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Rates for irreversible Gibbsian Ising models

Claude Godrèche

Institut de Physique Théorique, CEA Saclay and CNRS
91191 Gif-sur-Yvette cedex, France

Abstract. Dynamics under which a system of Ising spins relaxes to a stationary state with Boltzmann-Gibbs measure and which do not fulfil the condition of detailed balance are irreversible and asymmetric. We revisit the problem of the determination of rates yielding such a stationary state for models with single-spin flip dynamics. We add some supplementary material to this study and confirm that Gibbsian irreversible Ising models exist for one and two-dimensional lattices but not for the three-dimensional cubic lattice. We also analyze asymmetric Gibbsian dynamics in the limit of infinite temperature. We finally revisit the case of a linear chain of spins under asymmetric conserved dynamics.

1. Introduction

The one-dimensional Glauber-Ising model was probably the first example of a strongly interacting system with soluble dynamics showing how a system relaxes to equilibrium [1]. The preliminary question to solve was the choice of rates ensuring that a ferromagnetic chain of Ising spins relaxes towards equilibrium under single spin flip dynamics. The question is settled by requiring the rates at which spins flip to fulfil the condition of detailed balance with respect to the Hamiltonian defining the model [1].

Conversely, one may ask whether it is still possible for the system to reach a stationary state with the same Boltzmann-Gibbs measure by an appropriate choice of rates if one relinquishes this constraint, i.e., if only global balance is imposed. The dynamics now becomes generically irreversible and asymmetric: the flipping spin is not equally influenced by its neighbours. This question was addressed some time ago by Künsch [2], who exhibited examples of such a dynamics, in the particular case where it is totally asymmetric, in one and two dimensions. The problem was thoroughly revisited in ref. [3], with the following conclusions.

The study made in [3] shows that irreversible Gibbsian Ising models exist for one and two-dimensional lattices but not for the three-dimensional cubic lattice. More precisely, imposing the up-down spin symmetry, the rate function yielding an irreversible Gibbsian stationary state for the linear chain depends on 3 arbitrary parameters. In two dimensions, the number of arbitrary parameters is respectively equal to 10 for the square lattice, and to 35 for the triangular lattice. Yet, for the totally asymmetric dynamics where only half of the spins have an influence on the flipping spin, the rate function is *unique*, up to a time scale, for these three geometries. In contrast, for the cubic lattice no such rate function is found, i.e., global balance enforces detailed balance (see Table 4).

The aim of the present work is to add some supplementary material to the same study, making the method used more easy to grasp and illustrating its outcomes on more examples. In particular we give a fuller account of the method, which relies on linear algebra coupled to the properties of the system under translation invariance, in order to make clearer its generality. We come back on the interplay between coordination and dimension. We explain, on the example of the linear chain, the constraints imposed by the positivity of the rates. We shall also be concerned in restating the statement made in [3], that no such rates do exist for the case of the three-dimensional cubic lattice, as recalled above. To this end we shall give some more details on the analysis in order to substantiate its conclusion. We shall then give a critical reading of a recent paper [4], where it is claimed that there exist irreversible Gibbsian dynamics for the cubic lattice, in contradiction with the study made in [3], and shall dismiss its conclusion on this issue. We shall finally consider the case of Gibbsian asymmetric dynamics at infinite temperature. An appendix is devoted to the study of conserved Gibbsian asymmetric dynamics for the linear chain.†

† The author of ref. [4] recently issued an Erratum [5] where he corrects the claims which lead him to the incorrect prediction mentioned in the Introduction. We nevertheless kept the text of section 6 unchanged because the analysis presented there provides an interesting illustration, on the example chosen in ref. [4], of the fact that global balance enforces detailed balance for the cubic lattice, and explains the mechanism by which this occurs.

2. Starting point

Let us consider N Ising spins on a regular lattice of coordination z , in D dimensions, with periodic boundary conditions. The energy (Hamiltonian) of a configuration $\mathcal{C} = \{\sigma_1, \dots, \sigma_n, \dots, \sigma_N\}$ reads

$$E(\mathcal{C}) = -J \sum_{n,j} \sigma_n \sigma_j, \quad (2.1)$$

where n and j are nearest neighbours.

2.1. Master equation

The dynamics consists in flipping a spin, chosen at random, say spin n , with a rate $w(\mathcal{C}_n|\mathcal{C})$, corresponding to the transition between configurations \mathcal{C} and $\mathcal{C}_n = \{\sigma_1, \dots, -\sigma_n, \dots, \sigma_N\}$. At stationarity, the master equation expresses that losses are equal to gains, and reads

$$P(\mathcal{C}) \sum_n w(\mathcal{C}_n|\mathcal{C}) = \sum_n w(\mathcal{C}|\mathcal{C}_n) P(\mathcal{C}_n). \quad (2.2)$$

We want to find the rate function $w(\mathcal{C}_n|\mathcal{C})$ satisfying this equation when $P(\mathcal{C})$ is the Boltzmann-Gibbs distribution associated to the Hamiltonian (2.1),

$$P(\mathcal{C}) \propto e^{-E(\mathcal{C})/T}. \quad (2.3)$$

After division of both sides by the weight $P(\mathcal{C})$, eq. (2.2) can be rewritten as

$$\sum_n \left(w(\mathcal{C}_n|\mathcal{C}) - w(\mathcal{C}|\mathcal{C}_n) e^{-\Delta E/T} \right) = 0, \quad (2.4)$$

where the change in energy due to the flip reads

$$\Delta E = E(\mathcal{C}_n) - E(\mathcal{C}) = 2J \sigma_n h_n, \quad (2.5)$$

and h_n is the local field $h_n = \sum_j \sigma_j$, due to the z neighbours $\{\sigma_j\}$. We choose a rate function only depending on the local configuration $\{\sigma_n; \{\sigma_j\}\}$ of the central spin σ_n and of its neighbours, and simplify the notation accordingly,

$$w(\mathcal{C}_n|\mathcal{C}) = w(\sigma_n; \{\sigma_j\}). \quad (2.6)$$

Thus, denoting the balance term by

$$B(\sigma_n; \{\sigma_j\}) = w(\sigma_n; \{\sigma_j\}) - w(-\sigma_n; \{\sigma_j\}) e^{-2K\sigma_n h_n}, \quad (2.7)$$

where $K = J/T$, the balance equation (2.4) becomes

$$\sum_n B(\sigma_n; \{\sigma_j\}) = 0. \quad (2.8)$$

This equation can be satisfied either term by term, which gives the detailed balance condition on the rate function,

$$w(\sigma_n; \{\sigma_j\}) = w(-\sigma_n; \{\sigma_j\}) e^{-2K\sigma_n h_n}. \quad (2.9)$$

or as a whole, which is the global balance condition.

2.2. Representation of the rate function on a basis of spin operators

The number of values taken by the rate function is equal to the number of local configurations $\{\sigma_n; \{\sigma_j\}\}$ of the central spin and of its neighbours. There are 2^{z+1} such configurations, i.e., 8 for the chain, 32 for the square lattice, and 128 for the two-dimensional triangular lattice or for the cubic lattice. We hereafter consider the simpler case where we have up-down spin symmetry:

$$w(\sigma_n; \{\sigma_j\}) = w(-\sigma_n; \{-\sigma_j\}). \quad (2.10)$$

The number of possible values of the rate function is therefore halved and is equal to the number of different environments of the central spin σ_n , i.e., of configurations $\{\sigma_j\}$ of its neighbours. There are 2^z such configurations, labelled by the index α , i.e., 4 for the chain, 16 for the square lattice, and 64 for the triangular lattice or for the cubic lattice. We denote the 2^z rates with $\sigma_n = +1$ by w_α and the other 2^z rates, corresponding to $\sigma_n = -1$, by \bar{w}_α :

$$w_\alpha = w(\sigma_n = +1; \{\sigma_j\}_\alpha), \quad \bar{w}_\alpha = w(\sigma_n = -1; \{\sigma_j\}_\alpha). \quad (2.11)$$

The latter are obtained from the former by the spin symmetry relation (2.10), yielding

$$\bar{w}_\alpha = w_{2^z+1-\alpha}, \quad (2.12)$$

(see Tables 1 and 2). For instance, for the linear chain, the rates to be determined are

$$\begin{aligned} w_1 &= w(+; ++), & w_2 &= w(+; +-), \\ w_3 &= w(+; -+), & w_4 &= w(+; --). \end{aligned} \quad (2.13)$$

Table 1. List of local configurations and corresponding values of the rate function for the one-dimensional chain. There are 4 possible rates w_α , with $\sigma_n = +1$, corresponding to the 4 possible configurations $\{\sigma_j\}$, labelled by α , of the two neighbours of the central spin, taken in the order: left, right. The 4 remaining rates \bar{w}_α , with $\sigma_n = -1$, are deduced from the former, due to the spin symmetry (see (2.12)).

α	$\sigma_n; \{\sigma_j\}$	w_α	$\sigma_n; \{\sigma_j\}$	\bar{w}_α
1	$++$	w_1	$--$	$\bar{w}_1 = w_4$
2	$+-$	w_2	$-+$	$\bar{w}_2 = w_3$
3	$-+$	w_3	$++$	$\bar{w}_3 = w_2$
4	$--$	w_4	$+-$	$\bar{w}_4 = w_1$

When the spin symmetry is not imposed, the rate function depends on the values taken by the $z+1$ spins σ_n and $\{\sigma_j\}$, and can be decomposed on a basis of 2^{z+1} spin operators made of $0, 1, \dots, z+1$ spins. For instance, for the linear chain, these operators are: $\{1, \sigma_{n-1}, \sigma_n, \sigma_{n+1}, \sigma_n \sigma_{n+1}, \sigma_{n-1} \sigma_n, \sigma_{n-1} \sigma_{n+1}, \sigma_{n-1} \sigma_n \sigma_{n+1}\}$. In the present situation where spin symmetry holds, this decomposition can be restricted to 2^z even spin operators O_i , i.e.,

$$w(\sigma_n; \{\sigma_j\}) = \sum_{i=0}^{2^z-1} c_i O_i, \quad (2.14)$$

with $O_0 = 1$. The knowledge of the 2^z coefficients c_i is equivalent to the knowledge of the 2^z rates w_α . The coefficient c_0 fixes the scale of time.

Table 2. List of local configurations and corresponding values of the rate function for the 2D square lattice. There are 16 possible rates w_α , with $\sigma_n = +1$, corresponding to the 16 possible configurations $\{\sigma_j\}$, labelled by α , of the four neighbours of the central spin, taken in the order: east, north, west, south. The 16 remaining rates \bar{w}_α , with $\sigma_n = -1$, are deduced from the former, due to the spin symmetry (see (2.12)).

