beta_0}}(C_0)$ , satisfies the identity

$$\frac{P_{P_{\text{can}}^{\beta_0}}(Q_1, Q_2; t)}{P_{P_{\text{can}}^{\beta_0}}(-Q_1, -Q_2; t)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2)}. \quad (3.16)$$

Subsequently the measurable quantity  $\Delta_{\text{exch}}^{\text{excs}, \beta_0} S(Q_1, Q_2)$ , with the distribution probability  $P_{P_{\text{can}}^{\beta_0}}(\Delta_{\text{exch}}^{\text{excs}, \beta_0} S) = \sum_{Q_1, Q_2} \delta(\Delta_{\text{exch}}^{\text{excs}, \beta_0} S - (\beta_1 - \beta_0) Q_1 - (\beta_2 - \beta_0) Q_2) P_{P_{\text{can}}^{\beta_0}}(Q_1, Q_2; t)$  obeys the symmetry relation at any finite time, which may be referred to as a detailed fluctuation relation,

$$\frac{P_{P_{\text{can}}^{\beta_0}}(\Delta_{\text{exch}}^{\text{excs}, \beta_0} S)}{P_{P_{\text{can}}^{\beta_0}}(-\Delta_{\text{exch}}^{\text{excs}, \beta_0} S)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \beta_0} S}. \quad (3.17)$$

The latter relation itself entails the identity, which may be referred to as an integral fluctuation relation,

$$\left\langle e^{\Delta_{\text{exch}}^{\text{excs}, \beta_0} S} \right\rangle_{P_{\text{can}}^{\beta_0}} = 1. \quad (3.18)$$

By using Jensen's inequality we get the inequality  $-\langle \Delta_{\text{exch}}^{\text{excs}, \beta_0} S \rangle \geq 0$ . To our knowledge the two relations (3.17) and (3.18) have not appeared explicitly in the literature, though the calculations involved in the derivation of the present finite-time fluctuation relations are analogous to those that lead to finite-time detailed fluctuation relations for protocols where the system is in thermal contact with only one heat bath and is driven out of equilibrium by a time-dependent external parameter (see the argument first exhibited by Crooks [16] for work fluctuations and then Seifert [18] for the entropy production along a stochastic trajectory (see also the review [19])). The latter class of protocols is very different as for the physical mechanisms that they involve: the changes in energy level populations are caused by energy exchanges with only one thermal bath and the system is driven out of equilibrium by the time dependence of the energy levels enforced by external time-dependent forces [27]. Moreover, in Jarzynski-like protocols the system evolves from an initial equilibrium state and measurements are performed until work ceases to be provided to the system, which then relaxes to another equilibrium state. The present protocol does not either involve the comparison of forward and backward evolutions corresponding to two different series of experiments, as needed for Crooks relation. (In Crooks' argument the initial configurations for the forward and backward evolutions are distributed with different equilibrium probabilities,  $P_{\text{can}}^{\beta_0}$  and  $P_{\text{can}}^{\beta_f}$ , whereas forward and backward evolutions with the same initial distribution had already been considered in [28, 29]). In Hatano–Sasa-like protocols the system evolves from an initial non-equilibrium steady state to another one (and then housekeeping heats and excess heats are introduced as in the steady state thermodynamics introduced by Oono and Paniconi [30]). In the finite-time protocol considered here, the system starts in an equilibrium state and at time  $t$  it has not yet reached the steady state controlled by  $\beta_1$  and  $\beta_2$ . Moreover, the integral fluctuation relation (3.18) differs from the Hatano–Sasa relation [31] in the sense that the quantity to be averaged over repeated experiments does not involve the probability distribution of the system.

### 3.4. Symmetries in protocols starting from a stationary state with a canonical distribution

For some systems, such as the two-spin model studied in [14], the stationary distribution when the thermostats are at the inverse temperatures  $\beta_1$  and  $\beta_2$  proves to be a canonical distribution at the effective inverse temperature  $\beta_\star(\beta_1, \beta_2)$ .

When the system is prepared in a stationary state between two heat baths at the inverse temperatures  $\beta_1^0$  and  $\beta_2^0$  and then put in thermal contact with two thermostats at the inverse temperatures  $\beta_1$  and  $\beta_2$  at time  $t_0 = 0$ , the protocol describes the relaxation from a given stationary state corresponding to  $(\beta_1^0, \beta_2^0)$  to another stationary state corresponding to  $(\beta_1, \beta_2)$ . When the initial stationary state has the canonical distribution at the effective inverse temperature  $\beta_\star^0 = \beta_\star(\beta_1^0, \beta_2^0)$ , the argument of the previous subsection can be repeated and the equalities (3.17) and (3.18) still hold with  $\beta_0$  replaced by  $\beta_\star^0$  and  $\Delta_{\text{exch}}^{\text{excs}, \beta_0} S$  replaced by

$$\Delta_{\text{exch}}^{\text{excs}, \beta_\star^0} S(Q_1, Q_2) = (\beta_1 - \beta_\star^0) Q_1 + (\beta_2 - \beta_\star^0) Q_2. \quad (3.19)$$

