Entropy production for asymmetric diffusion of particles

M O Hase¹, T Tomé² and M J de Oliveira²

¹ Escola de Artes, Ciências e Humanidades, Universidade de São Paulo, Avenida Arlindo Béttio, 1000, 03828-000 São Paulo, São Paulo, Brazil
² Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05314-970 São Paulo, São Paulo, Brazil
E-mail: mhase@usp.br

Received 26 September 2015
Accepted for publication 28 October 2015
Published 10 December 2015

Abstract. We analyse a non-equilibrium exclusion process in which particles are created and annihilated in pairs and hop to the the right or to the left with different transition rates, \( p \) and \( q \), respectively. We have studied the dynamics of a single particle, and exactly determined the entropy, entropy production rate and entropy flux as functions of time. In the system of many particles, we have characterised the system by its probability distribution, as well as the entropy production rate in close forms, provided that \( p + q \) equals the sum of the dimers creation and annihilation rates. The general case, where this constraint is absent, was considered at a pair approximation level; the time-dependent behaviour of the system was analysed, and the stationary entropy production was determined. In all cases, in the stationary regime, we showed that the entropy production rate is a bilinear form in the current of particles and the force \( \ln(p/q) \).

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

Non-equilibrium statistical physics presents fundamental questions that may require the use of approaches and quantities which has no analogue in an equilibrium context. One of these quantities is the production of entropy, which vanishes in equilibrium and is positive in non-equilibrium and may thus characterise a system out of thermodynamic equilibrium. The time derivative of entropy $S$ of a system can be decomposed into two components \[ \frac{dS}{dt} = \Pi - \Phi, \] as

where one has the entropy production rate, $\Pi$, and entropy flux, $\Phi$. The former is the contribution to the entropy by the system itself and is always non-negative. The latter, the entropy flux, is the contribution due to the environment, and can have either signs: the flux is positive if the entropy leaves the system. These functions distinguish different dynamics regimes, since in the stationary state they are equal, $\Pi = \Phi$ (but not necessarily zero); furthermore, in equilibrium state, they both vanish, $\Pi = \Phi = 0$.

Equation (1) is useful in the study of models in statistical mechanics as long as we know the statistical definitions of the quantities $S$, $\Pi$ and $\Phi$ for systems out of equilibrium. Here we are interested in the models described by a continuous time Markovian process, that is, governed by the master equation \[ \frac{d}{dt} P_i(t) = \sum_j \left[ W_{ij} P_j(t) - W_{ji} P_i(t) \right], \]
where $P_i(t)$ is the probability of finding the system in state $i$ at time $t$ and $W_{ij}$ is the transition rate from state $j$ to state $i$. The definition of entropy $S$ in thermodynamic equilibrium or out of equilibrium is given by the Boltzmann–Gibbs expression

$$S(t) = -\sum_i P_i(t) \ln P_i(t),$$

and the entropy production rate is given by [4]

$$\Pi(t) = \frac{1}{2} \sum_{ij} [W_{ij} P_j(t) - W_{ji} P_i(t)] \ln \frac{W_{ij} P_j(t)}{W_{ji} P_i(t)},$$

an expression that has been considered by several authors [5–17].

From the time derivative of entropy,

$$\frac{dS}{dt} = \frac{1}{2} \sum_{ij} [W_{ij} P_j(t) - W_{ji} P_i(t)] \ln \frac{P_j(t)}{P_i(t)},$$

obtained by the use of the master equation, and the definition of $\Pi$, we find from (1) that the entropy flux is given by

$$\Phi(t) = \frac{1}{2} \sum_{ij} [W_{ij} P_j(t) - W_{ji} P_i(t)] \ln \frac{W_{ij}}{W_{ji}}.$$

It is seen that the entropy production rate given by expression (4) is non-negative. Moreover, it vanishes in thermodynamic equilibrium, in which case the detailed balance condition is fulfilled, that is, $W_{ij} P_j = W_{ji} P_i$. The expression analogous to (4) has also been obtained for systems described by a Fokker–Planck equation [18].