α	$\sigma_n; \{\sigma_j\}$	w_α	$\sigma_n; \{\sigma_j\}$	\bar{w}_α
1	++;++	w_1	-;++++	$\bar{w}_1 = w_{16}$
2	++;+-	w_2	-;+++-	$\bar{w}_2 = w_{15}$
3	++;-+	w_3	-;+-++	$\bar{w}_3 = w_{14}$
4	++;--	w_4	-;+--+	$\bar{w}_4 = w_{13}$
5	+;-++	w_5	-;-+++	$\bar{w}_5 = w_{12}$
6	+;-+-	w_6	-;-+-+	$\bar{w}_6 = w_{11}$
7	+;- -+	w_7	-;- -++	$\bar{w}_7 = w_{10}$
8	+;- --	w_8	-;- -+-	$\bar{w}_8 = w_9$
9	+;- -++	w_9	-;- -+++	$\bar{w}_9 = w_8$
10	+;- -+-	w_{10}	-;- -+-+	$\bar{w}_{10} = w_7$
11	+;- - -+	w_{11}	-;- - -++	$\bar{w}_{11} = w_6$
12	+;- - --	w_{12}	-;- - -+-	$\bar{w}_{12} = w_5$
13	+;- - -++	w_{13}	-;- - -+++	$\bar{w}_{13} = w_4$
14	+;- - -+-	w_{14}	-;- - -+-+	$\bar{w}_{14} = w_3$
15	+;- - - -+	w_{15}	-;- - - -++	$\bar{w}_{15} = w_2$
16	+;- - - --	w_{16}	-;- - - -+-	$\bar{w}_{16} = w_1$

For instance, for the linear chain,

$$w(\sigma_n; \{\sigma_j\}) = c_0 + c_1 \sigma_n \sigma_{n+1} + c_2 \sigma_{n-1} \sigma_n + c_3 \sigma_{n-1} \sigma_{n+1}, \quad (2.15)$$

i.e.,

$$O_1 = \sigma_n \sigma_{n+1}, \quad O_2 = \sigma_{n-1} \sigma_n, \quad O_3 = \sigma_{n-1} \sigma_{n+1}. \quad (2.16)$$

For the square lattice, we use the following notations. The central spin σ_n being located at \mathbf{x}_n , we denote by σ_{j_a} (resp. $\sigma_{j_{\bar{a}}}$) the neighbouring spins located at $\mathbf{x}_n + \mathbf{e}_a$ (resp. $\mathbf{x}_n - \mathbf{e}_a$), where \mathbf{e}_a ($a = 1, 2$) are the unit vectors spanning the square lattice. Thus σ_{j_1} , σ_{j_2} , $\sigma_{j_{\bar{1}}}$ and $\sigma_{j_{\bar{2}}}$ are the east, north, west and south spins, respectively. The list of even operators is given in Table 3.

In order to determine the rate function satisfying the global balance condition (2.8), or the detailed balance condition (2.9), we can proceed in either of two ways. The first one consists in finding the constraints on the rates $\{w_\alpha\}$, from which constraints on the coefficients $\{c_i\}$ ensue. The second one consists in finding the constraints on the coefficients $\{c_i\}$, from which constraints on the rates $\{w_\alpha\}$ ensue. These two ways are strictly equivalent because the rates $\{w_\alpha\}$ are linear combinations of the coefficients $\{c_i\}$, and both are equivalent representations of the rate function $w(\sigma_n; \{\sigma_j\})$.

We emphasize this equivalence as follows. Defining the indicator variables

$$I_\alpha = I(\sigma_n = +1; \{\sigma_j\}_\alpha), \quad \bar{I}_\alpha = I(\sigma_n = -1; \{\sigma_j\}_\alpha), \quad (2.17)$$

we have, using the notation (2.11),

$$w(\sigma_n; \{\sigma_j\}) = \sum_{\alpha=1}^{2^z} (I_\alpha w_\alpha + \bar{I}_\alpha \bar{w}_\alpha). \quad (2.18)$$

Table 3. List of the even operators made of the five spins $(\sigma_n; \{\sigma_j\})$. The central spin σ_n being located at \mathbf{x}_n , σ_{j_a} (resp. $\sigma_{j_{\bar{a}}}$) are the neighbouring spins located at $\mathbf{x}_n + \mathbf{e}_a$ (resp. $\mathbf{x}_n - \mathbf{e}_a$), where \mathbf{e}_a ($a = 1, 2$) are the unit vectors spanning the square lattice.

i	O_i
1	$\sigma_n \sigma_{j_1} \sigma_{j_2} \sigma_{j_{\bar{1}}}$
2	$\sigma_n \sigma_{j_1} \sigma_{j_2} \sigma_{j_{\bar{2}}}$
3	$\sigma_n \sigma_{j_1} \sigma_{j_{\bar{1}}} \sigma_{j_{\bar{2}}}$
4	$\sigma_n \sigma_{j_2} \sigma_{j_{\bar{1}}} \sigma_{j_{\bar{2}}}$
5	$\sigma_{j_1} \sigma_{j_2} \sigma_{j_{\bar{1}}} \sigma_{j_{\bar{2}}}$
6	$\sigma_n \sigma_{j_1}$
7	$\sigma_n \sigma_{j_2}$
8	$\sigma_n \sigma_{j_{\bar{1}}}$
9	$\sigma_n \sigma_{j_{\bar{2}}}$
10	$\sigma_{j_1} \sigma_{j_2}$
11	$\sigma_{j_2} \sigma_{j_{\bar{1}}}$
12	$\sigma_{j_1} \sigma_{j_{\bar{1}}}$
13	$\sigma_{j_1} \sigma_{j_{\bar{2}}}$
14	$\sigma_{j_1} \sigma_{j_2}$
15	$\sigma_{j_2} \sigma_{j_{\bar{2}}}$

Using the spin symmetry relation (2.12), we can rewrite the expression above as

$$w(\sigma_n; \{\sigma_j\}) = \sum_{\alpha=1}^{2^z} w_{\alpha} (I_{\alpha} + \bar{I}_{2^z+1-\alpha}), \quad (2.19)$$

where the two indicator variables in the bracket correspond to two opposite configurations. These indicator variables can be decomposed on the complete basis of 2^{z+1} spin operators made of $0, 1, \dots, z+1$ spins, however their sum only contains even operators O_i . For instance, for the linear chain,

$$\begin{aligned}
I_{\alpha} + \bar{I}_{2^z+1-\alpha} &= \frac{1 + \sigma_n}{2} \frac{1 + \text{sign}(\sigma_{n-1})_{\alpha} \sigma_{n-1}}{2} \frac{1 + \text{sign}(\sigma_{n+2})_{\alpha} \sigma_{n+1}}{2} \\
&+ \frac{1 - \sigma_n}{2} \frac{1 - \text{sign}(\sigma_{n-1})_{\alpha} \sigma_{n-1}}{2} \frac{1 - \text{sign}(\sigma_{n+2})_{\alpha} \sigma_{n+1}}{2} \\
&= \frac{1}{4} (1 + \text{sign}(\sigma_{n+1})_{\alpha} \sigma_n \sigma_{n+1} + \text{sign}(\sigma_{n-1})_{\alpha} \sigma_{n-1} \sigma_n \\
&+ \text{sign}(\sigma_{n-1} \sigma_{n+1})_{\alpha} \sigma_{n-1} \sigma_{n+1}) \\
&= \sum_{i=0}^{2^z-1} a_{i,\alpha} O_i, \quad (2.20)
\end{aligned}$$

where we have introduced the matrix of signs (up to the constant $1/2^z$)

$$A = (a_{i,\alpha}) = \frac{1}{2^z} O_i(\sigma_n = +1; \{\sigma_j\}_{\alpha}). \quad (2.21)$$

(The matrix $(a_{i,\alpha})$ for the linear chain is given in the Appendix.) One can thus rewrite (2.19) as

$$w(\sigma_n; \{\sigma_j\}) = \sum_{\alpha=1}^{2^z} w_{\alpha} \sum_{i=0}^{2^z-1} a_{i,\alpha} O_i. \quad (2.22)$$

Identifying (2.19) with (2.14) we obtain

$$c_i = \sum_{\alpha=1}^{2^z} a_{i,\alpha} w_\alpha. \quad (2.23)$$

The inverse relation reads

$$w_\alpha = \sum_{i=0}^{2^z-1} c_i O_i(\sigma_n = +1; \{\sigma_j\}_\alpha). \quad (2.24)$$

In other words $A^2 = I/2^z$, where I is the unit matrix.

2.3. Balance term

Starting from (2.14), then using the identity $e^{-a\sigma} = \cosh a - \sinh a \sigma$, we can decompose the balance term on the basis of spin operators as

$$B(\sigma_n; \{\sigma_j\}) = \sum_{i=0}^{2^z-1} E_i(\{c_i\}) O_i, \quad (2.25)$$

where the coefficients $E_i(\{c_i\})$ are linear combinations of the c_i , with coefficients depending on temperature through hyperbolic functions of $2K$. (See the Appendix for an illustration on the example of the linear chain.)

Let us now define

$$B_\alpha = w_\alpha - \bar{w}_\alpha e^{-\beta \Delta E_\alpha}, \quad \bar{B}_\alpha = \bar{w}_\alpha - w_\alpha e^{\beta \Delta E_\alpha}, \quad (2.26)$$

where ΔE_α is the change of energy associated to the rate w_α . Thanks to the symmetry relation (2.12) we have

$$\bar{B}_\alpha = B_{2^z+1-\alpha}. \quad (2.27)$$

For instance, for the linear chain, (2.27) reads

$$\begin{aligned} \bar{B}_1 &= \bar{w}_1 - e^{4K} w_1 = w_4 - e^{4K} \bar{w}_4 = B_4, \\ \bar{B}_2 &= \bar{w}_2 - w_2 = w_3 - \bar{w}_3 = B_3, \end{aligned} \quad (2.28)$$

and so on. Proceeding as for the rate function $w(\sigma_n; \{\sigma_j\})$, we can decompose the balance term $B(\sigma_n; \{\sigma_j\})$ as

$$B(\sigma_n; \{\sigma_j\}) = \sum_{i=0}^{2^z-1} F_i(\{B_\alpha\}) O_i, \quad (2.29)$$

where the coefficients $F_i(\{B_\alpha\})$ are linear combinations of the B_α ,

$$F_i = \sum_{\alpha=1}^{2^z} a_{i,\alpha} B_\alpha. \quad (2.30)$$

(See the Appendix for the example of the linear chain.) The sets E_i and F_i provide two equivalent representations of the linear decomposition of the balance term on the basis of spin operators, the former expressed in terms of the coefficients c_i , the latter in terms of the values B_α taken by the balance term.

3. Detailed balance

We start with the simple case of detailed balance, $B(\sigma_n; \{\sigma_j\}) = 0$, as a preparation for the sequel. This equation is satisfied by imposing $E_i = F_i = 0$ for all i .

3.1. Constraints on the rates or on the coefficients

The condition of detailed balance on the rate function (2.9) implies 2^z relations $\{B_\alpha = 0\}$, or equivalently, 2^z relations $\{F_i = 0\}$. However, thanks to the symmetry relation (2.27) these relations are redundant and only half of them remain. We thus get 2^{z-1} relations between pairs of rates:

$$w_\alpha = \bar{w}_\alpha e^{-\beta \Delta E_\alpha}, \quad (\alpha = 1, \dots, 2^{z-1}), \quad (3.1)$$

In return, using the spin operator representation (2.14) in these relations, the coefficients c_i are found to obey 2^{z-1} linear constraints.