When the system is already in the stationary state corresponding to the inverse temperatures  $\beta_1$  and  $\beta_2$  at time  $t_0 = 0$ , the equalities (3.17) and (3.18) for  $\Delta_{\text{exch}}^{\text{excs}, \beta_0} S$  still hold with  $\beta_\star(\beta_1, \beta_2)$  in place of  $\beta_0$ :

$$\frac{P_{\text{st}}(\Delta_{\text{exch}}^{\text{excs}, \beta_\star} S)}{P_{\text{st}}(-\Delta_{\text{exch}}^{\text{excs}, \beta_\star} S)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \beta_\star} S}, \quad (3.20)$$

where the subscript ‘st’ in the notation for the probability is a reminder of the fact that the initial configurations are distributed according to the stationary measure, which is equal to  $P_{\text{can}}^{\beta_\star}$  in the present case. Another detailed fluctuation relation involving the forward histories for the original dynamics and the backward histories for the dual reversed dynamics is derived in [32] for the case where the external parameters also vary during the time interval  $[t_0, t]$ ; these considerations are out of the scope of the present paper.

## 4. Extension of previous results to a larger class of models

### 4.1. Generic expression of exchange entropy variation

In this section we consider the generic case where the finite-size system  $S$  is made of  $\nu_s$  species of mobile elementary constituents and can occupy a domain whose boundaries may be mobile interfaces. The degrees of freedom of every elementary constituent involve the site where it sits in discretized space and some possible internal degrees of freedom. In the following we call degrees of freedom of a configuration  $C$  of the system  $S$  the degrees of freedom of the elementary constituents in this configuration. (The number of constituents of every species may vary from one configuration to another.) When some boundaries are mobile interfaces, the description of any configuration  $C$  of the system not only involves the values of its degrees of freedom but it is also specified by the positions of the interfaces that surround the domain, called  $D(C)$ , that the system  $S$  can occupy. For each configuration  $C$  one can define the following global quantities: the energy  $\mathcal{E}(C)$ , the volume  $v(C)$  of  $D(C)$  and the total number of elementary constituents  $n(C) = \sum_{s=1}^{\nu_s} n_s(C)$ , where  $n_s(C)$  is the number of elementary constituents of species  $s$  that sit in  $D(C)$ . All these quantities are assumed to take a finite number of values. The system  $S$  is in contact with several macroscopic bodies  $B_a$ s.

A crucial assumption is that in the course of the ergodic deterministic microscopic dynamics of the whole system ( $S$  and the large parts  $B_a$ ), for a given configuration  $C$ , the domain  $D(C)$  can be divided in several disjoint subdomains  $D_a(C)$  s such that some boundary portion of  $D_a(C)$  can move only thanks to a corresponding volume variation of large part  $B_a$ , and the values of the degrees of freedom that sit inside  $D_a(C)$  can vary only by exchanging microscopically conserved quantities (energy and/or matter) with the corresponding large part  $B_a$ . Then a jump of system  $S$  from configuration  $C$  to another one  $C'$  is allowed only if  $D(C)$  and  $D(C')$  differ by a displacement of some boundary portion of only one  $D_a(C)$  and by different values of the degrees of freedom inside  $D_a(C)$  and  $D_a(C')$ ; then we use the notation  $C' \in \mathbb{F}_a(C)$ . Moreover, the corresponding jump of the microscopic configuration of  $B_a$  is such that conservation rules hold for the sum of the energies of  $S$  and  $B_a$ ,  $\mathcal{E}(C') + E'_a = \mathcal{E}(C) + E_a$ , for the sum of the volumes that they occupy,  $v(C') + V'_a = v(C) + V_a$ , and for the sum of the numbers of elementary constituents of species  $s$  that they contain,  $n_s(C') + N'_{a,s} = n_s(C) + N_{a,s}$ , where  $E_a$ ,  $V_a$  and the  $N_{a,s}$  are the values of the extensive

parameters that characterize body  $B_a$  (and the prime denotes their values after the configuration jump). For instance, if system  $S$  is a mobile diathermal thin solid wall separating a vessel in two parts filled with gases kept at different temperatures and pressures, then  $S$  can be viewed as made of two layers of constituents, each of which interacts respectively with body  $B_1$  and  $B_2$ . Then an infinitesimal displacement of  $S$  such that the volume of  $B_1$  increases while that of  $B_2$  decreases by the same absolute amount can be decomposed into two microscopic configuration jumps of the global system: in the first (second) jump only the layer in contact with  $B_2$  ( $B_1$ ) moves and the volume of  $S$  increases (decreases), and after two jumps the volume of  $S$  has retrieved its initial value.