The calculation of the production of entropy of lattice models has been done in several models; in some cases, by the use of numerical simulations [7, 14, 16, 17]. In this paper we consider a system of particles moving along a one-dimensional lattice with periodic boundary conditions. They hop to the right or to the left with distinct rates denoted by $p$ and $q$, respectively, so that in the stationary state the system is not in thermodynamic equilibrium and the entropy production rate is non-zero. We analyse two models: the first is a system of non-interacting particles, in which case the problem is reduced to solving the master equation for just one particle that performs an asymmetric random walk along a chain of $L$ sites. The second model is a system of exclusion particles that hop to the right and left with transition rates $p$ and $q$ along a chain of $L$ sites. In addition, they may be created in pairs, with rate $c$, and annihilated in pairs, with rate $a$. Both models are solved exactly, the second with the condition $a + c = p + q$, but we have also analysed the case without this constraint in pair approximation. From the solutions, we have determined the entropy production rate. In the stationary state we show that it can be written in the bilinear form [17]

$$\Pi = L J X,$$

where $X = \ln(p/q)$ and $J$ is the current of particles which is shown to vanish when $p \rightarrow q$ as $J \sim X$. Therefore, near thermodynamic equilibrium, which occurs when $p = q$, the entropy production rate vanishes as $\Pi \sim X^2$. 

doi:10.1088/1742-5468/2015/12/P12004
2. One-particle system

2.1. Discrete formulation

A one-dimensional diffusive particle will be considered here. The state of this particle can be identified with the (discrete) position \( n \) it can occupy over a chain. The distribution probability \( P_n \) is governed by the master equation,

\[
\frac{d}{dt} P_n(t) = \sum_m [W_{nm} P_m(t) - W_{mn} P_n(t)],
\]

where \( W_{nm} \) is the transition rate from state \( m \) to \( n \), given by

\[
W_{nm} = \begin{cases} 
 p, & n - m = 1, \\
 q, & n - m = -1, \\
 0, & |n - m| > 1.
\end{cases}
\]

In this setup, the particle jumps to the right with rate \( p \) and to the left with rate \( q \). The parameters \( p \) and \( q \) will be taken to be both strictly positive. The transition is short-ranged in the sense that the particle moves to one of its neighbouring sites per movement. The master equation for this model can be restated as

\[
\frac{d}{dt} P_n(t) = pP_{n-1}(t) + qP_{n+1}(t) - (p + q)P_n(t),
\]

which can be solved exactly. If the initial condition is taken to be \( P_n(0) = \delta_{n0} \), the probability distribution is

\[
P_n(t) = e^{-(p+q)t} \left( \frac{p}{q} \right)^{n/2} I_n(2t\sqrt{pq}),
\]

where \( I_n(z) \) stands for a modified Bessel function (the first kind).

We start by calculating the entropy flux. Applying formula (6) to the present case, one has

\[
\Phi = \frac{1}{2} \sum_n [pP_n(t) - qP_{n+1}(t)] \ln \frac{p}{q} + \frac{1}{2} \sum_n [qP_n(t) - pP_{n-1}(t)] \ln \frac{q}{p},
\]

and it is straightforward to see that

\[
\Phi = (p-q) \ln \frac{p}{q}.
\]

Note that this value for the entropy flux does not depend on time and is a non-negative quantity.

Instead of using formula (4) to calculate the entropy production rate, we determine the entropy derivative \( dS/dt \) and sum to \( \Phi \) to get \( \Pi = \Phi + dS/dt \). Now from formula (5) we have
Entropy production for asymmetric diffusion of particles

\[ \frac{dS}{dt} = \sum_n [pP_n(t) - qP_{n+1}(t)] \ln \frac{P_n(t)}{P_{n+1}(t)}. \]  \hspace{1cm} (14)

Replacing (11) into (14) we may calculate \( dS/dt \). The graphs of \( dS/dt \) calculated numerically from (14) together with \( \Phi \) given by (13) and \( \Pi = \Phi + dS/dt \) are shown in figure 1, where one can see that the entropy production has the tendency to match the entropy flux with time, which leads the time derivative of entropy, \( dS/dt \), to zero, as expected. The system converges to a stationary state, and the way it reaches it is discussed in the next section, where a continuous version of the model is analysed by means of a Fokker–Planck equation.