One can also proceed in reverse order, determining first the constraints on the coefficients c_i , then deducing those for the rates from the former. Expressing that $B(\sigma_n; \{\sigma_j\})$ vanishes identically, and using (2.25) yields an homogeneous system of 2^z linear equations $\{E_i = 0\}$, which are not all independent. The rank of this system is necessarily equal to the rank of the system $\{F_i = 0\}$, i.e., to the number of relations between pairs of rates mentioned above, namely 2^{z-1} .

3.2. Examples

We illustrate the previous considerations by the following examples.

For the linear chain, the relations (3.1) are $B_1 = B_2 = 0$, i.e.,

$$\begin{aligned} w(+;++) &= e^{-4K} w(-; ++), \\ w(+;+-) &= w(-;+-). \end{aligned} \quad (3.2)$$

The constraints on the coefficients are either deduced from (3.2) or obtained from the solution of the 4 equations $\{E_i = 0\}$ (see Appendix A):

$$c_1 + c_2 + \gamma(c_0 + c_3) = 0, \quad c_1 = c_2, \quad (3.3)$$

where

$$\gamma = \tanh 2K. \quad (3.4)$$

The space of independent rates, or independent coefficients, has dimension 2. We thus find the most general rate function obeying detailed balance

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} (1 + \delta \sigma_{n-1} \sigma_{n+1} - \frac{\gamma}{2} (1 + \delta) \sigma_n (\sigma_{n-1} + \sigma_{n+1})), \quad (3.5)$$

where α and δ are the free parameters, recovering a result due to Glauber, written here with his notations [1].

On the square lattice, there are 8 constraints $B_1 = B_2 = \dots = B_8 = 0$, on the 16 rates w_α :

$$\begin{aligned} w_1 &= e^{-8K} \bar{w}_1, \\ w_\alpha &= e^{-4K} \bar{w}_\alpha, \quad (\alpha = 2, 3, 5), \\ w_\alpha &= \bar{w}_\alpha. \quad (\alpha = 4, 6, 7), \\ w_8 &= e^{4K} \bar{w}_8. \end{aligned} \quad (3.6)$$

We do not write down the corresponding 8 relations between the c_i because we will not use them in the sequel.

3.3. Symmetric rates

Let us consider the simpler case where the rates only depend on the variation of energy (2.5).

For the linear chain, the general form (3.5) automatically verifies this requirement. The so-called Glauber rate is obtained by fixing the parameter $\delta = 0$. It is the only such rate yielding linear equations for the temporal evolution of the observables. For instance, the Metropolis rate

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) &= \min(1, e^{-\Delta E/T}) \\ &= \frac{2 + \gamma}{2(1 + \gamma)} \left(1 - \frac{\gamma}{2 + \gamma} (\sigma_{n-1}\sigma_{n+1} + \sigma_n(\sigma_{n-1} + \sigma_{n+1})) \right) \end{aligned} \quad (3.7)$$

does not share this property.

For the square lattice, the requirement that the rates only depend on the variation of energy implies that the four neighbours of the central spin are equivalent, yielding 11 additional constraints

$$\begin{aligned} c_4 = c_3 = c_2 = c_1, \quad c_9 = c_8 = c_7 = c_6, \\ c_{15} = c_{14} = c_{13} = c_{12} = c_{11} = c_{10}. \end{aligned} \quad (3.8)$$

The remaining independent coefficients are $c_0, c_1, c_5, c_6, c_{10}$. The system of 16 equations $\{E_i = 0\}$ for these 5 coefficients only gives two constraints

$$\begin{aligned} c_1 + \frac{\gamma}{2}(c_5 - c_0) - c_6 &= 0, \\ \frac{\gamma^2}{6}c_0 - 2\frac{1 + \gamma^2}{3\gamma}c_1 - \frac{2 + \gamma^2}{6}c_5 - c_{10} &= 0. \end{aligned} \quad (3.9)$$

From this general solution one can extract some simpler expressions for the rate function. For instance, imposing $c_5 = c_{10} = 0$ yields

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) &= \frac{\alpha}{2} \left(1 - \frac{\gamma(2 + \gamma^2)}{4(1 + \gamma^2)} \sigma_n(\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_{\perp 1}} + \sigma_{j_{\perp 2}}) \right. \\ &\quad \left. + \frac{\gamma^3}{4(1 + \gamma^2)} \sigma_n(\sigma_{j_1}\sigma_{j_2}\sigma_{j_{\perp 1}} + \sigma_{j_2}\sigma_{j_{\perp 1}}\sigma_{j_{\perp 2}} + \sigma_{j_{\perp 1}}\sigma_{j_{\perp 2}}\sigma_{j_1} + \sigma_{j_{\perp 2}}\sigma_{j_1}\sigma_{j_2}) \right) \end{aligned} \quad (3.10)$$

which is the Glauber rate, usually written as

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} (1 - \sigma_n \tanh K(\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_{\perp 1}} + \sigma_{j_{\perp 2}})). \quad (3.11)$$

Another simple form is obtained by setting $c_1 = c_5 = 0$:

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) &= \frac{\alpha}{2} \left(1 - \frac{\gamma}{2} \sigma_n(\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_{\perp 1}} + \sigma_{j_{\perp 2}}) \right. \\ &\quad \left. + \frac{\gamma^2}{6} (\sigma_{j_1}\sigma_{j_2} + \sigma_{j_2}\sigma_{j_{\perp 1}} + \sigma_{j_{\perp 1}}\sigma_{j_{\perp 2}} + \sigma_{j_{\perp 2}}\sigma_{j_1} + \sigma_{j_2}\sigma_{j_{\perp 2}} + \sigma_{j_1}\sigma_{j_{\perp 1}}) \right). \end{aligned} \quad (3.12)$$

Let us finally note that the general form of a rate function satisfying detailed balance can be written as

$$w(\sigma_n; \{\sigma_j\}) = Q(\{\sigma_j\}) e^{-K\sigma_n h_n}, \quad (3.13)$$

where $Q(\{\sigma_j\})$ is a linear combination with arbitrary coefficients of the operators O_i not containing the central spin. This can be seen by multiplying both sides of (2.9) by $e^{K\sigma_n h_n}$ and observing that the product $w(\sigma_n; \{\sigma_j\}) e^{K\sigma_n h_n}$ is even in σ_n .

For instance, for the linear chain,

$$Q(\{\sigma_j\}) = a_0 + a_3 O_3, \quad (3.14)$$

where a_0 and a_3 are arbitrary, and simply related to c_0 and c_1 of (3.3): $a_0 = (c_0 - c_3 + (c_0 + c_3)/\cosh 2K)/2$, $a_3 = (c_3 - c_0 + (c_0 + c_3)/\cosh 2K)/2$.

For the square lattice,

$$Q(\{\sigma_j\}) = a_0 + a_5 O_5 + \sum_{i=10}^{15} a_i O_i \quad (3.15)$$

depends on 8 arbitrary parameters. If furthermore we ask that the rate function only depends on the variation of energy, then one should take

$$Q(\{\sigma_j\}) = a_0 + a_5 O_5 + a_{10} \sum_{i=10}^{15} O_i, \quad (3.16)$$

with arbitrary coefficients a_0, a_5, a_{10} . These are linearly related to the three independent parameters amongst $c_0, c_1, c_5, c_6, c_{10}$ related by (3.9).

4. Global balance

We now want to satisfy (2.8), not term by term but as a whole. As above we can solve the problem in either of two equivalent ways: by first finding the constraints on the rates $\{w_\alpha\}$, from which those on the coefficients $\{c_i\}$ ensue; or by first finding the constraints on the coefficients, from which those on the rates ensue. Both ways have to be implemented by formal computations, which are of equal algorithmic difficulty. We start with the second one, of easier presentation.

Table 4. Number of constraints (or rank) for dynamics on regular lattices. First column: linear chain ($z = 2$), square lattice ($z = 4$), triangular lattice ($z = 6$), cubic lattice ($z = 6$). The last line is for the hexagonal lattice (see text). Second and third columns: number of equations and rank of the system of equations for detailed balance (db). Fourth and fifth columns: same for global balance (gb). Last column: number of free parameters for global balance.

Lattice	2^z	Rank (db)	M	Rank (gb)	Free parameters (gb)
linear	4	2	3	1	3
square	16	8	12	6	10
triangular	64	32	49	29	35
cubic	64	32	55	32	32
hexagonal	8+8	8	12	8	8

4.1. Constraints on the coefficients

Remind that

$$B(\sigma_n; \{\sigma_j\}) = \sum_{i=0}^{2^z-1} E_i O_i, \quad (4.1)$$

Table 5. Number of constraints (or rank) and number of free parameters (gb) for dynamics on regular lattices at infinite temperature. Same examples as in Table 4.

Lattice	Rank (db)	Rank (gb)	Free parameters (gb)
linear	2	1	3
square	8	6	10
triangular	32	26	38
cubic	32	29	35
hexagonal	8	5	11

where the E_i are linear combinations of the c_i . The detailed balance condition is just $\{E_i = 0\}$ (see section 3). The sum in (2.8) can be rewritten as

$$\sum_n B(\sigma_n; \{\sigma_j\}) = N \sum_i E_i \overline{O_i}, \quad (4.2)$$

defining the spatial averages of the spin operators as

$$\overline{O_i} = \frac{1}{N} \sum_n O_i. \quad (4.3)$$

Taking into account the identities between the $\overline{O_i}$ due to translation invariance (see the examples below), the balance equation (2.8) finally reads

$$\sum_j \widetilde{E_j} \overline{O_j} = 0, \quad (4.4)$$

where the $\overline{O_j}$ are a subset of the $\overline{O_i}$, and with $\widetilde{E_0} \equiv E_0$. The size of this subset, i.e., the number M of terms in this sum, is equal to the difference between 2^z and the number of identities due to translation invariance. The M equations $\{\widetilde{E_j} = 0\}$ on the c_i are not all independent a priori. The rank of this system of equations is given in Table 4 for the various examples that we now present.