Then the mesoscopic Markovian dynamics defined according to the prescription of section 2.2 is such that, when energy, volume and matter are exchanged, the transition rates obey the microcanonical detailed balance

$$\frac{W(C', E'_a, V'_a, \{N'_{a,s}\} \leftarrow C, E_a, V_a, \{N_{a,s}\})}{W(C, E_a, V_a, \{N_{a,s}\} \leftarrow C', E'_a, V'_a, \{N'_{a,s}\})} = \frac{\Omega_a(E'_a, V'_a, \{N'_{a,s}\})}{\Omega_a(E_a, V_a, \{N_{a,s}\})} \quad (4.1)$$

with

$$\frac{\Omega_a(E'_a, V'_a, \{N'_{a,s}\})}{\Omega_a(E_a, V_a, \{N_{a,s}\})} \equiv e^{S_a^B(E'_a, V'_a, \{N'_{a,s}\}) - S_a^B(E_a, V_a, \{N_{a,s}\})}, \quad (4.2)$$

where  $\Omega_a(E_a, V_a, \{N_{a,s}\})$  is the number of configurations (or microstates) of large part  $B_a$  when it is isolated. In the following, in the spirit of the notations used by Callen [1], we denote by  $X_i^{(a)}$  the extensive macroscopic parameters of  $B_a$ , namely in the generic case

$$X_0^{(a)} \equiv E_a, \quad X_1^{(a)} \equiv V_a, \quad X_{1+s}^{(a)} = N_{a,s}. \quad (4.3)$$

The total number of elementary constituents in  $B_a$  is  $N_a = \sum_s N_{a,s}$ . The microscopic conservation rules that are associated with (4.1) read

$$X_i'^{(a)} - X_i^{(a)} = -[x_i(C') - x_i(C)] \quad \text{if } C' \in \mathbb{F}_a(C), \quad (4.4)$$

with the same notations for system  $S$  as those introduced in (4.3) for the macroscopic bodies.

If the bodies  $B_a$  are so large that they can be described by a thermodynamic limit, then, in a transient regime where the macroscopic extensive parameters  $X_i^{(a)}$  s have negligible relative variations,  $B_a$  remains at thermodynamic equilibrium. The thermodynamic entropy per elementary constituent,  $S_a^{TH}/N_a$ , coincides with the thermodynamic limit of the Boltzmann entropy per elementary constituent,  $S_a^B/N_a$ . The intensive thermodynamic parameter  $F_i^{(a)}$  conjugate to the extensive quantity  $X_i^{(a)}$  by  $F_i^{(a)} \equiv \partial S_a^{TH}/\partial X_i^{(a)}$  (with  $X_i^{(a)}$  defined in (4.3)) is given by

$$F_0^{(a)} \equiv \beta_a, \quad F_1^{(a)} \equiv \beta_a P_a, \quad F_{1+s}^{(a)} = -\beta_a \mu_{a,s}, \quad (4.5)$$

where  $\beta_a$  is the inverse thermodynamic temperature,  $P_a$  the thermodynamic pressure and  $\mu_{a,s}$  the chemical potential of species  $s$  in  $B_a$ . Then from the relations (4.1) and (4.2), one can show, as in section 2.3, that in the transient regime the transition rates obey the local detailed balance (2.26) where  $\delta_{\text{exch}} S(C' \leftarrow C)$  is opposite to the infinitesimal variation at fixed intensive parameters of the thermodynamic entropy of the reservoir  $B_a$  that causes the jump from  $C$  to  $C'$  under the conservation rules (4.4). Therefore, if  $C' \in \mathbb{F}_a(C)$

$$\delta_{\text{exch}} S(C' \leftarrow C) = \beta_a [\mathcal{E}(C') - \mathcal{E}(C)] + \beta_a P_a [v(C') - v(C)] - \beta_a \sum_s \mu_{a,s} [n_s(C') - n_s(C)]. \quad (4.6)$$

In the case of pure thermal contact, the volume of system  $S$  does not vary,  $v(C) = v(C')$ , and there is no matter exchange; then  $\delta_{\text{exch}} S(C' \leftarrow C) = \beta_a [\mathcal{E}(C') - \mathcal{E}(C)]$  coincides with  $\beta_a$  times the opposite of the variation of the internal energy of  $B_a$ , which is equal in that case to the heat given by  $B_a$  at constant volume. If system  $S$  and macroscopic body  $B_a$  are compressible, then, during energy exchanges such that the thermodynamic pressure  $P_a$  of  $B_a$  remains fixed, the variation of the internal energy of the macroscopic body  $B_a$  involves both heat and pressure work; then  $\delta_{\text{exch}} S(C' \leftarrow C) = \beta_a [\mathcal{E}(C') - \mathcal{E}(C)] + \beta_a P_a [v(C') - v(C)]$  coincides with  $\beta_a$  times the opposite of the variation of the enthalpy of  $B_a$ , which is equal in that case to the heat given by  $B_a$  at constant pressure. Moreover, system  $S$  may receive work from some conservative external forces  $f_b^{\text{ext}}$  (such as gravitational or electrical fields), each of which causes the variation of some global coordinate  $Z_b(C)$  of the system (such as its mass center or its electrical barycenter) but does not act upon the macroscopic bodies. In that case the mechanical energy  $\mathcal{E}(C)$  of system  $S$  in configuration  $C$  is the sum of its internal energy  $\mathcal{E}_{\text{int}}(C)$  and an external potential energy  $\mathcal{E}_{\text{ext}}(C)$ . In all these situations the distances between the possible energy levels  $\mathcal{E}$  are time-independent, and during the evolution only the occupation of the energy levels is modified, contrarily to the case where a time-dependent force acts on the system by changing the spacing between energy levels.