In the steady state \( \Pi = \Phi \) so that from (13) we find the result for the entropy production rate

\[ \Pi = (p - q) \ln \frac{P}{q}. \]  \hspace{1cm} (15)

Now the current of particles is \( J = (p - q)/L \) and we may write

\[ \Pi = L J X, \]  \hspace{1cm} (16)

where \( X = \ln(p/q) \).

2.2. Continuous formulation

In the continuous case, which means a (biased) random walk on the real line, one can pass from the master equation (10) to a Fokker–Planck equation. The continuous limit of the master equation is obtained as follows. We assume that the possible positions of the particle are \( x = bn \), where \( b \) is the spacing between consecutive positions. Writing \( P_n(t) = b P(x, t) \) and expanding \( P_{n+1}(t) = bP(x + b, t) \) and \( P_{n-1}(t) = bP(x - b, t) \) up to quadratic terms in \( b \), we get
where \( \gamma = (p - q)\beta \) and \( \Gamma = (p + q)\beta^2/2 \). The parameter \( \Gamma \) is the diffusion constant and \( \gamma \) controls the drift of the particle to the right if \( \gamma > 0 \) or to the left if \( \gamma < 0 \). Therefore, \( \gamma = 0 \) corresponds to \( p = q \) in the previous discrete model and \( p > q \) to positive values of \( \gamma \).

Defining the function

\[
J(x, t) = \gamma P(x, t) - \Gamma \frac{\partial}{\partial x} P(x, t),
\]

the Fokker–Planck equation can be cast as

\[
\frac{\partial}{\partial t} P(x, t) = -\frac{\partial}{\partial x} J(x, t),
\]

which is a continuity equation and \( J \) can be interpreted as a probability current. In this formulation, the entropy production is given by [18]

\[
\Pi = \frac{1}{\Gamma} \int dx \frac{[J(x, t)]^2}{P(x, t)},
\]

while the flux is

\[
\Phi = \frac{\gamma}{\Gamma} \int dx \ J(x, t).
\]

As usual, the entropy is given by

\[
S = -\int dx \ P(x, t) \ln P(x, t).
\]

The Fokker–Planck equation (17) can be solved by standard methods, and the probability distribution for the initial condition \( P(x, 0) = \delta(x) \) is

\[
P(x, t) = \frac{1}{\sqrt{4\pi\Gamma t}} \exp \left[ -\frac{(x - \gamma t)^2}{4\Gamma t} \right].
\]

The evaluation of entropy from the probability distribution, given by (23), yields

\[
S = \frac{1}{2} \ln(\Gamma t) + \frac{1}{2} \ln(d\pi e).
\]

Note that the time derivative of the entropy is

\[
\frac{dS}{dt} = \frac{1}{2t}.
\]

\[
doiz:10.1088/1742-5468/2015/12/P12004
\]

J. Stat. Mech. (2015) P12004
which decreases algebraically with time.

Inserting the probability distribution (23) into (20) and (21) gives, respectively, the entropy production rate,

$$\Pi = \frac{\gamma^2}{\Gamma} + \frac{1}{2t},$$

(26)

the entropy flux,

$$\Phi = \frac{\gamma^2}{\Gamma},$$

(27)

and shows that the entropy flux is independent of time as in the discrete case, and vanishes only if $\gamma = 0$. Note that $dS/dt = \Pi - \Phi$ as it should. In the stationary state, $\Pi = \gamma^2/\Gamma$ or yet $\Pi = 2(p - q)^2/(p + q)$.

3. Many-particles system

3.1. Formulation of the problem

The above analysis is extended to a system of many diffusive particles with excluded volume interactions. Consider a chain with $L$ sites, each one being occupied by a particle (●) or empty (○). The possible transitions with the respective rates are as follows:

- $\bullet \rightarrow \circ$ diffusion to the right,
- $\circ \rightarrow \bullet$ diffusion to the left,
- $\circ \rightarrow \circ$ creation,
- $\bullet \rightarrow \bullet$ annihilation.