4.2. Examples

For the linear chain, we have, with the notation (2.16),

$$\overline{O_1} = \overline{O_2}, \quad (4.5)$$

hence (4.4) reads

$$E_0 + (E_1 + E_2) \overline{O_1} + E_3 \overline{O_3} = 0. \quad (4.6)$$

The $M = 3$ equations $\{\widetilde{E_j} = 0\}$ yield only one condition: $E_0 = 0$ (see Appendix A). In other words, the rank of this system of 3 equations is equal to 1 (see Table 4). We find:

$$c_1 + c_2 + \gamma(c_0 + c_3) = 0, \quad (4.7)$$

which generalizes the result (3.3) found in the detailed balance case. Hence, setting $c_2/c_0 = \epsilon$, $c_3/c_0 = \delta$ and $c_0 = \alpha/2$, the most general rate function satisfying the condition of global balance reads

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} (1 - (\gamma(1 + \delta) + \epsilon) \sigma_n \sigma_{n+1} + \epsilon \sigma_{n-1} \sigma_n + \delta \sigma_{n-1} \sigma_{n+1}), \quad (4.8)$$

which depends on the 3 arbitrary parameters α, ϵ, δ . The corresponding dynamics is asymmetric and irreversible. Setting $\epsilon = -\gamma(1 + \delta)(1 - p)$, we can alternatively write:

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2}(1 - \gamma(1 + \delta)\sigma_n(p\sigma_{n-1} + (1 - p)\sigma_{n+1}) + \delta\sigma_{n-1}\sigma_{n+1}). \quad (4.9)$$

The general Glauber form (3.5) is recovered by setting $p = 1/2$. At the other end, the case of totally asymmetric dynamics where the central spin is only influenced by one of its neighbours leads, once a choice of neighbour is done, to a *unique* expression up to the time scale fixed by the coefficient α . For instance, if σ_n is only influenced by its left neighbour, setting $\delta = 0$ and $p = 1$ ($\epsilon = -\gamma$), we obtain

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2}(1 - \gamma\sigma_{n-1}\sigma_n). \quad (4.10)$$

Fixing the scale of time by the choice $\alpha = 2 \cosh 2K$, we obtain the exponential form

$$w(\sigma_n; \{\sigma_j\}) = e^{-2K\sigma_{n-1}\sigma_n}. \quad (4.11)$$

We shall comment further, in section 7, on the range of allowed parameters in (4.8) or (4.9).

Remark Eq. (4.7) can also be interpreted as the equation fixing the temperature of the model. Hence, for the linear chain, any generic rate depending on the 4 parameters c_0, c_1, c_2, c_3 leads to a Gibbsian stationary measure.

On the square lattice we have 4 identities due to translation invariance, which only involves two-spin operators,

$$\overline{O_6} = \overline{O_9}, \quad \overline{O_7} = \overline{O_8}, \quad \overline{O_{10}} = \overline{O_{13}}, \quad \overline{O_{11}} = \overline{O_{14}}, \quad (4.12)$$

with the notations of Table 3. The resulting system of $M = 12$ (16-4) linear equations $\{\widetilde{E}_j = 0\}$, has rank 6, yielding 6 equations of constraint on the c_i . In other words, 6 coefficients are expressed as linear combinations of the other 10 coefficients, which remain arbitrary. Totally asymmetric cases are obtained by asking the rate function to depend only on two or three of the neighbouring spins instead of four. For example keeping the east (σ_{j_1}) and north (σ_{j_2}) spins only, and cancelling the coefficients of the operators containing the two other spins $\sigma_{j_{\underline{1}}}$ and $\sigma_{j_{\underline{2}}}$, we obtain a *unique* rate function, up to a scale of time,

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2}(1 - \gamma\sigma_n(\sigma_{j_1} + \sigma_{j_2}) + \gamma^2\sigma_{j_1}\sigma_{j_2}). \quad (4.13)$$

Fixing this timescale by the choice $\alpha = 2 \cosh^2 2K$, allows to write (4.13) into the exponential form[‡]

$$w(\sigma_n; \{\sigma_j\}) = e^{-2K\sigma(\sigma_{j_1} + \sigma_{j_2})}. \quad (4.14)$$

For the 3D cubic lattice, amongst the $2^z = 64$ operators O_i , 18 are related, two by two, by translation invariance. They all belong to the group of $\binom{7}{2} = 21$ two-spin operators. The three two-spin operators of this group not related by translation invariance are

$$\sigma_{j_a}\sigma_{j_{\underline{a}}}, \quad (4.15)$$

for $a = 1, 2, 3$, with notations analogous to those of Table 3. So we have $M = 55$ (64 - 9) linear equations $\{\widetilde{E}_j = 0\}$ in the $\{c_i\}$ to solve. The rank of this system of M

[‡] This form, as well as (4.11), appear in [2] without the factor 2. The corresponding stationary states have their temperature halved.

equations is equal to 32, as for the case of detailed balance. The constraints are indeed found to be the same as when detailed balance holds (see also section 4.3 below). On the cubic lattice there is no irreversible Gibbsian dynamics.

It is striking to compare the former case of the 3D cubic lattice to the case of the 2D triangular lattice, for which the coordination is the same ($z = 6$). For the triangular lattice, there are 15 identities due to translational invariance satisfied by the spatial averages of a subset of the 64 operators O_i . These 15 identities correspond to the translations of $\sigma_n \sigma_{j_a}$, for $a = 1, 2, 3$ (9 relations), to the translations of $\sigma_{j_1} \sigma_{j_3}, \sigma_{j_2} \sigma_{j_1}, \sigma_{j_3} \sigma_{j_2}$ (3 relations), and to the translations of the four-spin operators, e.g., $\sigma_n \sigma_{j_3} \sigma_{j_1} \sigma_{j_2}$ (3 relations). Thus $M = 49$ ($64 - 15$), and the rank of this system of equations is found to be equal to 29. In this case, there do exist irreversible Gibbsian dynamics.

The totally asymmetric case involving the three spins $\sigma_{j_1}, \sigma_{j_2}, \sigma_{j_3}$ in the three unit directions is, again, determined *uniquely*, up to a time scale as

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) &= \frac{\alpha}{2} (1 - \gamma \sigma_n (\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_3}) \\ &\quad + \gamma^2 (\sigma_{j_1} \sigma_{j_2} + \sigma_{j_2} \sigma_{j_3} + \sigma_{j_1} \sigma_{j_3}) - \gamma^3 \sigma_n \sigma_{j_1} \sigma_{j_2} \sigma_{j_3}). \end{aligned} \quad (4.16)$$

This rate function can also be written in exponential form as

$$w(\sigma_n; \{\sigma_j\}) = e^{-2K \sigma_n (\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_3})}, \quad (4.17)$$

with the choice $\alpha = 2 \cosh^3 2K$.

4.3. Constraints on the rates

One can, of course, deduce the constraints on the rates from the above. Alternatively we can obtain these constraints directly by following the exact parallel of section 4.1. Remind that

$$B(\sigma_n; \{\sigma_j\}) = \sum_{i=0}^{2^z-1} F_i O_i, \quad (4.18)$$

where the F_i are linear combinations of the B_α . The detailed balance condition is just $\{F_i = 0\}$ (see section 3). The sum in (2.8) can be rewritten as

$$\sum_n B(\sigma_n; \{\sigma_j\}) = N \sum_i F_i \overline{O_i}. \quad (4.19)$$

Taking into account the identities between the $\overline{O_i}$ due to translation invariance, the balance equation (2.8) finally reads

$$\sum_j \widetilde{F_j} \overline{O_j} = 0, \quad (4.20)$$

where the $\overline{O_j}$ are a subset of the $\overline{O_i}$, and with $\widetilde{F_0} \equiv F_0$. The M equations $\{\widetilde{F_j} = 0\}$ on the B_α are equivalent to the equations $\{\widetilde{E_j} = 0\}$ on the c_i . However they yield constraints on the rates, instead of constraints on the coefficients.

Remark

One can recover (4.19) following a slightly different path, as follows§. For a given fixed configuration \mathcal{C} , the sum in (2.8) can be rewritten as

$$\sum_{\alpha=1}^{2^z} (N_\alpha B_\alpha + \bar{N}_\alpha \bar{B}_\alpha), \quad (4.21)$$

where N_α (resp. \bar{N}_α) is the number of occurrences in \mathcal{C} of the local configuration {central spin up (resp. down) with the z neighbours in configuration α }.

$$N_\alpha = \sum_n I(\sigma_n = +1; \{\sigma_j\}_\alpha), \quad \bar{N}_\alpha = \sum_n I(\sigma_n = -1; \{\sigma_j\}_\alpha). \quad (4.22)$$

Using the spin symmetry and regrouping terms, the sum can be rewritten as

$$\sum_{\alpha=1}^{2^z} (N_\alpha + \bar{N}_{2^z+1-\alpha}) B_\alpha. \quad (4.23)$$

The numbers N_α can be decomposed on the basis of spatial averages of all the spin operators. However, only the even operators remain in the sum $N_\alpha + \bar{N}_{2^z+1-\alpha}$ (see (2.20)). Finally the sum (4.23) yields (4.19).

4.4. Examples

We illustrate the method on the cases considered above, in one to three dimensions.

For the linear chain, (4.20) reads

$$F_0 + (F_1 + F_2) \overline{O_1} + F_3 \overline{O_3} = 0. \quad (4.24)$$

The 3 equations $\{\widetilde{F_j} = 0\}$ yield only one condition: $F_0 = 0$, hence the detailed balance condition $B_1 = w_1 - e^{-4K} \bar{w}_1 = 0$, i.e.,

$$w(+;++) = e^{-4K} w(-; ++), \quad (4.25)$$

which is equivalent to (4.7). The rank of this system of 3 equations is equal to 1, as already found above (see Appendix A).

On the square lattice, taking into account the identities (4.12) due to translation invariance, the resulting system of $M = 12$ linear equations in the B_α , $\{\widetilde{F_j} = 0\}$, has rank 6, yielding the following 6 equations of constraint:

$$\begin{aligned} w_1 - e^{-8K} \bar{w}_1 &= 0, \\ w_6 - \bar{w}_6 &= 0, \\ w_2 - e^{-4K} \bar{w}_2 + w_5 - e^{-4K} \bar{w}_5 &= 0, \\ e^{4K} w_3 - \bar{w}_3 - (w_8 - e^{4K} \bar{w}_8) &= 0, \\ w_2 - e^{-4K} \bar{w}_2 - (w_3 - e^{-4K} \bar{w}_3) + \frac{2}{1 + e^{4K}} (w_7 - \bar{w}_7) &= 0, \\ w_2 - e^{-4K} \bar{w}_2 + w_3 - e^{-4K} \bar{w}_3 - \frac{2}{1 + e^{4K}} (w_4 - \bar{w}_4) &= 0. \end{aligned} \quad (4.26)$$

The space of independent parameters has dimension 10, in agreement with what was found above.

§ This variant of the method was first introduced in [6].

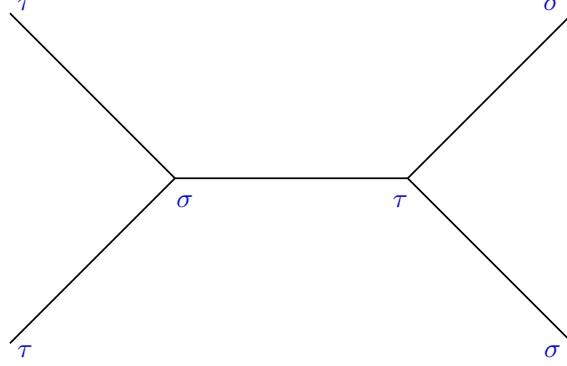


Figure 1. Two types of environments for the hexagonal lattice.