In order to handle compact notations for the successive variations  $\delta_{\text{exch}} S$  in the course of the history of system  $S$ , let us introduce the notation  $\delta\chi_i^{(a)}(C' \leftarrow C)$  for the quantity with index  $i$  received by the system from reservoir  $B_a$  when the system jumps from  $C$  to  $C'$ , with the same convention as in definition (2.24), namely

$$\begin{cases} \delta\chi_i^{(a)}(C' \leftarrow C) = x_i(C') - x_i(C) & \text{if } C' \in \mathbb{F}_a(C) \\ \delta\chi_i^{(a)}(C' \leftarrow C) = 0 & \text{otherwise} \end{cases}. \quad (4.7)$$

(In the case where  $C' \in \mathbb{F}_a(C)$  but where in fact reservoir  $B_a$  does not exchange quantity with index  $i$  in the jump from  $C$  to  $C'$ ,  $x_i(C') - x_i(C) = 0$ ). Then the exchange entropy variation in a jump takes the form

$$\delta_{\text{exch}} S(C' \leftarrow C) = \sum_i \sum_{a \in R(i)} F_i^{(a)} \delta\chi_i^{(a)}(C' \leftarrow C), \quad (4.8)$$

where the first sum runs over the indices  $i$  of the extensive quantities defined in (4.3), the second sum runs over the indices of the reservoirs that indeed can exchange quantity  $i$  with the system and  $R(i)$  denotes the set of the latter reservoirs.

#### 4.2. Consequences of LDB at finite time

In the form (2.26) where it involves the microscopic exchange entropy variation  $\delta_{\text{exch}} S(C' \leftarrow C)$  associated with a jump from configuration  $C$  to configuration  $C'$ , the local detailed balance entails the symmetry (3.9) between the probabilities for time-reversed histories. At a more mesoscopic level, let us compare the probability of all evolutions from configuration  $C_0$  to configuration  $C_f$ , in the course of which the system receives given cumulative quantities with index  $i$   $\mathcal{X}_i^{(a)} = \sum \delta\chi_i^{(a)}$  from each reservoir  $B_a$ , and the probability of the reversed evolutions, namely evolutions from  $C_f$  to  $C_0$  where the cumulative quantities are  $-\mathcal{X}_i^{(a)}$ s. The symmetry (3.11) written in the case of thermal contact takes the following form in the generic case

$$\frac{P\left(C_f \mid \left\{\mathcal{X}_i^{(a)}\right\}; t \mid C_0\right)}{P\left(C_0 \mid \left\{-\mathcal{X}_i^{(a)}\right\}; t \mid C_f\right)} = e^{-\Delta_{\text{exch}} S\left(\left\{\mathcal{X}_i^{(a)}\right\}\right)}, \quad (4.9)$$

with, according to (4.8),

$$\Delta_{\text{exch}} S\left(\left\{\mathcal{X}_i^{(a)}\right\}\right) = \sum_i \sum_{a \in R(i)} F_i^{(a)} \mathcal{X}_i^{(a)}. \quad (4.10)$$

In (4.9) and in the formulæ derived from it in the following,  $\mathcal{X}_i^{(a)}$  occurs only if reservoir  $\mathcal{B}_a$  indeed exchanges quantity with index  $i$ . The ratio of probabilities in (4.9) does not explicitly depend on the initial and final configurations  $C_0$  and  $C_f$ . There is only an implicit dependence on these configurations through the conservation rules that the cumulative exchange quantities  $\mathcal{X}_i^{(a)}$  for a given history must satisfy, namely  $\sum_{a \in R(i)} \mathcal{X}_i^{(a)} = x_i(C_f) - x_i(C_0)$ .

At the macroscopic level, namely when only the exchanges of extensive quantities with the reservoirs are measured, there appears a symmetry for transient regimes where the system is initially prepared in some equilibrium state with a fixed intensive parameter  $F_i^0$  for each configuration observable  $x_i$  and then is suddenly put into contact with reservoirs with thermodynamic parameters  $F_i^{(a)}$  s that drive the system into a non-equilibrium state. The symmetry involves the excess exchange entropy variation  $\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S$ , defined as the difference between the exchange entropy variation under the non-equilibrium external constraints  $F_i^{(a)}$  s, defined in (4.10), and the corresponding variation under the equilibrium conditions where for all reservoirs that exchange quantity with index  $i$  the thermodynamic parameter has the same value  $F_i^0$ ,

$$\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}}\left(\left\{\mathcal{X}_i^{(a)}\right\}\right) \equiv \Delta_{\text{exch}} S\left(\left\{\mathcal{X}_i^{(a)}\right\}\right) - \sum_i F_i^0 \sum_{a \in R(i)} \mathcal{X}_i^{(a)}. \quad (4.11)$$

