Irreversible models with Boltzmann–Gibbs probability distribution and entropy production

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Abstract. We analyze irreversible interacting spin models evolving according to a master equation with spin flip transition rates that do not obey detailed balance but obey global balance with a Boltzmann–Gibbs probability distribution. Spin flip transition rates with up–down symmetry are obtained for a linear chain, a square lattice, and a cubic lattice with a stationary state corresponding to the Ising model with nearest neighbor interactions. We show that these irreversible dynamics describes the contact of the system with particle reservoirs that cause a flux of particles through the system. Using a microscopic definition, we determine the entropy production rate of these irreversible models and show that it can be written as a macroscopic bilinear form in the forces and fluxes. Exact expressions for this property are obtained for the linear chain and the square lattice. In this last case the entropy production rate displays a singularity at the phase transition point of the same type as the entropy itself.

Keywords: exact results, stochastic particle dynamics (theory), stationary states
1. Introduction

When one thinks about thermodynamic equilibrium in microscopic terms, what comes to mind is the Boltzmann–Gibbs (BG) probability distribution. Indeed, any system in thermodynamic equilibrium is microscopically described by the BG distribution \[1\]. If one considers a description that takes into account the microscopic dynamics, such as that given by a stochastic Markovian process, the equilibrium is more properly characterized by the microscopic reversibility, or detailed balance \[2\], or yet by no entropy creation. If a system lacks detailed balance its stationary state is not an equilibrium state and entropy is continuously being produced. In this situation one usually expects a non-BG distribution to describe the static properties. However, this is not a necessary consequence of the lack of detailed balance. In fact there are examples of interacting spin models that lack detailed balance but are nonetheless described by a BG probability distribution \[3\]–\[6\]. This result has the important consequence that the BG distribution is a necessary but not a sufficient condition for the thermodynamic equilibrium of systems described by a dynamic theory.

Here we are concerned with the construction of irreversible interacting spin models evolving according to a master equation whose stationary state is described by a BG probability distribution. More precisely, we wish to set up transitions rates that do not
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obey detailed balance but still obey the global balance with a BG distribution. The models are defined on a regular lattice with a one spin flip transition rate and a BG probability distribution which is the same as that of the Ising model with nearest neighbor interactions and up–down symmetry. The lattices we consider are a linear chain and square and cubic lattices. This problem has recently been addressed by Godrèche and Bray [5] with a method that has similarities to the present approach. Although the present method is general and may be applied to any form of transition rate, we have only considered transition rates with up–down symmetry with a particular form, to be explained later, that suffices to take us to the desired transition rates.

The second purpose of this paper is the calculation of the production of entropy in the stationary state. Since the system is not in thermodynamic equilibrium, there will be a nonzero production of entropy. The entropy production rate is a measure of the irreversible character of a system and is here obtained by a microscopic expression introduced by Schnakenberg [7] for systems described by a master equation and considered by other authors [8]–[20]. The expression is nonnegative by definition and vanishes only when detailed balance is obeyed, that is, in thermodynamic equilibrium. From the Schnakenberg expression we determine the entropy production rate of the irreversible models in the steady state, particularly that of models with totally asymmetric dynamics. In two and three dimensions, when the system displays a symmetry breaking phase transition, we have found that the entropy production rate has a singularity at the critical point of the same type as the entropy itself.

We show that some of the irreversible dynamics with BG distribution can be interpreted as describing the contact of the system with particle reservoirs having distinct chemical potential so that a flux of particles sets in from one reservoir to the other through the system. The Schnakenberg microscopic expression for the production of entropy is also shown to have a macroscopic bilinear form in the forces and fluxes [21]–[24].

2. Method

Each site $i$ of a regular lattice of $N$ sites and periodic boundary conditions has a spin variable $\sigma_i$ that takes the values $\pm 1$. The whole configuration is denoted by the vector $\sigma = \{\sigma_i\}$. The system evolves in time according to a continuous time Markov process in which only one spin changes at each time step. That is, the evolution of the probability distribution $P(\sigma, t)$ of configuration $\sigma$ at time $t$ is governed by the master equation

$$\frac{d}{dt}P(\sigma, t) = \sum_i \{w_i(\sigma^i)P(\sigma^i, t) - w_i(\sigma)P(\sigma, t)\},$$

where $w_i(\sigma)$ is the one spin flip transition rate and the notation $\sigma^i$ stands for the vector obtained from $\sigma$ by changing the sign of the spin variable $\sigma_i$. In the stationary state the probability $P(\sigma)$ satisfies the global balance equation

$$\sum_i \{w_i(\sigma^i)P(\sigma^i) - w_i(\sigma)P(\sigma)\} = 0.$$
expression we start by rewriting equation (2) in the more convenient form
\[
\sum_i \left\{ w_i(\sigma^i) \frac{P(\sigma^i)}{P(\sigma)} - w_i(\sigma) \right\} = 0,
\]
(3)
obtained by dividing (2) by \( P(\sigma) \). Defining the function \( g_i(\sigma) \) by
\[
g_i(\sigma) = w_i(\sigma^i) \frac{P(\sigma^i)}{P(\sigma)} - w_i(\sigma),
\]
(4)
the global balance equation is written in the short form
\[
\sum_i g_i(\sigma) = 0.
\]
(5)
Next we write the function \( g_i(\sigma) \) as the expansion [25]
\[
g_i(\sigma) = \sum_R a_{i,R} \sigma_R,
\]
(6)
where the summation is over any cluster of sites \( R \) of the lattice and \( \sigma_R \) is the product of the spin variables associated with the sites belonging to the set \( R \), that is
\[
\sigma_R = \prod_{j \in R} \sigma_j.
\]
(7)
Given a function \( g_i(\sigma) \), the coefficients \( a_{i,R} \) are uniquely determined by the formula [25]
\[
a_{i,R} = 2^{-N} \sum_\sigma g_i(\sigma) \sigma_R.
\]
(8)
Summing up these coefficients and taking into account the global balance equation (5) we end up with the equation
\[
\sum_i a_{i,R} = 0,
\]
(9)
where the summation extends over all sites of the lattice. Equation (9) is then equivalent to global balance. Detailed balance means \( a_{i,R} = 0 \) for any \( i \).