To each site $n$ we associate a variable $s_n$ that takes the value $s_n = +1$ if the site is occupied (●) and the values $s_n = -1$ if the site is empty (○). In terms of these variables, the possible transitions are

$$ (+1, -1) \xrightarrow{p} (-1, +1) $$
$$ (-1, +1) \xrightarrow{q} (+1, -1) $$
$$ (-1, -1) \xrightarrow{c} (+1, +1) $$
$$ (+1, +1) \xrightarrow{a} (-1, -1) $$

From top to bottom in the above scheme, the particle jumps to the right with rate $p$, and hops to the left with rate $q$. Moreover, a pair of particles is created and annihilated with rate $c$ and $a$, respectively. Assuming a single transition per unit time, the transition rate $w_n(s)$ from $(s_n, s_{n+1})$ to $(-s_n, -s_{n+1})$, where $s = (s_1, \ldots, s_L)$, can be expressed as

$$ w_n(s) = A + Bs_n + Cs_{n+1} + Ds_ns_{n+1}, $$

(28)
where

\[ A = \frac{1}{4} (p + q + c + a), \]  

\[ B = \frac{1}{4} (p - q - c + a), \]  

\[ C = \frac{1}{4} (-p + q - c + a), \]  

\[ D = \frac{1}{4} (-p - q + c + a). \]  

The time evolution of probability distribution is given by the master equation

\[
\frac{d}{dt} P(s, t) = \sum_{n=1}^{L} \left[ w_n(s^{n,n+1}) P(s^{n,n+1}, t) - w_n(s) P(s, t) \right],
\]

where \( s^{n,n+1} \) denotes the vector \( s \) with the variables \( s_n \) and \( s_{n+1} \) replaced by \( -s_n \) and \( -s_{n+1} \), respectively.

### 3.2. Stationary solution

The model defined by the transition rate (28) becomes simpler when the condition \( D = 0 \) is imposed, because in this case the transition rate \( w_n \) becomes linear in the \( s_n \) and \( s_{n+1} \), that is,

\[ w_n(s) = A + B s_n + C s_{n+1}. \]  

The condition \( D = 0 \) is equivalent to the relation

\[ a + c = p + q, \]  

which means that the sum of the creation and annihilation rates is equal to the sum of the diffusion to the right and to the left.

The stationary probability distribution can be shown to be of the form [19, 20]

\[ P(s) = \frac{1}{Z} e^{h(s_1 + s_2 + \ldots + s_L)}, \]  

where \( Z = (2 \cosh h)^L \) and \( h \) is a parameter to be determined. To this end, we replace (36) into the stationary master equation

\[
\sum_{n=1}^{L} \left[ w_n(s^{n,n+1}) P(s^{n,n+1}, t) - w_n(s) P(s) \right] = 0,
\]

where \( w_n(s) \) is given by (28). This equation is to be solved with a periodic boundary condition. After substitution we get

\[ \text{doi:10.1088/1742-5468/2015/12/P12004} \]
Entropy production for asymmetric diffusion of particles

\[ \sum_{n=1}^{L} [(A - B s_n - C s_{n+1}) e^{-2h(s_n + s_{n+1})} - (A + B s_n + C s_{n+1})] = 0. \] (38)

Defining \( u = \cosh 2h \) and \( v = \sinh 2h \), and using a periodic boundary condition we may write

\[ \sum_{n=1}^{L} (A v + B u + C u) [v(1 + s_n s_{n+1}) - 2u s_n] = 0. \] (39)

Therefore, the distribution (36) is the solution of the stationary master equation if \( A v + B u + C u = 0 \), that is, if

\[ \frac{v}{u} = \frac{-B - C}{A} = \frac{c - a}{c + a}, \] (40)

or \( \tanh 2h = (c - a)/(c + a) \), which determines the parameter \( h \) in terms of the rates \( c \) and \( a \).