When the system is prepared in the equilibrium state with probability distribution  $P_{\text{eq}}(\{F_i^0\})$  and put into contact with reservoirs with thermodynamic parameters  $F_i^{(a)}$  s at the initial time of the measurements of exchanged quantities, the joint probability for the cumulative exchange quantities  $\mathcal{X}_i^{(a)}$  obeys the symmetry relation at any finite time,

$$\frac{P_{P_{\text{eq}}(\{F_i^0\})}\left(\left\{\mathcal{X}_i^{(a)}\right\}\right)}{P_{P_{\text{eq}}(\{F_i^0\})}\left(\left\{-\mathcal{X}_i^{(a)}\right\}\right)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S\left(\left\{\mathcal{X}_i^{(a)}\right\}\right)}. \quad (4.12)$$

As a consequence, the excess exchange entropy variation  $\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S$  obeys the symmetry relation at any finite time, or ‘detailed fluctuation relation’,

$$\frac{P_{P_{\text{eq}}(\{F_i^0\})}\left(\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S\right)}{P_{P_{\text{eq}}(\{F_i^0\})}\left(-\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S\right)} = e^{-\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S}. \quad (4.13)$$

The latter relation itself entails the identity, or ‘integral fluctuation relation’,

$$\left\langle e^{\Delta_{\text{exch}}^{\text{excs}, \{F_i^0\}} S} \right\rangle_{P_{\text{eq}}(\{F_i^0\})} = 1. \quad (4.14)$$

We notice that a relation similar to (4.12) has been derived from the fluctuation relation for the entropy production [18, 19] in a slightly different protocol where several reservoirs



exchange both energy and matter with the system of interest and the system is prepared at equilibrium with one reservoir [33].

## Appendix A. Property of the coarse grained dynamics

In the present appendix we derive the property (2.5) valid over a period of the ergodic deterministic microscopic dynamics  $\mathcal{T}$  when  $\mathcal{T}$  respects both the conservation of  $E_{\text{dec}}$  and the interaction pattern specified when the conservation law (2.2) was introduced.

Though we believe that a general development could be pursued, we prefer to concentrate on a specific model at this point. The system is made of two large parts and a small one, which is reduced to two Ising spins  $\sigma_1, \sigma_2 = \pm 1$ , each one directly in contact with one of the large parts. So a configuration  $C$  can be written as  $C = (C_1, \sigma_1, \sigma_2, C_2)$ . We assume that, when the small part is isolated, its energy  $\mathcal{E}(\sigma_1, \sigma_2)$  does not describe independent spins. Moreover, the microscopic dynamics  $\mathcal{T}$  conserves the energy  $E_{\text{dec}}(C)$  where the interactions between parts is neglected, namely  $E_{\text{dec}}(C) \equiv E_1(C_1) + E_2(C_2) + \mathcal{E}(\sigma_1, \sigma_2)$ . The remnant of interactions between the parts is embodied in the following restrictions. For any  $C$ ,  $\mathcal{T}(C)$  is obtained from  $C$  by one of the following operations:

- (I) a flip of spin  $\sigma_1$  together with a change in  $C_1$  and a possible change in  $C_2$  such that  $E_1(C_1) + \mathcal{E}(\sigma_1, \sigma_2)$  and  $E_2(C_2)$  both remain constant (i.e. the energy needed to flip the spin  $\sigma_1$  entirely comes from or goes to large part 1).
- (II) a flip of spin  $\sigma_2$  together with a change in  $C_2$  and a possible change in  $C_1$  such that  $E_1(C_1)$  and  $E_2(C_2) + \mathcal{E}(\sigma_1, \sigma_2)$  both remain constant (i.e. the energy needed to flip the spin  $\sigma_2$  entirely comes from or goes to large part 2).
- (III) a change in  $C_1$  and/or  $C_2$  but no flip of  $\sigma_1$  or  $\sigma_2$ , such that  $E_1(C_1)$  and  $E_2(C_2)$  both remain constant, as well as  $\mathcal{E}(\sigma_1, \sigma_2)$ .

In order to build an effective mesoscopic dynamics we just keep track of  $(E_1, \sigma_1, \sigma_2, E_2)$  as a function of time. Therefore during the time evolution of a given configuration  $C$  of the whole system we concentrate only on time steps at which a change of type (I) or (II) occurs, namely when either spin  $\sigma_1$  or spin  $\sigma_2$  is flipped with known corresponding variations in  $E_1$  and  $E_2$ . We do not follow precisely the changes (III) that modify the configurations of large parts without changing the energy of any part (either  $E_1$ ,  $E_2$  or  $\mathcal{E}(\sigma_1, \sigma_2)$ ). The possible changes are

$$\begin{aligned} (E_1, \sigma_1, \sigma_2, E_2) &\rightarrow (E'_1, -\sigma_1, \sigma_2, E_2) \quad \text{with} \\ E'_1 &= E_1 + \mathcal{E}(\sigma_1, \sigma_2) - \mathcal{E}(-\sigma_1, \sigma_2) \quad \text{type(I)} \end{aligned} \quad (\text{A.1})$$

and

$$\begin{aligned} (E_1, \sigma_1, \sigma_2, E_2) &\rightarrow (E_1, \sigma_1, -\sigma_2, E'_2) \quad \text{with} \\ E'_2 &= E_2 + \mathcal{E}(\sigma_1, \sigma_2) - \mathcal{E}(\sigma_1, -\sigma_2) \quad \text{type(II)} \end{aligned} \quad (\text{A.2})$$