A more useful form of equation (9) is obtained by exploiting the translation invariance of \( a_{i,R} \). To this end let us denote by \( R + j \) the set of sites obtained by translation of the sites of \( R \) by the vector \( j \). Translation invariance means that \( a_{i,R} = a_{i+j,R+j} \) and, in particular, \( a_{i,R} = a_{0,R-i} \). Using this property, equation (9) becomes
\[
\sum_i a_{0,R-i} = 0,
\]
(10)
which must be satisfied for each set of sites \( R \). Equation (10) involves only the coefficients of \( g_0(\sigma) \) and is the basis of our approach in seeking spin flip transition rates that do not obey detailed balance.
3. Transition rate

We will consider as the stationary probability distribution the following BG probability distribution with up–down symmetry, that is, invariant under the change of sign of all spin variables,

\[ P(\sigma) = \frac{1}{Z} e^{K \sum_{\langle i,j \rangle} \sigma_i \sigma_j}, \tag{11} \]

where the summation is over the pairs of nearest neighbor sites of a regular lattice with periodic boundary conditions and \( K \) is a parameter which we call the coupling constant. It is the same probability distribution that describes the static properties of the Ising model with nearest neighbor interaction at a temperature proportional to the inverse of the coupling constant.

Taking into account the probability given by (11) and the definition of \( g_i(\sigma) \), given by equation (4), we may write

\[ g_i(\sigma) = w_i(\sigma^i) e^{-2K\sigma_i \sum_\delta \sigma_{i+\delta} - w_i(\sigma)}, \tag{12} \]

where \( \delta \) is any one of the vectors connecting a central site to a nearest neighboring site. If detailed balance holds, that is if \( g_i = 0 \), then

\[ \frac{w_i(\sigma)}{w_i(\sigma^i)} = e^{-2K\sigma_i \sum_\delta \sigma_{i+\delta}}, \tag{13} \]

from which follows that the spin flip rate obeying detailed balance has the general form

\[ w_i(\sigma) = K_i(\sigma) e^{-K\sigma_i \sum_\delta \sigma_{i+\delta}}, \tag{14} \]

where \( K_i(\sigma) \) does not depend on \( \sigma_i \).

Several spin flip transition rates used in Monte Carlo calculations are indeed of this form. They are distinguished by the factor \( K_i(\sigma) \). For the Glauber transition rate [26]

\[ w_i(\sigma) = \alpha \min\{1, e^{-2K\sigma_i \sum_\delta \sigma_{i+\delta}}\} \tag{15} \]

the factor is

\[ K_i(\sigma) = \alpha e^{-|K\sum_\delta \sigma_{i+\delta}|}. \tag{16} \]

For the Metropolis transition rate [27]

\[ w_i(\sigma) = \alpha \min\{1, e^{-2K\sigma_i \sum_\delta \sigma_{i+\delta}}\} \tag{17} \]

the factor is

\[ K_i(\sigma) = \alpha e^{-|K\sum_\delta \sigma_{i+\delta}|}. \tag{18} \]

For the following spin flip transition rate,

\[ w_i(\sigma) = \alpha e^{-K\sigma_i \sum_\delta \sigma_{i+\delta}}, \tag{19} \]

the factor is simply \( K_i(\sigma) = \alpha \).

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Figure 1. The central site and its nearest neighbor sites for the linear chain, the square lattice and the cubic lattice.

Here, however, we wish to set up transition rates that do not obey detailed balance. To this end we assume the following form for the spin flip transition rate

$$w_i(\sigma) = K_i(\sigma)e^{-\sigma_i \sum \delta A\sigma_{i+\delta}}.$$  \hspace{1cm} (20)

where $K_i(\sigma)$ does not depend on $\sigma_i$ and $A$ are parameters. We consider only regular lattices with an inversion center like those shown in figure 1. For those lattices, to each neighboring site $i + \delta$ there corresponds an opposite site $i - \delta$ in relation to the central site $i$. We further assume that

$$A_{-\delta} + A_{\delta} = 2K.$$  \hspace{1cm} (21)

When $A_{-\delta} = A_{\delta}$ we recover detailed balance, since in this case $A_{-\delta} = A_{\delta} = K$ and (20) reduces to (14).

The function $K_i(\sigma)$ is assumed to depend only on the nearest neighbor spins $\sigma_{i+\delta}$ and to be invariant under the inversion operation $\sigma_{i+\delta} \to \sigma_{i-\delta}$, for all $\delta$. We assume in addition that $K_i(\sigma)$ has the up–down symmetry which amounts to saying that $w_i(\sigma)$ also has this symmetry. Expression (20), together with the restrictions imposed on $K_i(\sigma)$, is not the most general form for $w_0(\sigma)$ but will suffice to set up spin flip transition rates that do not obey detailed balance but still obey the global balance (2) with the BG probability distribution (11).