From the stationary distribution we may find the magnetisation \( m = \langle s_n \rangle = \tanh h \), which is

\[ m = \frac{\sqrt{c} - \sqrt{a}}{\sqrt{c} + \sqrt{a}}. \] (41)

We may also determine the pair correlation function \( r = \langle s_n s_{n+1} \rangle = \langle s_n \rangle \langle s_{n+1} \rangle = m^2 \). Note that the density of particles is \( \rho = P(+) \), or

\[ \rho = \frac{\sqrt{c}}{\sqrt{c} + \sqrt{a}}. \] (42)

3.3. Flux and production of entropy

The entropy flux, defined by (12), of a system that has its dynamics governed by the rule (28) is given by

\[ \Phi = \sum_s \sum_n w_n(s) P(s) \ln \frac{w_n(s)}{w_n(s^n,n+1)}, \] (43)

which can be written as the average

\[ \Phi = \sum_n \left\langle w_n(s) \ln \frac{w_n(s)}{w_n(s^n,n+1)} \right\rangle, \] (44)

so that

\[ \Phi = \frac{L}{4} \left[ (c - a) \ln \frac{c}{a} + (p - q) \ln \frac{p}{q} \right] - \frac{L}{2} \left[ (c + a) \ln \frac{c}{a} \right] m \] (45)
Entropy production for asymmetric diffusion of particles

\[ + \frac{L}{4} \left( (c - a) \ln \frac{c}{a} - (p - q) \ln \frac{p}{q} \right) r, \]  

(46)

where the translational invariance was invoked.

This equation for \( \Phi \) is valid at any time as long as the constraint \( a + c = p + q \) is fulfilled. In the stationary state we use the result (41) and \( r = m^2 \) to get, after some algebraic manipulations, the result

\[ \Pi = L \frac{\sqrt{ca}}{(\sqrt{c} + \sqrt{a})^2} (p - q) \ln \frac{p}{q}. \]

When \( a = c \) the entropy production rate per particle coincides with the entropy production rate obtained from the one-particle case (13).

The current of particles \( J \) is given by \( pP(+, -) - qP(-+) \). But from the stationary solution (36) we get \( P(+, -) = P(-+) = P(+)P(-) = \rho(1 - \rho) \) so that, \( J = \rho(1 - \rho)(p - q) \), or, using (42),

\[ J = \frac{\sqrt{ca}}{(\sqrt{c} + \sqrt{a})^2} (p - q), \]

(47)

and we may write the entropy production rate as

\[ \Pi = LJX, \]

(48)

where \( X = \ln(p/q) \).

4. Pair approximation

In this section, we will consider again the general problem of one-dimensional diffusion (with the creation and annihilation of particles) where the restriction (35) is removed, which means that the transition rate is

\[ w_n(s) = A + BS_n + Cs_{n+1} + Ds_n s_{n+1}. \]  

(49)

The dynamics of the site magnetisation \( m(t) := \langle s_i(t) \rangle \) and pair correlation \( r := \langle s_i(t) s_{i+1}(t) \rangle \) in this model will be analysed through the pair approximation, and we will assume translational invariance. Multiplying (33) by \( s_n \) and taking the trace yields

\[ \frac{d}{dt} m = -2(B + C) - 4(A + D)m - 2(B + C)r. \]

(50)

Multiplying now (33) by \( s_n s_{n+1} \), and taking the trace yields

\[ \frac{d}{dt} r = -4Ar - 2(B + C)m - 2(B + C)r_{123} - 4Dr_{13}, \]

(51)
Entropy production for asymmetric diffusion of particles

where \( r_{123} := \langle s_{n-1}s_n s_{n+1} \rangle = \langle s_n s_{n+1} s_{n+2} \rangle \) and \( r_{13} := \langle s_{n-1}s_{n+1} s_{n+2} \rangle = \langle s_n s_{n+2} \rangle \). In order to close the equations (50) and (51), we will express both \( r_{123} \) and \( r_{13} \) as functions of \( m \) and \( r \) following the prescription of pair approximation [21, 22]. Let us consider, without a lack of generality, three consecutive spins, \( s_1, s_2 \) and \( s_3 \), and the marginal distribution \( P(s_1, s_2, s_3) \), which is obtained by summing \( P(s_1, ..., s_L) \) over all the other spins. The pair approximation assumes that

\[
P(s_1, s_2, s_3) = P(s_1, s_3 | s_2) P(s_2) \approx P(s_1 | s_2) P(s_3 | s_2) P(s_2) = \frac{P(s_1, s_2) P(s_2, s_3) P(s_2)}{P(s_2)},
\]