Starting from some initial configuration  $(E_1^0, \sigma_1^0, \sigma_2^0, E_2^0)$ , some set of possible  $(E_1, \sigma_1, \sigma_2, E_2)$  will be visited during the time evolution over a period of  $\mathcal{T}$ , and it is useful to view this set as the vertices of a graph whose edges connect two vertices if the system can jump from one to the other by a single change of type (I) or (II). This graph can be chosen to be unoriented because a transformation of type (I) or of type (II) is its own inverse. Then a trajectory over a period of the underlying deterministic dynamics corresponds to a closed walk on this graph, which summarizes the coarse graining due to the macroscopic description

of the large parts. During a period of the microscopic dynamics the closed walk on the graph goes through each edge a number of times.

The main observation is that, since energy  $\mathcal{E}(\sigma_1, \sigma_2)$  does not describe independent spins, the graph has the topology of a segment. Indeed, the graph is connected by construction, but each vertex has at most two neighbors. So the graph is either a segment or a circle. Let us suppose that it is a circle. Then one can go from  $(E_1^0, \sigma_1^0, \sigma_2^0, E_2^0)$  to itself by visiting each edge exactly once, i.e. by an alternation of moves of type (I) and (II). After two steps both spins in the small part are flipped, so the total length of the circle is a multiple of 4. But after 4 steps a definite amount of energy has been transferred between the two large parts, namely the energy in the first large part has changed by  $\mathcal{E}(\sigma_1, \sigma_2) - \mathcal{E}(-\sigma_1, \sigma_2) + \mathcal{E}(-\sigma_1, -\sigma_2) - \mathcal{E}(\sigma_1, -\sigma_2)$  and a trivial computation shows that this cannot vanish unless  $\mathcal{E}(\sigma_1, \sigma_2)$  describes two independent spins, a possibility which has been discarded. This excludes the circle topology.

Since the graph is a segment, any closed walk on the graph traverses a given edge the same number of times in one direction and in the other one. As a consequence, during a period of the microscopic dynamics  $\mathcal{T}$ , the motion induced by  $\mathcal{T}$  on the graph is such that the number of transitions of type (I)  $(E_1, \sigma_1, \sigma_2, E_2) \rightarrow (E_1', -\sigma_1, \sigma_2, E_2)$  is equal to the number of their inverse transitions  $(E_1', -\sigma_1, \sigma_2, E_2) \rightarrow (E_1, \sigma_1, \sigma_2, E_2)$ , where the relation between  $E_1'$  and  $E_1$  is given in (A.1). The same considerations apply for transition rates associated with the flipping of  $\sigma_2$ . The result is summarized in (2.5).

For a more general discrete system, the mesoscopic time evolution can again be characterized by the time steps where the small system variables are flipped while the changes in the large parts are only macroscopically described by their net energies. An analogous graph can be constructed but it can be much harder to analyze its topology, which is the crucial knowledge needed to exploit the consequences of ergodicity. These consequences are most stringent for a tree. There is no reason *a priori* why the graph should be a tree, but what this implies, namely that ratios for the transition rates involving the small part and a large part are given by ratios of energy level degeneracies in the large part, is physically quite appealing.

## Appendix B. The Markovian approximation

This appendix is a short digression on mathematics. The aim is to briefly recall a trick allowing us to replace a fixed sequence of symbols by a random one with ‘analogous’ statistical properties, and then to combine this trick with a coarse graining procedure.

### B.1. Discrete time stochastic approximation

Suppose  $w \equiv x_1 x_2 \dots x_N$  is a given finite sequence of elements of a finite set  $S$ . It is convenient to assume that this sequence is periodic, i.e. that  $x_{N+1} \equiv x_1$ . For  $x \in S$ , set  $N_x \equiv \#\{i \in [1, N], x_i = x\}$ , i.e.  $N_x$  is the number of occurrences of  $x$  in the sequence  $w$ . There is no loss of generality in assuming that  $N_x \neq 0$  for every  $x \in S$ , should it lead to consider a smaller  $S$ . For  $x, x' \in S$  set  $N_{xx'} \equiv \#\{i \in [1, N], x_i = x, x_{i+1} = x'\}$ , i.e.  $N_{xx'}$  is the number of occurrences of the pattern  $xx'$  in the sequence  $w$ . Notice that we accept that  $x = x'$  in this definition. Of course, we could look at the occurrence of more general patterns. By definition, we have  $\sum_{x' \in S} N_{xx'} = \sum_{x' \in S} N_{x'x} = N_x$ . The result we want to recall is the following.