Introducing (20) into (12), the function $g_i(\sigma)$ becomes

$$g_i(\sigma) = K_i(\sigma)\{e^{-\sigma_i \sum \delta A_{-\delta}\sigma_{i+\delta}} - e^{-\sigma_i \sum \delta A_{\delta}\sigma_{i+\delta}}\}.$$  \hspace{1cm} (22)

Notice that $g_i(\sigma)$ should have up–down symmetry because $K_i(\sigma)$ holds this symmetry. Since the expression inside the curls of equation (22) changes sign and $K_0(\sigma)$ remains invariant under the inversion operation, the function $g_i(\sigma)$ changes sign under this operation. Due to the change of sign of $g_i(\sigma)$ under the inversion operator it follows from (8) that the coefficients $a_{i,R}$ and $a_{i,-R}$, where $-R$ stands for the set of sites obtained from $R$ by the inversion operator, are related by

$$a_{i,R} + a_{i,-R} = 0.$$  \hspace{1cm} (23)

Our approach will be as follows. We first determine the coefficients $a_{0,R}$ of $g_0(\sigma)$ in terms of the parameters appearing in the right-hand side of expression (22) by the use of equation (8). Due to the translation invariance it suffices to focus on a given site which we choose to be the site $i = 0$. If $R$ is invariant under the inversion operation, it follows
immediately from (23) that $a_{0,R}$ vanishes. Therefore the possible surviving coefficients $a_{0,R}$ are those for which $R$ is not invariant under the inversion operation. Let us suppose that two coefficients $a_{0,R}$ and $a_{0,R^*}$ of the sum in equation (10) are such that $R^*$ and $R$ are the inverse of each other, that is $R^* = -R$. It follows from (23) that they cancel each other. We are left in equation (10) with those coefficients $a_{0,R}$ such that the set $-R$ obtained from $R$ by the inversion operation is not a set $R + i$ obtained from $R$ by any translation operator. Our method consists then in imposing the constraint

$$a_{0,R} = 0$$

(24)
on the coefficients of this type so that equation (10) becomes fulfilled.

4. Linear chain

The stationary BG distribution for this case is

$$P(\sigma) = \frac{1}{Z} e^{K \sum_i \sigma_i \sigma_{i+1}}.$$  

(25)

We will focus on a particular site of the lattice which we denoted by $i = 0$. Its two nearest neighbors are denoted by $i = 1$ and $2$ as shown in figure 1. Using this convention the spin flip rate for the linear chain is of the form

$$w_0(\sigma) = K_0(\sigma)e^{-\sigma_0(A_1\sigma_1 + A_2\sigma_2)},$$

(26)

where $A_1 + A_2 = 2K$. The function $K_0(\sigma)$, which depends on $\sigma_1$ and $\sigma_2$, has up–down symmetry and is invariant by the inversion operation $\sigma_1 \leftrightarrow \sigma_2$. Its most general form is

$$K_0(\sigma) = b_0 + b_1\sigma_1\sigma_2.$$  

(27)

The function $g_0(\sigma)$ has up–down symmetry and changes sign by the inversion operation $\sigma_1 \leftrightarrow \sigma_2$. From these properties, its general expression is

$$g_0(\sigma) = a\sigma_0(\sigma_1 - \sigma_2),$$

(28)

so that equation (10) is satisfied. Although it is unnecessary at this point, the coefficient $a$ can be determined explicitly and is given by

$$a = (b_0 - b_1) \sinh(A_1 - A_2).$$

(29)

It follows therefore that

$$w_0(\sigma) = (b_0 + b_1\sigma_1\sigma_2)e^{-\sigma_0(A_1\sigma_1 + A_2\sigma_2)}$$

(30)

is the desired spin flip transition for the linear chain, valid for any values of $b_0$, $b_1$, $A_1$ and $A_2$ as long as

$$A_1 + A_2 = 2K.$$  

(31)

Detailed balance occurs when $A_1 = A_2$.

The transition rate (30) can also be written in the equivalent form [5]

$$w_0(\sigma) = \alpha(1 - \gamma_1\sigma_0\sigma_1 - \gamma_2\sigma_0\sigma_2 + r\sigma_1\sigma_2),$$

(32)
where the parameters $\gamma_1$, $\gamma_2$ and $r$ are related to $b_0$, $b_1$ and $A_1$ and $A_2$ by

\[
\frac{\gamma_1 + \gamma_2}{1 + r} = \tanh(A_1 + A_2), \tag{33}
\]

\[
\frac{\gamma_1 - \gamma_2}{1 - r} = \tanh(A_1 - A_2), \tag{34}
\]

\[
1 - r = \frac{(b_0 - b_1) \cosh(A_1 - A_2)}{(b_0 + b_1) \cosh(A_1 + A_2)}, \tag{35}
\]

and to the coupling constant $K$ by

\[
\gamma_1 + \gamma_2 = (1 + r) \tanh 2K. \tag{36}
\]

Detailed balance is recovered when $\gamma_1 = \gamma_2$.

A totally asymmetric transition rate [5], that is, a rate that does not depend on the spin at the left of the central site, is obtained by setting $b_1 = 0$ and $A_2 = 0$, in which case $A_1 = 2K$ so that

\[
w_0(\sigma) = b_0 e^{-2K \sigma_0 \sigma_1}, \tag{37}
\]

or in an equivalent way, by setting $r = 0$ and $\gamma_2 = 0$ in which case $\gamma_1 = \tanh 2K$ and

\[
w_0(\sigma) = a(1 - \gamma_1 \sigma_0 \sigma_1). \tag{38}
\]

### 5. Square lattice

The stationary BG distribution for this case is given by (11), defined on a square lattice, and again we focus on a particular site denoted by $i = 0$. Its four nearest neighbors are denoted by $i = 1, 2, 3, 4$ as shown in figure 1. Using this convention the spin flip transition is given by

\[
w_0(\sigma) = K_0(\sigma) e^{-\sigma_0(A_1 \sigma_1 + A_2 \sigma_2 + A_3 \sigma_3 + A_4 \sigma_4)}, \tag{39}
\]

where

\[
A_1 + A_2 = 2K, \quad A_3 + A_4 = 2K. \tag{40}
\]

The function $K_0(\sigma)$, which depends on $\sigma_1$, $\sigma_2$, $\sigma_3$ and $\sigma_4$, is invariant under the inversion operation $\sigma_1 \leftrightarrow \sigma_2$ and $\sigma_3 \leftrightarrow \sigma_4$ and has up–down symmetry. Its most general form is

\[
K_0(\sigma) = b_0 + b_1 \sigma_1 \sigma_2 + b_2 \sigma_3 \sigma_4 + b_3 (\sigma_1 \sigma_3 + \sigma_2 \sigma_4) + b_4 (\sigma_1 \sigma_4 + \sigma_2 \sigma_3) + b_5 \sigma_1 \sigma_2 \sigma_3 \sigma_4. \tag{41}
\]