where \( P(x | y) \) stands for the conditional probability of an event \( x \), given \( y \). Furthermore, since

\[
P(s_2) = \frac{1}{2} (1 + ms_2)
\]

and

\[
P(s_1, s_3) = \frac{1}{4} [1 + m(s_1 + s_3) + rs_1 s_3],
\]

one has

\[
r_{123} = \sum_{s_1, s_2, s_3} s_1 s_2 s_3 P(s_1, s_2, s_3) \approx \sum_{s_1, s_2, s_3} s_1 s_2 s_3 \frac{P(s_1, s_2) P(s_2, s_3)}{P(s_2)} = \frac{2m(2r - m^2 - r^2)}{1 - m^2} \quad (55)
\]

and

\[
r_{13} = \sum_{s_1, s_2, s_3} s_1 s_3 P(s_1, s_2, s_3) \approx \sum_{s_1, s_2, s_3} s_1 s_3 \frac{P(s_1, s_2) P(s_2, s_3)}{P(s_2)} = \frac{2(m^2 - 2m^2r + r^2)}{1 - m^2}. \quad (56)
\]

The set of differential equations (50) and (51) in the pair approximation becomes, therefore,

\[
\begin{align*}
\frac{d}{dt} m &= (c - a) - 2(c + a)m + (c - a)r \\
\frac{d}{dt} r &= (c - a)m + 2(c - a) \frac{m(2r - m^2 - r^2)}{1 - m^2} \\
&\quad + 4(p + q - c - a) \frac{m^2 - 2m^2r + r^2}{1 - m^2} - (p + q + c + a)r
\end{align*}
\]

in the original parameters \( p, q, c \) and \( a \), introduced in section 3.1. The entropy flux per site is given by
Entropy production for asymmetric diffusion of particles

\[
\Phi(t) = \frac{1}{4} \left[ (p - q) \ln \frac{p}{q} + (c - a) \ln \frac{c}{a} \right] - m(t) \left( \frac{c + a}{2} \right) \ln \frac{c}{a} - \frac{1}{4} \left[ (p - q) \ln \frac{p}{q} - (c - a) \ln \frac{c}{a} \right] r(t),
\]

(58)

and its time evolution can be obtained numerically from the system (57) above, as shown in figure 2.

Nevertheless, some analytical results are available from the above equations in the stationary regime. Let us denote by \( m_\infty \) and \( r_\infty \) the stationary magnetisation and pair correlation, respectively. If \( a = c = \frac{p + q}{2} \), the stationary solution is trivial, \( m_\infty = r_\infty = 0 \). On the other hand, if \( a = c \) with \( a \neq \frac{p + q}{2} \), then \( m_\infty = 0 \), but there are two possibilities for \( r_\infty \): besides the trivial solution \( r_\infty = 0 \), there is another one, which is

\[
r_\infty = \frac{p + q + 2c}{4(p + q - 2c)} \quad \left( a = c \neq \frac{p + q}{2} \right).
\]

(59)

The stability analysis shows that the point \((m_\infty, r_\infty) = (0, 0)\) is a stable point, while \((m_\infty, r_\infty) = \left(0, \frac{p + q + 2c}{4(p + q - 2c)}\right)\) is a saddle point.

When \( a = c \), the entropy flux can be written as

\[
\frac{\Phi(\infty)}{L} = \frac{1}{4} (1 - r_\infty)(p - q) \ln \frac{p}{q} \quad (a = c),
\]

(60)

and the entropy production has the same value, \( \Pi(\infty) = \Phi(\infty) \) in the stationary state.