For the 2D triangular lattice, one recovers the results presented above: the 15 identities satisfied by the spatial averages of a subset of the $2^z = 64$ operators O_i yield a system of $M = 49$ equations, the rank of which is equal to 29.

For the 3D cubic lattice, we have $M = 55$ ($64 - 9$) linear equations in the B_α , ($\alpha = 1, \dots, 64$), to solve. The constraints found are the 32 detailed balance conditions $B_\alpha = 0$, in agreement with what was found above.

4.5. Special case of the hexagonal lattice

On the hexagonal lattice one has to distinguish two kinds of spins, named respectively σ and τ , corresponding to two types of environments (figure 1). Spin σ_n , located at \mathbf{x}_n , is surrounded by τ_{j_1} , τ_{j_2} and τ_{j_3} with notations analogous to those of Table 3, where \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 are the unit vectors spanning the hexagonal lattice. Spin $\tau_n \equiv \tau_{j_1}$, located at \mathbf{y}_n , distant from \mathbf{x}_n by one unit, is surrounded by σ_{k_1} (which is σ_n), σ_{k_2} and σ_{k_3} in the respective directions $-\mathbf{e}_1$, $-\mathbf{e}_2$ and $-\mathbf{e}_3$. To these two spins correspond two rates $w^\sigma(\sigma; \{\tau\})$ and $w^\tau(\tau; \{\sigma\})$, skipping the indices. The balance equation (4.4) now reads

$$\widetilde{E}_0^\sigma + \widetilde{E}_0^\tau + \sum_j \left(\widetilde{E}_j^\sigma \overline{O_j^\sigma} + \widetilde{E}_j^\tau \overline{O_j^\tau} \right) = 0, \quad (4.27)$$

where the operators O^σ are the three $\sigma_n \tau_{j_a}$, the three $\tau_{j_a} \tau_{j_b}$ and $\sigma_n \tau_{j_1} \tau_{j_2} \tau_{j_3}$. The operators O^τ are defined analogously. In (4.27) the identities due to translation invariance have been taken into account:

$$\overline{\sigma_n \tau_{j_2}} = \overline{\tau_n \sigma_{k_2}}, \quad \overline{\sigma_n \tau_{j_3}} = \overline{\tau_n \sigma_{k_3}}. \quad (4.28)$$

Moreover $\overline{\sigma_n \tau_{j_1}}$ and $\overline{\tau_n \sigma_{k_1}}$ represent the same operator and $\widetilde{E}_0^\sigma + \widetilde{E}_0^\tau = 0$ counts for one equation only. The system of 12 resulting equations yield 8 constraints, identical to the detailed balance constraints. Thus, on the hexagonal lattice, there is no irreversible Gibbsian dynamics, i.e., global balance enforces detailed balance, as long as temperature is finite (see below).

4.6. Infinite temperature

When temperature is infinite, the balance term takes the simpler form

$$B(\sigma_n; \{\sigma_j\}) = w(\sigma_n; \{\sigma_j\}) - w(-\sigma_n; \{\sigma_j\}), \quad (4.29)$$

which only involves the operators containing the central spin. Likewise, the only identities between operators due to translation invariance to be considered are those involving the central spin.

For instance, for the linear chain, $B(\sigma_n; \{\sigma_j\})$ only involves the two operators O_1 and O_2 . The identity $O_1 = O_2$ still holds, thus the balance equation $(c_1 + c_2)O_1 = 0$ yields the constraint $c_1 + c_2 = 0$, which is the limit of (4.7) for $\gamma = 0$. The rate function reads

$$w(\sigma_n; \{\sigma_j\}) = c_0 + c_3 O_3 + c_1 (O_1 - O_2). \quad (4.30)$$

The sum of the first two terms represent the infinite-temperature reversible rate function $Q(\{\sigma_j\})$ (see (3.13)). If furthermore the dynamics is totally asymmetric, then one should impose $c_1 = c_3 = 0$, i.e., $w(\sigma_n; \{\sigma_j\}) = c_0$, in agreement with the infinite-temperature limit of (4.10). In this limit the dynamics is reversible.

For the square lattice, $B(\sigma_n; \{\sigma_j\})$ only involves the 8 operators O_1 to O_4 , and O_6 to O_9 . The identities to be considered are (see (4.12))

$$\overline{O_6} = \overline{O_9}, \quad \overline{O_7} = \overline{O_8}. \quad (4.31)$$

The balance equation thus imposes the 6 constraints

$$c_1 = c_2 = c_3 = c_4 = 0, \quad c_6 + c_9 = 0, \quad c_7 + c_8 = 0. \quad (4.32)$$

This number of constraints is the same as at finite temperature. The rate function reads

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) &= c_0 + c_5 O_5 + \sum_{i=10}^{15} c_i O_i \\ &\quad + c_6 (O_6 - O_9) + c_7 (O_7 - O_8). \end{aligned} \quad (4.33)$$

As above, the first line can be identified with the infinite-temperature reversible rate function $Q(\{\sigma_j\})$ defined in (3.13). The second line is a linear combination of the operators $\sigma_n(\sigma_{j_a} - \sigma_{j_{\underline{a}}})$ ($a = 1, 2$). If the dynamics is totally asymmetric, for instance keeping only the east and north spins, then one should impose the vanishing of the coefficients corresponding to operators containing the west or south spins, i.e., c_5, c_6, c_7 as well as c_{11} to c_{15} . Thus

$$w(\sigma_n; \{\sigma_j\}) = c_0 + c_{10} O_{10}, \quad (4.34)$$

which corresponds to a reversible dynamics, as can be seen by comparing to the first line of (4.33). This should be contrasted with the infinite-temperature limit of (4.13) which yields $w(\sigma_n; \{\sigma_j\}) = c_0$. There is no continuity of the finite-temperature result in this situation, when $T \rightarrow \infty$.

For the triangular lattice, the balance term involves 32 operators containing the central spin. Only 6 symmetry relations remain, thus finally there are 26 constraints to satisfy. In other words there are more arbitrary parameters in the definition of the rate function satisfying global balance at infinite temperature than at finite temperature. As for the square lattice, the rate is equal to the sum of $Q(\{\sigma_j\})$ (32 free parameters), of a linear combination of operator differences $\sigma_n(\sigma_{j_a} - \sigma_{j_{\underline{a}}})$ ($a = 1, 2, 3$) (3 free parameters), and of a linear combination of operator differences

of the type $\sigma_n(\sigma_1\sigma_2\sigma_3 - \sigma_3\sigma_1\sigma_2)$ (3 free parameters). If the dynamics is totally asymmetric, for instance keeping only the spins in the direction $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, and taking into account the identities due to translation invariance, the resulting rate depends on 4 arbitrary coefficients, namely c_0 and the 3 coefficients corresponding to the 3 operators $\sigma_{j_1}\sigma_{j_2}, \sigma_{j_1}\sigma_{j_3}, \sigma_{j_2}\sigma_{j_3}$. Again this dynamics is reversible but is different from the limit obtained from the finite-temperature result (4.16) at $T \rightarrow \infty$, which yields $w(\sigma_n; \{\sigma_j\}) = c_0$.

For the cubic lattice, again the balance term involves 32 operators containing the central spin. Only 3 symmetry relations remain, thus there are finally 29 constraints to satisfy. Detailed balance is no longer enforced by global balance at infinite temperature. The rate has the same form as for the triangular lattice, except that the four-spin operators do not enter the expression. The case of totally asymmetric dynamics is identical to that found for the triangular lattice.

For the hexagonal lattice, as for the case of the cubic lattice, detailed balance is no longer enforced by global balance at infinite temperature.

Table 5 summarizes the results for the various examples that we considered.

5. Special forms of the rate function

5.1. Totally asymmetric dynamics

For the totally asymmetric dynamics satisfying global balance encountered so far, the rate function could always be written in exponential form as

$$w(\sigma_n; \{\sigma_j\}) = e^{-2K\sigma_n h_n^+}, \quad (5.1)$$

where $h_n = h_n^+ + h_n^-$ is decomposed into two components related by inversion through the central spin see (4.11), (4.14) and (4.17). For instance on the square lattice, $h_n^+ = \sigma_{j_1} + \sigma_{j_2}$, $h_n^- = \sigma_{j_1} - \sigma_{j_2}$.

Reciprocally, assume that the rate function has the form (5.1) [3]. Then the balance term reads

$$B(\sigma_n; \{\sigma_j\}) = e^{-2K\sigma_n h_n^+} - e^{-2K\sigma_n h_n^-}. \quad (5.2)$$

Expanding the two exponential terms in the right side, the analysis confirms the fact that on 1D and 2D lattices such rates satisfy the balance equation (2.8), but shows that this is not the case for the 3D cubic lattice, or more generally for lattices of coordination $z \geq 8$ [3].

5.2. A restricted representation of the rate function

In preparation of the discussion of section 6, we now want to investigate whether there are representations of the rate function that generalize both the form (5.1) and the form encountered when detailed balance holds, namely (3.13). Let us consider, along the lines of Ref. [4], the following a priori representation of the rate function, instead of the general expression (2.14):

$$w(\sigma_n; \{\sigma_j\}) = Q(\{\sigma_j\})e^{-\sigma_n H_n}, \quad (5.3)$$

where $Q(\{\sigma_j\})$ is a linear combination of the operators O_i not involving the central spin, and where

$$H_n = \sum_{a=1}^D (A_a \sigma_{j_a} + A_{\underline{a}} \sigma_{j_{\underline{a}}}), \quad (5.4)$$

and $A_a + A_{\underline{a}} = 2K$. We remind that σ_{j_a} is the spin located at $\mathbf{x}_n + \mathbf{e}_a$, and $\sigma_{j_{\underline{a}}}$ is the spin located at $\mathbf{x}_n - \mathbf{e}_a$. Setting

$$A_a = K + L_a, \quad A_{\underline{a}} = K - L_a, \quad (5.5)$$

we can rewrite the rate function as

$$w(\sigma_n; \{\sigma_j\}) = Q(\{\sigma_j\}) e^{-K\sigma_n h_n} e^{-\sigma_n \sum_a L_a (\sigma_{j_a} - \sigma_{j_{\underline{a}}})}. \quad (5.6)$$

If the L_a vanish, one recovers the detailed balance form (3.13), made of the two first factors in the right side of this equation. At the other end, if $L_a = \pm K$, and if $Q(\{\sigma_j\})$ is reduced to a constant, then one recovers (5.1). However thus far this form is only an a priori representation of the rate function, on which one should now impose the global balance condition. In so doing, we find the following:

- 1D** The form (5.3) is faithful and equivalent to the previous result (4.8). The constraint of global balance is automatically encoded in this form, where the prefactor $Q(\{\sigma_j\}) = a_0 + a_3 O_3$, with arbitrary coefficients a_0 and a_3 .
- 2D** Let us take the example of the square lattice. The constraints of global balance fixes 4 linear relations on the $\{a_j\}$ defining $Q(\{\sigma_j\})$ (see (3.15)). Thus the form (5.3) provides examples of rate functions satisfying global balance [4]. The reciprocal is not true, i.e., any rate function satisfying global balance is not of the form (5.3). For instance (5.3) implies the following relation amongst the rates:

$$\frac{\bar{w}_2}{w_2} = e^{8K} \frac{w_5}{\bar{w}_5}, \quad (5.7)$$

which does not hold in general.