The most general form of $g_0(\sigma)$, which changes sign under the inversion operation $\sigma_1 \leftrightarrow \sigma_2$ and $\sigma_3 \leftrightarrow \sigma_4$ and has the up–down symmetry, is

\[
g_0(\sigma) = a_1 \sigma_0 (\sigma_1 - \sigma_2) + a_2 \sigma_0 (\sigma_3 - \sigma_4) + a_3 (\sigma_1 \sigma_3 - \sigma_2 \sigma_4) + a_4 (\sigma_1 \sigma_4 - \sigma_2 \sigma_3) + a_5 \sigma_0 (\sigma_1 - \sigma_2) \sigma_3 \sigma_4 + a_6 \sigma_0 \sigma_1 \sigma_2 (\sigma_3 - \sigma_4). \tag{42}
\]

Each cluster of spins appearing on the right-hand side of this expansion is shown in table 1 together with the respective coefficients. When equation (10) is applied to each one of the clusters in the four first columns of table 1, it becomes fulfilled because the inversions of
these clusters are identified as translation clusters. Applying equation (10) to the clusters in the fifth and sixth columns gives the conditions \( a_5 = 0 \) and \( a_6 = 0 \).

The coefficients \( a_i \) are determined by means of formula (8) and are given by

\[
a_1 = (S_1 C_2 - C_1 S_2)[C_3 C_4(b_0 - b_1) + S_3 S_4(b_2 - b_3)] + (C_1 C_2 - S_1 S_2)(S_3 C_4 - C_3 S_4)(b_3 - b_4),
\]

\[
a_2 = (S_3 C_4 - C_3 S_4)[C_1 C_2(b_0 - b_2) + S_1 S_2(b_1 - b_3)] + (S_1 C_2 - C_1 S_2)(C_3 C_4 - S_3 S_4)(b_3 - b_4),
\]

\[
a_3 = (S_1 C_2 S_3 S_4 - C_1 S_2 S_3 C_4)(b_1 - b_2) + (S_1 C_2 S_3 C_4 - C_1 S_2 S_3 S_4)(b_5 - b_6),
\]

\[
a_4 = (S_1 C_2 S_3 S_4 - C_1 S_2 S_3 S_4)(b_1 - b_2) + (S_1 C_2 S_3 C_4 - C_1 S_2 S_3 S_4)(b_5 - b_6),
\]

\[
a_5 = (C_3 S_4 - S_3 C_4)[(b_2 - b_0)S_1 S_2 + (b_5 - b_1)C_1 C_2] + (S_1 C_2 - C_1 S_2)(C_3 C_4 - S_3 S_4)(b_3 - b_4),
\]

\[
a_6 = (C_1 S_2 - S_1 C_2)[(b_1 - b_0)S_3 S_4 + (b_5 - b_2)C_2 C_4] + (C_1 C_2 - S_1 S_2)(C_3 S_4 - S_3 C_4)(b_3 - b_4),
\]

where \( C_i = \cosh A_i \) and \( S_i = \sinh A_i \).

Setting \( a_5 = 0 \) and \( a_6 = 0 \) we get the desired conditions on the coefficients \( b_i \) and \( A_i \). A trivial solution is \( A_1 = A_2 = A_3 = A_4 = K \), which gives a transition rate obeying detailed balance. But we are interested in solutions other than the trivial that will lead us to transition rates that do not obey detailed balance. In this case we have four constraints given by \( a_5 = 0 \) and \( a_6 = 0 \) and by the two equations (40), and 10 parameters \( b_i, i = 0-5 \) and \( A_i, i = 1-4 \). We are left therefore with six independent parameters. In what follows we consider particular solutions leading to a reduced number of independent parameters.

5.1. Example 1

In this section we restrict ourselves to the case in which \( b_4 = b_3 \), reducing the dynamics to five independent parameters. The transition rate becomes

\[
w_0(\sigma) = \mathcal{K}_0(\sigma) e^{-\sigma_0(A_1 \sigma_1 + A_2 \sigma_2 + A_3 \sigma_3 + A_4 \sigma_4)},
\]

\[
\mathcal{K}_0(\sigma) = b_0 + b_1 \sigma_1 \sigma_2 + b_2 \sigma_3 \sigma_4 + b_3 (\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4) + b_5 \sigma_1 \sigma_2 \sigma_3 \sigma_4,
\]

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with the restrictions
\[
\frac{b_2 - b_5}{b_1 - b_0} = \tanh A_3 \tanh A_4, \tag{51}
\]
\[
\frac{b_1 - b_5}{b_2 - b_0} = \tanh A_1 \tanh A_2, \tag{52}
\]
in addition to (40). The parameter \(b_3\) is free.

5.2. Example 2

A simpler dynamics is obtained by setting \(A_3 = A_1\) and \(A_4 = A_2\) from which follows that \(b_2 = b_1\). In this case we are left with five independent parameters and

\[
w_0(\sigma) = K_0(\sigma)e^{-\sigma_0[A_1(\sigma_1 + \sigma_3) + A_2(\sigma_2 + \sigma_4)]}, \tag{53}
\]
\[
K_0(\sigma) = b_0 + b_1(\sigma_1 \sigma_2 + \sigma_3 \sigma_4) + b_3(\sigma_1 \sigma_3 + \sigma_2 \sigma_4) + b_4(\sigma_1 \sigma_4 + \sigma_2 \sigma_3) + b_5 \sigma_1 \sigma_2 \sigma_3 \sigma_4, \tag{54}
\]
with the restriction
\[
\frac{b_1 - b_5 + b_4 - b_3}{b_1 - b_0 + b_4 - b_3} = \tanh A_1 \tanh A_2, \tag{55}
\]
in addition to \(A_1 + A_2 = 2K\).