There is a single time-homogeneous irreducible Markov matrix on  $S$  that fulfils the following two requirements. First, in the stationary state of the corresponding discrete-time

stochastic evolution, the probability  $P_{\text{st}}(x', i + 1; x, i)$  that a sample  $\hat{x}$  takes the value  $x$  at time  $i$  and the value  $x'$  at time  $i + 1$ <sup>11</sup> is equal to the frequency of the pattern  $xx'$  in the sequence  $w$ , namely

$$P_{\text{st}}(x', i + 1; x, i) = \frac{N_{xx'}}{N}. \quad (\text{B.1})$$

Second, the stationary probability that the random variable  $\hat{x}$  takes the value  $x$  at any time  $i$  is equal to the frequency of  $x$  in the sequence  $w$ , namely

$$P_{\text{st}}(x) = \frac{N_x}{N}. \quad (\text{B.2})$$

In fact (B.2) is a consequence of (B.1), because of the relations  $P_{\text{st}}(x) = \sum_{x' \in S} P_{\text{st}}(x', i + 1; x, i)$  and  $\sum_{x' \in S} N_{xx'} = N_x$ . To say it in words, there is a unique time-homogeneous irreducible Markov chain whose stationary statistics for patterns of length 1 or 2 is the same as the corresponding statistics in  $w$ .

The proof is elementary. By the Markov property, the Markov matrix element from  $x$  to  $x'$ , denoted by  $T(x' \leftarrow x)$ , must satisfy the relation  $P_{\text{st}}(x', i + 1; x, i) = T(x' \leftarrow x)P_{\text{st}}(x)$ , so the only candidate is

$$T(x' \leftarrow x) = \frac{N_{xx'}}{N_x}. \quad (\text{B.3})$$

Conversely, the corresponding matrix is obviously a Markov matrix ( $\sum_{x' \in S} T(x' \leftarrow x) = 1$  since  $\sum_{x' \in S} N_{xx'} = N_x$ ), and it is irreducible, because, as  $w$  contains all elements of  $S$ , transitions within  $w$  allow us to go from every element of  $S$  to every other one. Checking that for this Markov matrix the stationary measure, namely the solution of  $\sum_{x \in S} T(x' \leftarrow x)P_{\text{st}}(x) = P_{\text{st}}(x')$ , is given by (B.2) boils down to the identity  $\sum_{x \in S} N_{xx'} = N_{x'}$  recalled above, and then the two-point property (B.1) follows. This finishes the proof.

In the very specific case where  $x_1, x_2, \dots, x_N$  are all distinct, i.e.  $|S|$ , the cardinal of  $S$ , is equal to  $N$ ,  $N_x = 1$  for all  $x \in S$  and  $N_{xx'} = \delta_{x', x_{i+1}}$  where  $i$  is such that  $x_i = x$ . Then the only randomness lies in the choice of the initial distribution, and each trajectory of the Markov chain reproduces  $w$  up to a translation of all indices. If  $N$  is large and  $|S|$  is  $\sim N$ , slightly weaker but analogous conclusions survive. A more interesting case is when  $|S| \ll N$  by many orders of magnitude as discussed in next subsection.

This trick has been used, for instance, to write a random text ‘the Shakespeare way’ by computing the statistics of sequences of two words in one of his books.

By definition, the Markovian approximation reproduces the statistics of the original sequence only for length 1 and length 2 patterns. It is a delicate issue to decide whether or not it also does a reasonable job for other patterns. For instance, the random Shakespeare book certainly looks queer. Various physical but heuristic arguments suggest that, for the kind of sequences  $w$  relevant for this work, the Markov approximation is quite good, but we shall not embark on that.

## B.2. Continuous time approximation

By the very same argument, there is a time-homogeneous irreducible Markov transition matrix on  $S$  (unique up to a time scale  $\tau$ ) such that, in the stationary state of the corresponding continuous-time stochastic evolution, the expected number of transitions from  $x$  to  $x' \neq x$  per

<sup>11</sup> In the whole paper we use the convention that the evolution (here given by the joint probability  $P_{\text{st}}(x', i + 1; x, i)$  or the transition matrix  $T$ ) is written from the right to the left as in quantum mechanics.

unit time is  $N_{xx'}/\tau$ . The formula one finds for the transition rate is

$$W(x' \leftarrow x) = \frac{N_{xx'}}{\tau N_x} \text{ for } x \neq x'. \quad (\text{B.4})$$

The continuous-time approximation becomes more natural in the case when  $|S|$ , the cardinal of  $S$ , is such that  $|S| \ll N$ , while for all  $x$   $N_{xx} \sim N_x$  and for all  $x \neq x'$   $N_{xx'} \ll N_x$ , which means that transitions are rare and most of the time  $x$  follows  $x$  in the sequence  $w$ . Again, one can argue that for the kind of sequences  $w$  relevant for this work, this is guaranteed by physics. Then taking  $\tau$  (in some macroscopic time unit) of the order of the largest value of the  $N_{xx'}/N_x$ ,  $x \neq x'$ , one ends with a Markov transition matrix with elements of order unity (in some macroscopic inverse time unit), and  $t_i = \tau i$  can be taken as the physical macroscopic time.

To summarize, in this work, we shall systematically associate to certain sequences  $w$  a continuous-time Markov process and exploit properties of  $w$  to constrain the structure of  $W(x' \leftarrow x)$ .