One could also have argued differently by noting that the form (5.3), which depends on 10 arbitrary parameters a priori, actually depends on 6 parameters once the 4 constraints on the $\{a_j\}$ are imposed, namely the four remaining arbitrary $\{a_j\}$ and the two parameters L_1 and L_2 , while the general rate function obeying global balance depends on 10 arbitrary parameters (see section 4.2). This form therefore only represents a subset of the most general rate functions obeying global balance.

- 3D** Since we already stated that there is no Gibbsian irreversible dynamics for the cubic lattice, *the form (5.3) cannot represent a rate function satisfying global balance*. Since the constraint of global balance enforces detailed balance, it must necessarily suppress the dependence of $w(\sigma_n; \{\sigma_j\})$ in the parameters L_a . In other words, $Q(\{\sigma_j\})$ must vanish for any configuration of the neighbours $\{\sigma_j\}$ such that $\sigma_{j_a} \neq \sigma_{j_{\underline{a}}}$ for $a = 1, 2, 3$. For the configurations such that the equality holds, i.e., $\sigma_{j_a} = \sigma_{j_{\underline{a}}}$ for all $a = 1, 2, 3$, detailed balance automatically holds, as it should. This is illustrated by an explicit example in section 6.

5.3. Interpolating schemes

For the linear chain, (4.9) gives an interpolation between the totally asymmetric cases and the symmetric one.

In similar fashion there are forms of the rate function in 2D, which interpolate between the totally asymmetric expression (4.13) and one of the forms valid under detailed balance. For instance, for the square lattice,

$$\begin{aligned} w(\sigma_n; \{\sigma_j\}) = & \frac{\alpha}{2} (1 - \gamma p \sigma_n (\sigma_{j_1} + \sigma_{j_2}) - \gamma (1 - p) \sigma_n (\sigma_{j_{\underline{1}}} + \sigma_{j_{\underline{2}}})) \\ & + \gamma^2 p \sigma_{j_1} \sigma_{j_2} + \gamma^2 (1 - p) \sigma_{j_{\underline{1}}} \sigma_{j_{\underline{2}}}. \end{aligned} \quad (5.8)$$

The totally asymmetric forms are obtained for $p = 1$ or 0 . For $p = 1/2$, the rate function satisfies detailed balance, without being of the form (3.16). This expression is convenient when investigating the physical consequences of irreversibility for the two-dimensional Ising model with asymmetric dynamics [7].

6. Review of Ref. [4] and the question of the rates for the cubic lattice

Reference [4] is chiefly concerned with the computation of the entropy production rate for irreversible Ising models with Gibbsian stationary states. The rate function considered in this reference is of the form (5.3), which is well adapted to the computation of the entropy production rate. As said above, this choice is not restrictive in 1D, but does not account for the most general rate function satisfying global balance for the square lattice. The expression obtained in [4] for the entropy production rate of the linear chain generalizes a result of [8]; the computation of the entropy production rate of the square lattice is done for the totally asymmetric case (4.14).

We now turn to the treatment of the 3D case given in [4]. Ref. [4] claims that *there exist* irreversible Ising models on the cubic lattice, with Gibbsian stationary measure with respect to the Hamiltonian (2.1), contradicting the results found in Ref. [3] and recalled in the present work. This statement is actually untrue and relies on an incomplete analysis, as we now demonstrate. (See also [5].)

The rate function chosen in [4] for the 3D case is of the form (5.3) with the particular choice $L_1 = L_2 = L_3 = L$, and where $Q(\{\sigma_j\})$ is a linear combinations of operators, not involving the central spin and satisfying some additional symmetry requirements, with coefficients named b_0, b_1, \dots, b_5 (see eq. (67) in [4]). It is an easy task to solve the problem of determining these unknown coefficients if one imposes the global balance condition, using the general methods described in section 4. We find the following constraints on the coefficients b_0, b_1, \dots, b_5 ,

$$b_5 = b_0, \quad b_4 = b_2 = \frac{3b_1 - b_0}{2}, \quad b_3 = b_1, \quad (6.1)$$

independently of the value of the parameter L . One can then check that, taking into account the constraints (6.1), the rate function thus obtained either satisfies the detailed balance condition, when $\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_3} = \sigma_{j_1} + \sigma_{j_2} + \sigma_{j_3}$, or vanishes when this condition does not hold, because the prefactor $Q(\{\sigma_j\})$ vanishes itself. This is equivalent to saying that, for this choice of rate function, the condition of global balance enforces the condition of detailed balance.

These results are in agreement with the general statement, made in [3] and in section 4, that there are no Gibbsian irreversible models for the cubic lattice, and therefore no entropy production for dynamics of the form (5.3) in this case.

7. Positivity of the rates

The rate functions found by the method above must satisfy the additional constraint of positivity for the various possible configurations.

|| We also checked that the equations of constraint on b_0, b_1, \dots, b_5 written in [4] lead to the result (6.1). In [4] the determination of these equations of constraint is done by identification of two forms of the balance term, the first one deduced from the choice made for the rate w , the other one is a linear combination of a subset of the operators O_i chosen according to some symmetry requirements.

We illustrate the issue on the 1D case, using (4.8). The allowed region in the plane of the two parameters (δ, ϵ) yielding positive rates is the triangle depicted in figure 2. The sides of the triangle correspond to the vanishing of one of the rates w_α . The segment joining the two points $(-1, -1)$ and $(1, -\gamma)$ corresponds to $w_2 \equiv w(+; +-) = 0$. The segment joining the two points $(-1, 1)$ and $(1, -\gamma)$ corresponds to $w_3 \equiv w(+; -+) = 0$. Finally the vertical segment at $\delta = -1$ corresponds to $w_1 = w_4 = 0$, i.e., $w(+; ++) = w(+; --) = 0$.

All rates on the line joining $(-1, 0)$ to $(1, -\gamma)$ satisfy detailed balance. For example, the point marked M corresponds to the Metropolis rate (3.7). All rates with $\delta = 0$ lead to linear equations for the temporal evolution of the observables [9]. The point G , located at $(0, -\gamma/2)$ and corresponding to the Glauber rate, is the only point where both detailed balance and linearity hold.

The two ends of the green segment are the totally asymmetric points $(0, -\gamma)$ and $(0, 0)$, corresponding respectively to values of the interpolating parameter $p = 0$ and $p = 1$ in (4.9). The range of allowed values with $\delta = 0$ goes beyond this segment. It is comprised between the two extreme points $(0, -(1 + \gamma)/2)$ and $(0, (1 - \gamma)/2)$ which correspond respectively to the values $p = (\gamma - 1)/(2\gamma)$, which is negative, and $p = (\gamma + 1)/(2\gamma)$, which is larger than 1. For those points and more generally for the range of values depicted in red in figure 2 the magnetization of the linear chain exhibits an oscillating relaxation [10]. For instance, for the point $(0, -(1 + \gamma)/2)$, the rate function (4.8) becomes

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} \left(1 + \sigma_n \left(\frac{1 - \gamma}{2} \sigma_{n+1} - \frac{1 + \gamma}{2} \sigma_{n-1} \right) \right). \quad (7.1)$$

8. Discussion

Let us come back on the interplay between irreversibility and asymmetry of the dynamics in the present context. We recall that the dynamics is symmetric if the rates are given by a symmetric function of the neighbouring spins $\{\sigma_j\}$ of the flipping spin σ_n . In other words under symmetric dynamics the neighbouring spins have equal influence on the flipping spin. We ask:

- (i) Can a dynamics be both irreversible and symmetric?
- (ii) Can a dynamics be both reversible and asymmetric?

A negative answer to the first question means that irreversibility necessarily implies asymmetry. A negative answer to the second question means that reversibility necessarily implies symmetry, which is the reciprocal of (i). We illustrate the issue on the examples of the linear chain and of the square lattice.

For the linear chain the answer to the two questions is negative. Reversibility and symmetry are equivalent. Symmetry of the dynamics for the linear chain requires $c_1 = c_2$ (see (3.3)), which appears also as a constraint imposed by the condition of detailed balance.

For the square lattice, the answer to the two questions is positive.

- (i) Firstly, symmetry of the dynamics does not imply reversibility. Indeed, starting from the generic rate function depending on 16 parameters, if one imposes symmetry, then only 5 independent parameters remains, which are the coefficients $c_0, c_1, c_5, c_6, c_{10}$ (see (3.8)). If no further condition is imposed, the dynamics is

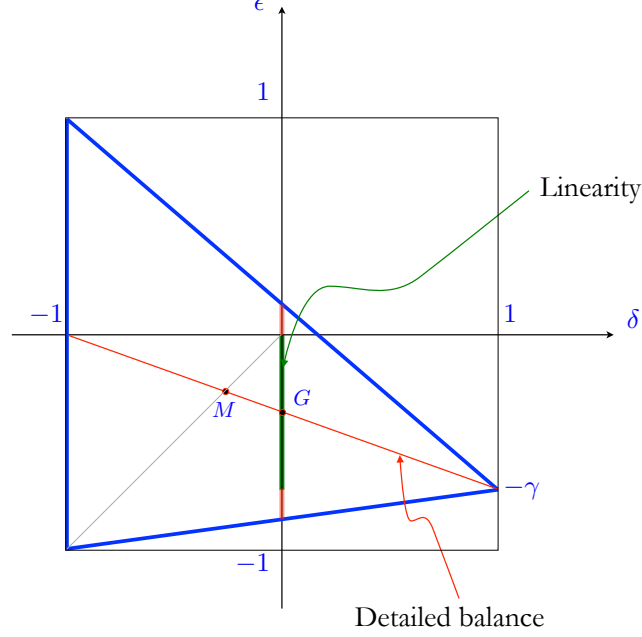


Figure 2. Constraints due to positivity for the linear chain: allowed values of the parameters yielding positive rates and satisfying global balance are inside the triangle.

generically irreversible. The voter model [12] and the broader class of models defined by the rate function [13, 14]

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2}(1 - \sigma_n \tanh[\beta(h_n) h_n]), \quad (8.1)$$

where $h_n = \sum_j \sigma_j$ (choosing $J = 1$), provide examples of such a situation. The inverse temperature takes three values, according to the value of the local field h_n : $\beta(0)$, $\beta(2) = \beta(-2)$ and $\beta(4) = \beta(-4)$. This rate function is clearly symmetric in the neighbouring spins. It can be rewritten as

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} \left(1 + \frac{1}{4} \left(\gamma_2 - \frac{\gamma_4}{1 + \gamma_4^2} \right) (O_1 + O_2 + O_3 + O_4) - \frac{1}{4} \left(\gamma_2 + \frac{\gamma_4}{1 + \gamma_4^2} \right) (O_6 + O_7 + O_8 + O_9) \right), \quad (8.2)$$

where $\gamma_2 = \tanh 2\beta(2)$, $\gamma_4 = \tanh 2\beta(4)$. Note that we have $c_5 = c_{10} = 0$. These models correspond to genuinely irreversible dynamics since the rates do not even satisfy the constraints of global balance (4.26), hence their stationary measure is unknown. The voter model corresponds to the choice $\gamma_2 = 1/2$, $\gamma_4 = 1$. The noisy voter model corresponds to the choice $\gamma_2 = \gamma_4/(1 + \gamma_4^2)$. The Glauber rate function (3.10) or (3.11) is recovered by fixing $\gamma_2 = \gamma_4 = \gamma$.