5.3. Example 3

Another simpler dynamics is obtained by setting \(A_4 = 0\) and \(b_4 = b_3\). In this case, \(A_3 = 2K\) and \(b_5 = b_2\) and the transition rate becomes

\[
w_0(\sigma) = K_0(\sigma)e^{-\sigma_0(A_1(\sigma_1 + 2K \sigma_3 + A_2 \sigma_4))}, \tag{56}
\]
\[
K_0(\sigma) = b_0 + b_1 \sigma_1 \sigma_2 + b_2(\sigma_3 \sigma_4 + \sigma_1 \sigma_2 \sigma_3 \sigma_4) + b_3(\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4), \tag{57}
\]
with the restriction
\[
\frac{b_1 - b_2}{b_2 - b_0} = \tanh A_1 \tanh A_2, \tag{58}
\]
in addition to \(A_1 + A_2 = 2K\). The parameter \(b_3\) is free.

From this case we obtain a transition rate in which the central spin is influenced by the left, top and right spins [5] by setting in addition \(b_2 = b_3 = 0\), in which case the transition rate is reduced to

\[
w_0(\sigma) = (b_0 + b_1 \sigma_1 \sigma_2)e^{-\sigma_0(A_1 \sigma_1 + 2K \sigma_3 + A_2 \sigma_2)}, \tag{59}
\]
with the restrictions
\[
\frac{b_1}{b_0} = -\tanh A_1 \tanh A_2, \tag{60}
\]
and \(A_1 + A_2 = 2K\). In this case, we are left with two independent parameters. The transition rate can also be written in the equivalent form

\[
w_0(\sigma) = \alpha e^{-B \sigma_1 \sigma_2 - \sigma_0(A_1 \sigma_1 + 2K \sigma_3 + A_2 \sigma_2)}, \tag{61}
\]
where the parameter \(B\) is related to \(A_1\) and \(A_2\) by
\[
\tanh B = \tanh A_1 \tanh A_2. \tag{62}
\]
5.4. Example 4

An even simpler dynamics is obtained if we set $A_3 = A_1$ and $A_4 = A_2 = 0$, from which it follows that $A_1 = A_2 = 2K$ and $b_1 + b_4 = b_5 + b_3$, which is the only constraint. Setting $b_4 = b_3$ we get $b_5 = b_3$ and the spin flip rate is reduced to the expression

$$w_0(\sigma) = K_0(\sigma)e^{-2K\sigma_0(\sigma_1 + \sigma_3)},$$

(63)

$$K_0(\sigma) = b_0 + b_1(\sigma_1\sigma_2 + \sigma_3\sigma_4 + \sigma_1\sigma_2\sigma_3\sigma_4) + b_3(\sigma_1 + \sigma_2)(\sigma_3 + \sigma_4),$$

(64)

with three free parameters $b_0$, $b_1$ and $b_3$.

The simplest spin flip transition is obtained by further setting $b_3 = b_1 = 0$ leading to

$$w_0(\sigma) = b_0e^{-2K\sigma_0(\sigma_1 + \sigma_3)}.$$ 

(65)

This is a totally asymmetric dynamics defined on a square lattice, in which the central spin is influenced only by the right and top spins, introduced by Künsch [3] and also obtained by Godrèche and Bray [5].

6. Cubic lattice

The stationary BG distribution for this case is given by (11), defined on a cubic lattice, and again we consider a particular site $i = 0$ and its six nearest neighbors, denoted by $i = 1–6$ according to the convention of figure 1. For this case we will consider a simpler form for $w_0(\sigma)$. We assume that it is also invariant under the permutations among $\sigma_1$, $\sigma_3$ and $\sigma_5$ and the permutations among $\sigma_2$, $\sigma_4$ and $\sigma_6$. It is given by

$$w_0(\sigma) = K_0(\sigma)e^{-\sigma_0[A_1(\sigma_1 + \sigma_3 + \sigma_5) + A_2(\sigma_2 + \sigma_4 + \sigma_6)]},$$

(66)

where $A_1 + A_2 = 2K$. We use the following specific expression for $K_0(\sigma)$ which is also invariant under the permutations just defined,

$$K_0(\sigma) = b_0 + b_1x_1x_2 + b_2(y_1 + y_2) + b_3y_1y_2 + b_4(x_1z_2 + z_1x_2) + b_5z_1z_2,$$

(67)

where

$$x_1 = \sigma_1 + \sigma_3 + \sigma_5, \quad x_2 = \sigma_2 + \sigma_4 + \sigma_6,$$

(68)

$$y_1 = \sigma_1\sigma_3 + \sigma_1\sigma_5 + \sigma_3\sigma_5, \quad y_2 = \sigma_2\sigma_4 + \sigma_2\sigma_6 + \sigma_4\sigma_6,$$

(69)

$$z_1 = \sigma_1\sigma_3\sigma_5, \quad z_2 = \sigma_2\sigma_4\sigma_6.$$ 

(70)

From (22) and (67) we get the following form for $g_0(\sigma)$ which is also invariant under the permutations defined above, besides changing sign under the transformation $\sigma_1 \leftrightarrow \sigma_2$, $\sigma_3 \leftrightarrow \sigma_4$, and $\sigma_5 \leftrightarrow \sigma_6$ and being invariant under the up–down transformation,

$$g_0(\sigma) = a_1\sigma_0(x_1 - x_2) + a_2(y_1 - y_2) + a_3\sigma_0(z_1 - z_2) + a_4\sigma_0(x_1y_2 - y_1x_2) + a_5(x_1z_2 - z_1x_2) + a_6\sigma_0(y_1z_2 - z_1y_2).$$

(71)

Each cluster of spins appearing on the right-hand side of this expansion is shown in table 2 together with the respective coefficients. When the equation (10) is applied to each of the clusters in the two first columns it becomes fulfilled because the inversions of these
clusters are identified as translation clusters. Applying equation (10) to the clusters in the third, fourth, fifth and sixth columns, we get the constraints $a_3 = 0$, $a_4 = 0$, $a_5 = 0$ and $a_6 = 0$.