A natural application of the above ideas is to the case where the sequence  $w$  arises from some coarse graining procedure. One starts from a sequence  $\omega = \xi_1 \xi_2 \dots \xi_N$  where  $\xi_1, \xi_2, \dots, \xi_N$  belong to a set  $\Sigma$  that is so large that  $\omega$  cannot be stored, and that only some of its features can be kept. Say we partition  $\Sigma \equiv \bigcup_{x \in S} \Sigma_x$  where  $S$  is of reasonable size. Then all we keep of  $\omega$  is  $w = x_1 x_2 \dots x_N$  where, for  $i \in [1, N]$ ,  $x_i$  is substituted for  $\xi_i$  when  $\xi_i \in \Sigma_{x_i}$ . In the applications we have in mind,  $\Sigma$  is an  $N$ -element set, i.e. all terms in the sequence  $\omega$  are distinct. In that case, even if  $\omega$  is constructed in a perfectly deterministic way, by saying who follows who in the sequence, such a description is unavailable on  $w$ , and  $w$  may well look quite random, so the Markov chain approximation is worth a try. In fact,  $|S| \ll N$  and we shall take as a physical input that transitions are rare, so that the (continuous-time) Markov process is an excellent approximation to the (discrete time) Markov chain.

### Appendix C. Microcanonical detailed balance and time reversal invariance in Hamiltonian dynamics

A microcanonical detailed balance similar to (2.11) can be derived in another context where the discrete microscopic variables of the whole system evolving under an ergodic energy-conserving map are replaced by continuous microscopic coordinates  $\xi$  in phase space evolving under a deterministic dynamics whose Hamiltonian  $H[\xi]$  is an even function of momenta, and where the role of the mesoscopic configurations  $(C, \underline{E})$  is played by some continuous mesoscopic variables  $x[\xi]$  that are even functions of momenta (with the same notations as in section 2.2.1).

A summary of the argument is the following. From the viewpoint of the statistical ensemble theory, the initial position of the whole system in phase space is not known, and it is assumed to be uniformly randomly distributed in the energy shell  $E = H[\xi]$ , where  $E$  is the value of the energy of the full system at the initial time  $t = 0$ . In other words, the initial probability distribution  $P_0(\xi)$  is such that  $d\xi P_0(\xi) \equiv d\xi \delta(H[\xi] - E) / \int d\xi' \delta(H[\xi'] - E)$ . Since both the Liouville measure  $d\xi$  and the energy  $H[\xi]$  are conserved when the system evolves in phase space from an initial position  $\xi$  at time  $t=0$  to a position  $f_t(\xi)$  at time  $t$ ,  $P_0(\xi)d\xi$  is conserved by the Hamiltonian dynamics. As a consequence the probability that at time  $t$  the set of mesoscopic variable  $x$  takes the value  $x_1$ , defined as  $P_0(x_1, t) \equiv \int d\xi P_0(\xi) \delta(x[f_t(\xi)] - x_1)$  is in fact independent of time, and it coincides with the microcanonical distribution  $P_{mc}(x_1) \equiv \int d\xi P_0(\xi) \delta(x[\xi] - x_1)$ .

Moreover, since the Hamiltonian is assumed to be an even function of momenta, the microscopic dynamics is invariant under time reversal:  $[Rf_i Rf_i](\xi) = \xi$ , where  $R$  is the operator that changes every momentum into its opposite. As a consequence, if the mesoscopic variables  $x[\xi]$  are even functions of momenta, the time-displaced joint probability that the set  $x$  takes the value  $x_1$  at time  $t = 0$  and the value  $x_2$  at time  $t$ , defined as  $P_{\tilde{h}}(x_2, t; x_1, 0) = \int d\xi P_0(\xi) \delta(x[f_t(\xi)] - x_2) \delta(x[\xi] - x_1)$ , is invariant under the exchange of the times at which  $x_1$  and  $x_2$  occur,

$$P_{\tilde{h}}(x_2, t; x_1, 0) = P_{\tilde{h}}(x_1, t; x_2, 0). \quad (\text{C.1})$$

Moreover, the displaced joint probability is invariant under time translation.

Then the approximation scheme by a Markov process for the time-displaced joint probability of the continuous mesoscopic variables  $x$  is the same as that we have used for the two-body ergodic average of the discrete mesoscopic configurations  $(C, \underline{E})$  in section 2.2.1. One assumes that the evolution of the mesoscopic variable  $x$  described by  $P_{\tilde{h}}(x_2, t; x_1, 0)$  can be approximated by an homogeneous Markovian stochastic process whose stationary distribution  $P_{st}(x)$  is the time-independent probability  $P_{\tilde{h}}(x)$  and whose transition rates, denoted by  $W(x' \leftarrow x)$ , are determined by the identification  $P_{\tilde{h}}(x', dt; x, 0) \equiv W(x' \leftarrow x) P_{\tilde{h}}(x) \times dt$ . Then the time reversal symmetry property (C.1) for the joint probability of  $x$  and  $x'$  at different times and the fact that  $P_{\tilde{h}}(x)$  coincides with the microcanonical distribution  $P_{mc}(x)$  lead to the microcanonical detailed balance

$$W(x' \leftarrow x) P_{mc}(x) = W(x \leftarrow x') P_{mc}(x'). \quad (\text{C.2})$$

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