Let us finally mention that imposing global balance on a generic symmetric rate function yields the two constraints (3.9), i.e., reversibility is recovered. In other words, irreversible Gibbsian dynamics are necessarily asymmetric.

- (ii) Secondly, reversibility does not imply symmetry of the dynamics. Indeed any generic reversible rate function depends on 8 parameters (see for example (3.15)). On the other hand the number of independent parameters corresponding to reversible symmetric dynamics is equal to 3 (see (3.16)). Thus generically any rate function satisfying detailed balance is asymmetric. For instance the rate function

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} \left(1 - \frac{\gamma}{2} \sigma_n (\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_\perp} + \sigma_{j_\parallel}) + \frac{\gamma^2}{2} (\sigma_{j_1} \sigma_{j_\perp} + \sigma_{j_2} \sigma_{j_\parallel}) \right) \quad (8.3)$$

provides an example of a reversible asymmetric process. In particular w_4 is not equal to w_6 , as would be the case for a fully symmetric dynamics. Eq. (5.8) is another example where, when $p = 1/2$, the dynamics is reversible but not fully symmetric. Yet another example is

$$w(\sigma_n; \{\sigma_j\}) = \frac{\alpha}{2} \left(1 - \frac{\gamma}{2 - \gamma^2} \sigma_n (\sigma_{j_1} + \sigma_{j_2} + \sigma_{j_\perp}) + \frac{\gamma^2}{2 - \gamma^2} (\sigma_{j_1} \sigma_{j_2} + \sigma_{j_1} \sigma_{j_\perp} + \sigma_{j_2} \sigma_{j_\perp}) - \frac{\gamma^3}{2 - \gamma^2} \sigma_n \sigma_{j_1} \sigma_{j_2} \sigma_{j_\perp} - \frac{1 - \gamma^2}{2 - \gamma^2} \sigma_n \sigma_{j_\parallel} \right), \quad (8.4)$$

which illustrates the fact that, even for reversible dynamics, one of the neighbouring spins (here σ_{j_2}) can play a role different from the other ones.

It is however easy to convince oneself, using (3.13), that reversibility and total asymmetry are incompatible, except at infinite temperature, as demonstrated by (4.34).

9. Conclusion

The present work is a completion of [3]. One of the questions raised and solved in this reference concerned the possible existence of irreversible single-spin flip dynamics with Gibbsian stationary states for ferromagnetic Ising systems. The motivation was twofold.

On the one hand, a natural question raised by the examples given in the past by Künsch [2] for totally asymmetric dynamics in one and two dimensions, is to what extent are these examples unique, and can they be extended to higher dimensions than two. The result of [3], completed here, is that, as long as the dynamics is not totally asymmetric, the space of parameters defining the rate function allowing irreversible Gibbsian Ising models is large (see Table 4). However, imposing total asymmetry of the dynamics yields a unique solution, up to a time scale, for the examples considered (linear chain, square and triangular lattices). The answer to the second part of the question is presumably negative. Indeed, firstly, there is no such Gibbsian irreversible dynamics for the cubic lattice; secondly, one can argue that there are neither totally asymmetric Gibbsian dynamics for lattices of coordination

$z \geq 8$ [3]. A novel outcome of the present work is that the situation can be different at infinite temperature (see Table 5).

On the other hand, the models thus defined are interesting laboratories for the study of the physical consequences of irreversibility, in particular of the properties of the resulting nonequilibrium stationary state. For instance, for the linear chain, though the stationary measure is Boltzmann-Gibbs, the dynamical properties of the relaxing system are changed [9]. Irreversibility also implies a non-vanishing entropy production rate in the stationary state which can be exactly computed for irreversible Gibbsian models since the stationary measure is known [4, 8].

The method used in [3] and in the present work for the solution of the question raised above relies on linear algebra and properties of the system under translations. This implies solving the system of linear equations of constraint on the rates by a formal computation. It would be desirable to answer the same question by other means which would in some sense generalize the argument recalled above for lattices with coordination number $z \geq 8$.

Acknowledgments

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Appendix A. Linear chain

Hereafter we give some details on the case of the linear chain.

We use the identity

$$e^{-2K\sigma_n h_n} = \frac{1}{1-\gamma^2} (1-\gamma O_1)(1-\gamma O_2) \quad (\text{A.1})$$

($\gamma = \tanh 2K$) to obtain the decomposition (2.25) of the balance term $B(\sigma_n; \{\sigma_j\})$ on the basis of operators O_i . The coefficients E_i thus obtained are, up to a global constant equal to $1/(1-\gamma^2)$,

$$\begin{aligned} E_0 &= -\gamma(c_1 + c_2 + \gamma(c_0 + c_3)), \\ E_1 &= 2c_1 - \gamma^2(c_1 - c_2) + \gamma(c_0 + c_3), \\ E_2 &= 2c_2 + \gamma^2(c_1 - c_2) + \gamma(c_0 + c_3), \\ E_3 &= E_0, \end{aligned} \quad (\text{A.2})$$

from which the relation $E_0/\gamma + (E_1 + E_2)/2 = 0$ is seen to hold. Hence the rank of the system $\{E_i = 0\}$ is equal to 2.

The matrix $A = (a_{i,\alpha})$ with $0 \leq i \leq 3$, and $1 \leq \alpha \leq 4$, which relates the coefficients c_i to the rates w_α , reads

$$A = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \quad (\text{A.3})$$

Hence, using (2.30), we have, for the coefficients F_i defined in (2.29),

$$F_0 = (B_1 + B_2 + B_3 + B_4)/4,$$

$$\begin{aligned}
F_1 &= (B_1 - B_2 + B_3 - B_4)/4, \\
F_2 &= (B_1 + B_2 - B_3 - B_4)/4, \\
F_3 &= (B_1 - B_2 - B_3 + B_4)/4.
\end{aligned} \tag{A.4}$$

Noting that $B_2 + B_3 = 0$, we obtain, up to a global constant equal to $1/4$,

$$\begin{aligned}
F_0 &= (1 - e^{4K})(w_1 - e^{-4K}\bar{w}_1), \\
F_1 &= (1 + e^{4K})(w_1 - e^{-4K}\bar{w}_1) - 2(w_2 - \bar{w}_2), \\
F_2 &= (1 + e^{4K})(w_1 - e^{-4K}\bar{w}_1) + 2(w_2 - \bar{w}_2), \\
F_3 &= F_0,
\end{aligned} \tag{A.5}$$

thus we have the relation $F_0/\gamma + (F_1 + F_2)/2 = 0$. Hence the rank of the system $\{F_i = 0\}$ is equal to 2.

The two writings (A.2) and (A.5) can be identified by using (2.15), i.e.,

$$w(\sigma_n; \{\sigma_j\}) = c_0 + c_1 \sigma_n \sigma_{n+1} + c_2 \sigma_{n-1} \sigma_n + c_3 \sigma_{n-1} \sigma_{n+1}. \tag{A.6}$$

Appendix B. Asymmetric Gibbsian conserved dynamics for the linear chain

In this appendix we use the methods of the present paper to determine the rate function when the dynamics is conserved and satisfies global balance. So doing we recover the results of a previous work, which were established by a variant of the present method, and written differently [6].

Appendix B.1. Basic facts

The dynamics of the chain consists in flipping a bond chosen at random, say bond (σ_n, σ_{n+1}) , if the two spins σ_n and σ_{n+1} are anti-aligned: either $+-$ flips into $-+$, or $-+$ flips into $+-$. The change in energy is equal to

$$\Delta E = 2J(\sigma_{n-1}\sigma_n + \sigma_{n+1}\sigma_{n+2}). \tag{B.1}$$

This is done with a rate $w(\sigma_n, \sigma_{n+1}; \{\sigma_j\})$, where $\{\sigma_j\}$ is a notation for the two neighbours σ_{n-1} and σ_{n+2} . The number of values taken by the rate function is therefore equal to 8. We denote the 4 rates with $(\sigma_n = +1, \sigma_{n+1} = -1)$ by w_α and the other 4 rates, corresponding to $(\sigma_n = -1, \sigma_{n+1} = +1)$, by \bar{w}_α :

$$w_\alpha = w(+--; \{\sigma_j\}_\alpha), \quad \bar{w}_\alpha = w(-+; \{\sigma_j\}_\alpha), \tag{B.2}$$

(see Table B1).

Let us introduce the basis of 16 spin operators O_1, \dots, O_{15} , made of the 4 spins $\sigma_{n-1}, \dots, \sigma_{n+2}$, with $O_0 = 1$ (see Table B2). We define the indicator variables

$$\begin{aligned}
I_\alpha &= I(+--; \{\sigma_j\}_\alpha) = \frac{1 + \sigma_n}{2} \frac{1 - \sigma_{n+1}}{2} J_\alpha, \\
\bar{I}_\alpha &= I(-+; \{\sigma_j\}_\alpha) = \frac{1 - \sigma_n}{2} \frac{1 + \sigma_{n+1}}{2} J_\alpha,
\end{aligned} \tag{B.3}$$

where J_α denotes the indicator variable of the event $\{\{\sigma_j\} \text{ in configuration } \alpha\}$. We thus have, using the notation (B.2),

$$w(+--; \{\sigma_j\}) = \sum_{\alpha=1}^4 J_\alpha w_\alpha, \quad w(-+; \{\sigma_j\}) = \sum_{\alpha=1}^4 J_\alpha \bar{w}_\alpha. \tag{B.4}$$

Table B1. List of local configurations and corresponding values of the rate function for the one-dimensional chain with conserved dynamics. There are 4 possible rates w_α , with $(\sigma_n = +1, \sigma_{n+1} = -1)$, corresponding to the 4 possible configurations $\{\sigma_j\}$, labelled by α , of the two neighbours of the flipping bond, taken in the order: left, right. The 4 remaining rates \bar{w}_α correspond to $(\sigma_n = -1, \sigma_{n+1} = +1)$.