Let us define the auxiliary quantities

$$h_1 = C_1^2 C_2^2 (C_1 S_2 - S_1 C_2),$$

$$h_2 = C_1 C_2 (S_1^2 C_2^2 - C_1^2 S_2^2),$$

$$h_3 = (C_1 S_2^2 - S_1 C_2^2),$$

$$h_4 = C_1 S_1 C_2 S_2 (C_1 S_2 - S_1 C_2),$$

$$h_5 = S_1 S_2 (S_1^2 C_2^2 C_1^2 S_2^2),$$

$$h_6 = S_1^2 S_2^2 (C_1 S_2 - S_1 C_2),$$

where $S_i = \sinh A_i$ and $C_i = \cosh A_i$. The six coefficients are written as

$$a_1 = -h_1 b_0 + 3(h_1 - 2h_4) b_1 - 3(h_6 - 2h_4) b_3 - (h_3 + 2h_1 - 3h_4) b_2 + (h_3 + 2h_6 - 3h_4) b_4 - h_6 b_5,$$

$$a_2 = -h_2 (b_0 + 2b_2 - 3b_3) + h_5 (b_5 + 2b_4 - 3b_1),$$

$$a_3 = -3(h_1 + h_6) (b_2 - b_4) - h_3 (b_0 - b_5) - 9h_4 (b_1 - b_3),$$

$$a_4 = (2h_1 + 2h_6 + h_3 - 4h_4) (b_1 - b_3) + (h_1 - 4h_4 + h_6) (b_4 - b_2) + h_4 (b_0 - b_5),$$

$$a_5 = h_2 (3b_1 - 2b_4 - b_5) + h_5 (b_0 + 2b_2 - 3b_3),$$

$$a_6 = h_1 (3b_3 - 2b_4 - b_5) + 6h_4 (b_1 - b_3) + (3h_4 - h_3) (b_4 - b_2) + h_6 (b_0 - 3b_1 + 2b_2).$$

Taking into account the four constraints $a_3 = 0$, $a_4 = 0$, $a_5 = 0$, $a_6 = 0$ and $A_1 + A_2 = 2K$, there are eight parameters and five equations, giving therefore three
free parameters. It is possible to find solutions as long as $A_1 \neq 0$ and $A_2 \neq 0$. However, no solution exists when $A_1 = 0$ or $A_2 = 0$ leading to the conclusion that, within the assumed form (20) of the transition rate, there can be no totally asymmetric dynamics for the cubic lattice, in agreement with Godrèche and Bray [5].

7. Entropy production

In this section we determine the entropy production rate $\Pi$ in the stationary regime of the nonequilibrium models defined in the previous sections. To determine the entropy production rate we use an expression introduced by Schnakenberg and considered by several authors. For the present case of a one spin flip dynamics given by the master equation (1) this expressions reads

$$\Pi = \frac{k_B}{2} \sum_\sigma \sum_i \{w_i(\sigma^j)P(\sigma^j) - w_i(\sigma)P(\sigma)\} \ln \frac{w_i(\sigma^j)P(\sigma^j)}{w_i(\sigma)P(\sigma)}, \quad (84)$$

where $k_B$ is the Boltzmann constant; this expression is is always nonnegative and vanishes only when detailed balance is obeyed. In the stationary state this expression is equivalent to

$$\Pi = \frac{k_B}{2} \sum_\sigma \sum_i \{w_i(\sigma^j)P(\sigma^j) - w_i(\sigma)P(\sigma)\} \ln \frac{w_i(\sigma^j)}{w_i(\sigma)}. \quad (85)$$

To show this it suffices to observe that the difference between these two expression vanishes in the steady state, a result that can be obtained by the use of the global balance (2).

The entropy production rate can be written in the simpler form

$$\Pi = k_B \sum_\sigma \sum_i w_i(\sigma)P(\sigma) \ln \frac{w_i(\sigma)}{w_i(\sigma^j)}. \quad (86)$$

Taking into account the translation invariance, we may write the entropy production rate per site $\Pi_0 = \Pi/N$ as

$$\Pi_0 = k_B \left\langle w_0(\sigma) \ln \frac{w_0(\sigma)}{w_0(\sigma^0)} \right\rangle, \quad (87)$$

or

$$\Pi_0 = \frac{k_B}{2} \left\langle g_0(\sigma) \ln \frac{w_0(\sigma)}{w_0(\sigma)} \right\rangle. \quad (88)$$

In the last equation we have used the definition of the function $g_i(\sigma)$ given by (4).

Using the general form (20) for the spin flip transition rate we get

$$\Pi_0 = k_B \sum_\delta A_\delta \langle g_0(\sigma)\sigma_0\sigma_\delta \rangle. \quad (89)$$

Taking into account that $g_0(\sigma)$ changes sign under the inversion operation we may write $\Pi_0$ as

$$\Pi_0 = k_B \sum_{\delta > 0} (A_\delta - A_{-\delta}) \langle g_0(\sigma)\sigma_0\sigma_\delta \rangle, \quad (90)$$

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where the summation in $\delta$ extends over half of the nearest neighbor sites. This expression shows that the rate of entropy production is a bilinear form

$$
\Pi_0 = \sum_{\delta > 0} X_\delta \mathcal{J}_\delta,
$$

(91)
in terms of forces,

$$
X_\delta = k_B(A_\delta - A_{-\delta}),
$$

(92)
and fluxes,

$$
\mathcal{J}_\delta = \langle g_0(\sigma)\sigma_0\sigma_\delta \rangle.
$$

(93)
We remark that, when $A_{-\delta} = A_\delta$, that is when detailed balance is obeyed, $g_0(\sigma)$ vanishes so that the fluxes $\mathcal{J}_\delta$ vanish. Therefore when the forces $X_\delta$ vanish, the fluxes vanish as well. We point out in addition that the expression (90) of the entropy production rate in terms of forces and fluxes is valid for any transition rate of the form (20) no matter whether the stationary state is of the BG type or not.

7.1. Contact with particle reservoirs

It is possible to interpret the transition rate (20) as describing the contact of the system to particle reservoirs. Let us consider first the one-dimensional dynamics defined by the transition rate given by (26). We assume the system to be in contact with two particle reservoirs. The contact with one reservoir is represented by the transition rate

$$
w^+_0(\sigma) = K_0(\sigma)e^{-\sigma_0[J(\sigma_1+\sigma_2)+H]/k_B T},
$$

(94)
and should be used when the configurations are $(\sigma_1, \sigma_2) = (-,-)$ and $(+,-)$, and the contact with the other is represented by

$$
w^-_0(\sigma) = K_0(\sigma)e^{-\sigma_0[J(\sigma_1+\sigma_2)-H]/k_B T},
$$

(95)
which should be used when the configurations are $(\sigma_1, \sigma_2) = (-,+)$ and $(+,+)$.

The parameter $T$ is the temperature of the reservoirs, considered to be the same, and $H$ and $-H$ are the fields related to each of the reservoirs. Comparing the transition rates (94) and (95) with (26) we get

$$
\frac{2J - H}{k_B T} = A_1 + A_2 = 2K, \quad \frac{H}{k_B T} = A_1 - A_2.
$$

(96)
In the case of a totally asymmetric transition rate $A_2 = 0$, so that $H = J$.

According to present interpretation the quantity $\mathcal{J}_1$ above will be the flux of particles through the system from one reservoir to the other.

We consider now the two-dimensional case and in particular the transition rate (53). In this case we assume that the system is in contact with three particle reservoirs, all with the same temperature $T$. The contact with the first is described by the transition rate

$$
w^+_0(\sigma) = K_0(\sigma)e^{-\sigma_0[J(\sigma_1+\sigma_2+\sigma_3+\sigma_4)+H]/k_B T},
$$

(97)
with the second by

$$
w^-_0(\sigma) = K_0(\sigma)e^{-\sigma_0[J(\sigma_1+\sigma_2+\sigma_3+\sigma_4)-H]/k_B T},
$$

(98)
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Figure 2. Local configurations associated with the first reservoir (on the left), to the second reservoir (center) and to the third reservoir (on the right). A dot represents the site to be updated, that can be in the plus or minus state.

and with the third by

\[ w_0^0(\sigma) = K_0(\sigma) e^{-\sigma_0 J (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) / k_BT}, \]  
(99)

and they should be used according to configurations shown in figure 2. Comparing the rates (97)–(99) with (53), we obtain the following relations

\[ \frac{4J - H}{2k_BT} = A_1 + A_2 = 2K, \quad \frac{H}{2k_BT} = A_1 - A_2. \]  
(100)

In the totally asymmetric case \( A_2 = 0 \) and we conclude that \( H = 2J \).

Again, according to the present interpretation, the quantity \( J_1 \) is the flux of particles through the system between the first reservoir and the second reservoir.

If we define a temperature \( T_s \) of the system by \( K = J / k_BT_s \) we come to the conclusion that \( T_s \) is in general distinct, in both cases examined above, from the temperature \( T \) of the reservoir, as can be inferred from the relations (96) and (100).

7.2. Linear chain

We determine here the entropy production for the one-dimensional system defined by the transition rate given by (30) which is

\[ w_0(\sigma) = (b_0 + b_1 \sigma_1 \sigma_2) e^{-\sigma_0 (A_1 \sigma_1 + A_2 \sigma_2)}. \]  
(101)

This dynamics lacks detailed balance for \( A_1 \neq A_2 \) and its stationary probability is the BG distribution

\[ P(\sigma) = \frac{1}{Z} e^{K \sum \sigma_i \sigma_{i+1}}, \]  
(102)

where the coupling constant \( K \) is related to \( A_1 \) and \( A_2 \) by \( A_1 + A_2 = 2K \).

Using expression (93) and the result (28) we get

\[ J_1 = a (1 - \langle \sigma_1 \sigma_2 \rangle), \]  
(103)

which involves the next nearest neighbor two-site correlation \( \langle \sigma_1 \sigma_2 \rangle \). The value of this correlation is obtained from the solution of the one-dimensional Ising model defined by (102) and is \( \langle \sigma_1 \sigma_2 \rangle = (\tanh K)^2 \). Therefore,

\[ J_1 = \frac{a}{(\cosh K)^2}. \]  
(104)

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Remembering that \( a \) has been calculated previously and is given by (29) we get
\[
\mathcal{J}_1 = \frac{(b_0 - b_1) \sinh (A_1 - A_2)}{(\cosh K)^2},
\]  
(105)
and
\[
\Pi_0 = \frac{k_B (b_0 - b_1)(A_1 - A_2) \sinh (A_1 - A_2)}{(\cosh K)^2}.
\]  
(106)

Since \( b_0 \geq b_1 \), because otherwise \( w_0 \) could be negative, it follows that \( \Pi_0 \geq 0 \), as it should be.

The entropy production rate of the totally asymmetric dynamics is obtained from this expression by setting \( b_1 = 0 \), \( A_2 = 0 \) and \( A_1 = 2K \) leading to
\[
\Pi_0 = 4k_B b_0 K \tanh K.
\]  
(107)

7.3. Square lattice

For the square lattice we will only consider the case of totally asymmetric dynamics whose spin flip transition rate is
\[
w_0(\sigma) = b_0 e^{-2K\sigma_0(\sigma_1+\sigma_3)},
\]  
(108)
and the stationary state is the BG distribution corresponding to the Ising model on a square lattice with nearest neighbor interactions,
\[
P(\sigma) = \frac{1}{Z} e^{K \Sigma_{\langle ij \rangle} \sigma_i \sigma_j},
\]  
(109)
where \( K \) is the coupling constant. Notice that in this case there is a symmetry breaking phase transition occurring at a value of \( K \) given by \( K_c = (1/2) \ln(1 + \sqrt{2}) \) [28].