α	$\sigma_n, \sigma_{n+1}; \{\sigma_j\}$	w_α	$\sigma_n, \sigma_{n+1}; \{\sigma_j\}$	\bar{w}_α
1	$+-; ++$	w_1	$-+; ++$	\bar{w}_1
2	$+-; +-$	w_2	$-+; +-$	\bar{w}_2
3	$+-; -+$	w_3	$-+; -+$	\bar{w}_3
4	$+-; --$	w_4	$-+; --$	\bar{w}_4

Table B2. List of operators made of the 4 spins $\sigma_{n-1}, \dots, \sigma_{n+2}$.

i	O_i
1	$\sigma_{n-1}\sigma_n\sigma_{n+1}\sigma_{n+2}$
2	$\sigma_{n-1}\sigma_n\sigma_{n+1}$
3	$\sigma_{n-1}\sigma_n\sigma_{n+2}$
4	$\sigma_{n-1}\sigma_{n+1}\sigma_{n+2}$
5	$\sigma_n\sigma_{n+1}\sigma_{n+2}$
6	$\sigma_{n-1}\sigma_n$
7	$\sigma_{n-1}\sigma_{n+1}$
8	$\sigma_{n-1}\sigma_{n+2}$
9	$\sigma_n\sigma_{n+1}$
10	$\sigma_n\sigma_{n+2}$
11	$\sigma_{n+1}\sigma_{n+2}$
12	σ_{n-1}
13	σ_n
14	σ_{n+1}
15	σ_{n+2}

Alternatively, we have

$$\begin{aligned} w(+-, \{\sigma_j\}) &= c_0 + c_8 O_8 + c_{12} O_{12} + c_{15} O_{15}, \\ w(-+, \{\sigma_j\}) &= d_0 + d_8 O_8 + d_{12} O_{12} + d_{15} O_{15}. \end{aligned} \quad (\text{B.5})$$

Finally we can write the rate function as

$$\begin{aligned} w(\sigma_n, \sigma_{n+1}; \{\sigma_j\}) &= \frac{1 + \sigma_n}{2} \frac{1 - \sigma_{n+1}}{2} w(+-, \{\sigma_j\}) \\ &\quad + \frac{1 - \sigma_n}{2} \frac{1 + \sigma_{n+1}}{2} w(-+, \{\sigma_j\}). \end{aligned} \quad (\text{B.6})$$

The balance term reads

$$\begin{aligned} B(\sigma_n, \sigma_{n+1}; \{\sigma_j\}) &= w(\sigma_n, \sigma_{n+1}; \{\sigma_j\}) \\ &\quad - w(-\sigma_n, -\sigma_{n+1}; \{\sigma_j\}) e^{-\Delta E/T}, \end{aligned} \quad (\text{B.7})$$

with

$$e^{-\Delta E/T} = \frac{1}{1 - \gamma^2} (1 - \gamma O_6)(1 - \gamma O_{11}), \quad (\text{B.8})$$

($\gamma = \tanh 2K$). Using (B.5), (B.6) and (B.8), we obtain a decomposition of the balance term (B.7) on the basis of operators of Table B2:

$$B(\sigma_n, \sigma_{n+1}; \{\sigma_j\}) = E_0 + \sum_{i=1}^{15} E_i O_i. \quad (\text{B.9})$$

Appendix B.2. Symmetries

We analyze the constraints induced on the rate function by the two following symmetries.

Symmetry under P , the spatial left-right parity

The constraint induced by this symmetry reads

$$w(+--; \sigma_{n-1}, \sigma_{n+2}) = w(-+; \sigma_{n+2}, \sigma_{n-1}), \quad (\text{B.10})$$

which imposes

$$d_0 = c_0, \quad d_8 = c_8, \quad d_{12} = c_{15}, \quad d_{15} = c_{12}, \quad (\text{B.11})$$

or

$$w_1 = \bar{w}_1, \quad w_2 = \bar{w}_3, \quad w_3 = \bar{w}_2, \quad w_4 = \bar{w}_4. \quad (\text{B.12})$$

Symmetry under CP

This symmetry is the product of C and P , where the charge conjugation C changes the spins into their opposites. In other words, the rates are the same for $+$ going to the right or for $-$ going to the left, with the environment of the latter conjugated to the environment of the former. The constraints induced by this symmetry read

$$\begin{aligned} w(+--; \sigma_{n-1}, \sigma_{n+2}) &= w(+--; -\sigma_{n+2}, -\sigma_{n-1}), \\ w(-+; \sigma_{n-1}, \sigma_{n+2}) &= w(-+; -\sigma_{n+2}, -\sigma_{n-1}). \end{aligned} \quad (\text{B.13})$$

This fixes

$$c_{12} + c_{15} = 0, \quad d_{12} + d_{15} = 0, \quad (\text{B.14})$$

or

$$w_1 = w_4, \quad \bar{w}_1 = \bar{w}_4. \quad (\text{B.15})$$

Appendix B.3. Detailed balance

The detailed balance condition imposes $B(\sigma_n, \sigma_{n+1}; \{\sigma_j\}) = 0$, i.e., $E_i = 0$ for all i . We thus obtain the 4 constraints

$$\begin{aligned} d_0 &= \frac{1}{1-\gamma^2} (c_0 - \gamma(\gamma c_8 - c_{12} + c_{15})), \\ d_8 &= \frac{1}{1-\gamma^2} (c_8 - \gamma(\gamma c_0 + c_{12} - c_{15})), \\ d_{12} &= \frac{1}{1-\gamma^2} (c_{12} - \gamma(\gamma c_{15} - c_0 + c_8)), \\ d_{15} &= \frac{1}{1-\gamma^2} (c_{15} - \gamma(\gamma c_{12} + c_0 - c_8)), \end{aligned} \quad (\text{B.16})$$

which express the equalities

$$w_1 = \bar{w}_1, \quad w_2 = \bar{w}_2 e^{-4K}, \quad w_3 = \bar{w}_3 e^{4K}, \quad w_4 = \bar{w}_4. \quad (\text{B.17})$$

We now restrict the rate function furthermore by symmetry requirements.

Symmetry under P , the spatial left-right parity

The additional constraint induced by this symmetry is

$$\gamma(c_0 - c_8) + c_{12} - c_{15} = 0, \quad (\text{B.18})$$

which expresses the equality $w_2 = e^{-4K}w_3$. The resulting rate function can be read off from (B.5) and (B.6):

$$\begin{aligned} w(+; \{\sigma_j\}) &= c_0 + c_8\sigma_{n-1}\sigma_{n+2} + c_{12}\sigma_{n-1} + (\gamma(c_0 - c_8) + c_{12})\sigma_{n+2}, \\ w(-; \{\sigma_j\}) &= c_0 + c_8\sigma_{n-1}\sigma_{n+2} + c_{12}\sigma_{n+2} + (\gamma(c_0 - c_8) + c_{12})\sigma_{n-1}. \end{aligned} \quad (\text{B.19})$$

It depends on 3 arbitrary coefficients.

Symmetry under CP

The constraints on the rate function are the three first lines of (B.16) with $c_{12} + c_{15} = 0$ and d_{15} is fixed equal to $-d_{12}$. Again the resulting rate function depends on 3 free coefficients.

Appendix B.4. Global balance

We now turn to the global balance condition. Translation invariance imposes

$$\begin{aligned} \overline{O_2} &= \overline{O_5}, & \overline{O_6} &= \overline{O_9} = \overline{O_{11}}, & \overline{O_7} &= \overline{O_{10}}, \\ \overline{O_{12}} &= \overline{O_{13}} = \overline{O_{14}} = \overline{O_{15}}. \end{aligned} \quad (\text{B.20})$$

Solving the system of equations $\widetilde{E}_j = 0$ (see (4.4)) yields 2 constraints:

$$\begin{aligned} d_8 &= \frac{1}{1 - \gamma^2}(c_8 - \gamma(\gamma c_0 + c_{12} - c_{15})), \\ \gamma d_0 - d_{12} + d_{15} &= \frac{1}{1 - \gamma^2}(-c_{12} + c_{15} - \gamma(c_0 - (2 - \gamma^2)c_8)), \end{aligned} \quad (\text{B.21})$$

which express the relations between rates

$$\begin{aligned} w_2 - \bar{w}_2 e^{-4K} + \bar{w}_3 - w_3 e^{-4K} &= 0 \\ w_1 - \bar{w}_1 + w_4 - \bar{w}_4 + \bar{w}_2(1 + e^{-4K}) - w_2(1 + e^{4K}) &= 0. \end{aligned} \quad (\text{B.22})$$

The number of free coefficients is equal to 6.

Symmetry under P , the spatial left-right parity

This again imposes $\gamma(c_0 - c_8) + c_{12} - c_{15} = 0$, and the resulting rate function is the same as for the case of detailed balance with P symmetry (see (B.19)).

Symmetry under CP

This imposes the two additional constraints (B.14) on (B.21), or (B.15) on (B.22). The resulting rate function depends on 4 free parameters.

Appendix B.5. Totally asymmetric dynamics

For instance, only the flipping of $+-$ into $-+$ is allowed. Hence $w(-+; \{\sigma_j\}) = 0$, or $\bar{w}_\alpha = 0$. We thus set the two left sides of (B.21) to zero, since $d_0 = d_8 = d_{12} = d_{15} = 0$, from which it results that

$$c_8 = 0, \quad \gamma c_0 + c_{12} - c_{15} = 0, \quad (\text{B.23})$$

or equivalently

$$w_1 + w_4 - w_2 - w_3 = 0, \quad w_2 = w_3 e^{-4K}. \quad (\text{B.24})$$

The resulting rate function reads

$$w(+--; \{\sigma_j\}) = c_0 + c_{12}\sigma_{n-1} + (\gamma c_0 + c_{12})\sigma_{n+2}, \quad (\text{B.25})$$

which depends on 2 free coefficients. Imposing the CP symmetry fixes $c_{12} = -\gamma c_0/2$. The solution found is therefore unique, up to the global time scale c_0 :

$$w(+--; \{\sigma_j\}) = c_0 \left(1 - \frac{\gamma}{2}(\sigma_{n-1} - \sigma_{n+2})\right). \quad (\text{B.26})$$

Partially asymmetric dynamics

A partial asymmetry with uniform bias [11] translates into the condition

$$\frac{w(-+; \sigma_{n-1}, \sigma_{n+2})}{w(+--; \sigma_{n+2}, \sigma_{n-1})} = \frac{1 - V}{1 + V}, \quad (\text{B.27})$$

where $0 \leq V \leq 1$. This condition yields

$$\begin{aligned} w(+--; \{\sigma_j\}) &= c_0 + c_{12}\sigma_{n-1} + (\gamma c_0 + c_{12})\sigma_{n+2}, \\ w(-+; \{\sigma_j\}) &= \frac{1 - V}{1 + V} (c_0 + (\gamma c_0 + c_{12})\sigma_{n-1} + c_{12}\sigma_{n+2}), \end{aligned} \quad (\text{B.28})$$

which depend on 3 parameters: c_0, c_{12} and V . Eqs. (B.24) still hold. The limiting case $V = 0$ is included in the solution (B.19) of the fully symmetric case. The totally asymmetric limit $V = 1$ reproduces the result (B.25). Imposing the CP invariance on the rate function again fixes $c_{12} = -\gamma c_0/2$.

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