The calculation of \( \Pi_0 \) becomes easier if we use expression (87), from which we get
\[
\Pi_0 = 4k_B b_0 K [\sinh 4K (1 + \langle \sigma_1 \sigma_3 \rangle) - 2 \cosh 4K \langle \sigma_0 \sigma_1 \rangle],
\]  
(110)
where \( \langle \sigma_0 \sigma_1 \rangle \) and \( \langle \sigma_1 \sigma_3 \rangle \) are the nearest and next nearest neighbor correlations on a square lattice. These two correlations can be calculated exactly so that the entropy production rate is exactly determined (see figure 3). From the exact solution of the Ising model on a square lattice [28] the correlations are as follows. For \( K < K_c \)
\[
\langle \sigma_0 \sigma_1 \rangle = \coth 2K \left[ \frac{1}{2} + \frac{1}{\pi}(\sinh^2 2K - 1)\mathcal{K}(k_>) \right],
\]  
(111)
\[
\langle \sigma_1 \sigma_3 \rangle = \frac{2}{\pi k_>}[\mathcal{E}(k_>) + (k_>^2 - 1)\mathcal{K}(k_>)].
\]  
(112)
For \( K > K_c \)
\[
\langle \sigma_0 \sigma_1 \rangle = \coth 2K \left[ \frac{1}{2} + \frac{1}{\pi}(2 - \coth^2 2K)\mathcal{K}(k_<) \right],
\]  
(113)
\[
\langle \sigma_1 \sigma_3 \rangle = \frac{2}{\pi} \mathcal{E}(k_<)
\]  
(114)
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Figure 3. Entropy production rate per site as a function of $\theta = 1/K$ where $\zeta = \Pi_0/b_0k_B$ according to the exact expression (110). There is a singularity at $\theta_c = 1/K_c = 2/\ln(1 + \sqrt{2}) = 2.269185$.

where $k_\triangleright = 1/k_\triangleleft = \sinh^2 2K$. The functions $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind, given by

$$K(k) = \int_0^{\pi/2} (1 - k^2 \sin^2 \phi)^{-1/2} d\phi, \quad (115)$$

$$E(k) = \int_0^{\pi/2} (1 - k^2 \sin^2 \phi)^{1/2} d\phi. \quad (116)$$

The correlations are finite but have a singularity of the type [28]

$$|K - K_c| \ln |K - K_c|, \quad (117)$$

around the critical point. Therefore the rate of entropy production for the totally asymmetric model on a square lattice also has the same type of singularity. The same type of singularity is to be expected for other transition rates that do not obey detailed balance.

7.4. Cubic lattice

From the expression (90) it becomes evident that the entropy production rate is a sum of short range correlations involving an even number of spins of the set composed by a central spin and its nearest neighbors. In one and two dimensions it was possible to determine these correlations exactly. In three dimensions the exact closed forms for the correlations are unknown but it is well known that the even short range correlations of
the Ising model are finite and have a singularity around the critical point of the type
\[ |K - K_c|^{1-\alpha}, \]
where \( \alpha < 1 \) is the critical exponent related to the specific heat. Therefore, we expect the same behavior for the entropy production rate in the cubic lattice, that is, \( \Pi_0 \) is finite with a singularity of the type above.

8. Conclusion

We have constructed spin flip dynamics for irreversible spin models, that do not obey detailed balance but, despite that, are described by a stationary BG probability distribution. The existence of such irreversible dynamics means that the BG distribution is a necessary but not sufficient condition for thermodynamic equilibrium. The necessary and sufficient condition is detailed balance or, in an equivalent way, the vanishing of the entropy production rate. The method we use has similarities to that advanced by Godrèche and Bray [5]. Both methods use as starting point the global balance equation for the BG distribution in the form given by equation (3). However, the two approaches are distinct in the way the constraint equations are obtained. In our method, we set up constraint equations in terms of the parameters \( b_i \) and \( A_i \) entering the transition rate. In their method, they set up constraint equations for the rates by determining the number of motifs. We have considered a particular form of the transition rate, with up–down symmetry, but our approach is general and can be used in association with any transition rate. Within the assumed form (20) of the transition rate, we confirm the findings of Godrèche and Bray [5], that there are totally asymmetric dynamics for the linear and square lattice but not for the cubic lattice.

We point out that we have considered here only the case of one-spin flip dynamics. The case of spin exchange, a two-spin flip dynamics, has been discussed by Spohn [29] by the use of a gradient condition, which seems to be similar to the condition (10). The following conclusions are drawn for the spin exchange case [29]. In one dimension it is possible to find many irreversible dynamics with a GB probability distribution. In two or more dimensions the only possible solution corresponds to a trivial GB probability distribution with vanishing coupling constants. Our results for the one-spin flip dynamics are much less restrictive. We have found irreversible dynamics with non-trivial GB probability distribution, that is, with nonzero coupling constants, not only in one dimension but also in two and three dimensions. Moreover, an irreversible transition rate for the trivial GB probability distribution exists in any dimension. Indeed, it is straightforward to show that the transition rate
\[ w_0(\sigma) = b_0 - \sigma_0 \sum_{\delta > 0} b_\delta (\sigma_\delta - \sigma_{-\delta}), \]
defined on a hypercubic lattice, corresponds to a trivial GB probability distribution with vanishing coupling constant.

We have also determined the entropy production rate at the stationary state and have shown that it can be written as a macroscopic bilinear form in the forces and fluxes. The entropy production rate was determined as a function of the parameters entering the transition rates or in an equivalent way as a function of parameters defining
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the reservoirs. The entropy production rate was determined exactly for the general expression for the linear chain. For the square lattice we used the spin flip transition rate corresponding to the totally asymmetric dynamics from which we determined exactly the entropy production rate. In this case we have shown that the entropy production rate displays a singularity of the same type as the entropy itself (or energy, since both have the same critical behavior). Although we did not calculate the entropy production rate for the three-dimensional case we argued that it should also have the same critical behavior as entropy or energy, that is, associated with a critical exponent $1 - \alpha$.

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