Finally, the condition \( a \neq c \) leads to

\[
\begin{align*}
\left\{ \begin{array}{l}
r_\infty - 2 \left( \frac{c + a}{c - a} \right) m_\infty + 1 = 0 \\
m_\infty + \frac{2m_\infty(2r_\infty - m_\infty^2 - r_\infty^2)}{1 - m_\infty^2} - \left( \frac{c + a}{c - a} \right) r_\infty = 0
\end{array} \right.
\end{align*}
\]

(61)

and one should solve a polynomial equation of third order to obtain an analytical result. The entropy flux, which is equal to the entropy production, is

\[
\frac{\Phi(\infty)}{L} = \frac{1}{2} \left[ 1 - \left( \frac{c + a}{c - a} \right) m_\infty \right] (p - q) \ln \frac{p}{q}.
\]

(62)

Note that the behaviour of the magnetisation, pair correlation and entropy are invariant under the exchange \( p \leftrightarrow q \). Moreover, the form

\[
\Pi(\infty) \propto L(p - q) \ln \frac{p}{q}
\]

(63)

in the pair approximation also recovers the dependence on \( p \) and \( q \) seen in the previous section for the entropy production.
5. Discussion

The dynamics of an asymmetric exclusion process was considered on a ring. In the case where the dynamics was restricted to a single particle, the entropy flux $\Phi$, which turned out to be a constant, was determined. This constant is zero in the symmetric case, as expected. The entropy production, on the other hand, was evaluated in the continuous approximation, and it was shown that it decays algebraically to $\Phi$, which is again constant during the whole dynamics. In the case of many particles with the constraint $a + c = p + q$, we have determined the stationary probability in a closed form from which we have found the entropy production rate. The general many-particles case, where this constraint is absent, was treated at a pair approximation level, and we could characterise numerically the time-dependent behaviour of the entropy flux and determine analytically its stationary value, which coincides with the stationary entropy production. It is worth mentioning that although the stationary distribution has the Boltzmann–Gibbs form, the system is not thermodynamic equilibrium if $p \neq q$. From the thermodynamic point of view, the asymmetric exclusion process should thus

Figure 2. Graphs of $m(t)$, $r(t)$ and $\Phi(t)$ with time in pair approximation with $p = 0.7$ and $q = 0.3$. 2a) $c = 0.8$, $a = 0.5$ and initial condition $m(0) = r(0) = 0.0$. 2b) $c = 0.2$, $a = 0.5$ and initial condition $m(0) = r(0) = 0.0$. 2c) $c = 0.8$, $a = 0.5$ and initial condition $m(0) = 0.99$ and $r(0) = 0.99^2$. 2d) $c = 0.2$, $a = 0.5$ and initial condition $m(0) = 0.99$ and $r(0) = 0.99^2$. 
be considered a non-equilibrium system. Finally, in all the models studied here, the entropy production rate, in the stationary state, has a bilinear form in the current $J$ and the force $X$.

References

[1] Nicolis G and Prigogine I 1977 *Self-Organization in Nonequilibrium Systems* (New York: Wiley)
[2] van Kampen N G 1981 *Stochastic Processes in Physics and Chemistry* (Amsterdam: North-Holland)
[3] Tomé T and de Oliveira M J 2015 *Stochastic Dynamics and Irreversibility* (Heidelberg: Springer)
[4] Schnakenberg J 1976 Rev. Mod. Phys. 48 571
[5] Jiu-Li L, Van den Broeck C and Nicolis G 1984 Z. Phys. B 56 165
[6] Mou C Y, Luo J-L and Nicolis G 1986 J. Chem. Phys. 84 7011
[7] Crochik L and Tomé T 2005 Phys. Rev. E 72 057103
[8] Zia R K P and Schmittmann B 2006 J. Phys. A: Math. Gen. 39 L407
[9] Andrieux D and Gaspard P 2006 Phys. Rev. E 74 011906
[10] Schmiedl T and Seifert U 2007 J. Chem. Phys. 126 044101
[11] Zia R K P and Schmittmann B 2007 J. Stat. Mech. P07012
[12] Esposito M, Lindenberg K and Van den Broeck C 2009 Phys. Rev. Lett. 102 130602
[13] Tomé T and de Oliveira M J 2010 Phys. Rev. E 82 021120
[14] de Oliveira M J 2011 J. Stat. Mech. P12012
[15] Esposito M 2012 Phys. Rev. E 85 041125
[16] Hase M O and de Oliveira M J 2012 J. Phys. A 45 165003
[17] Tomé T and de Oliveira M J 2012 Phys. Rev. Lett. 108 020601
[18] Tomé T 2006 Braz. J. Phys. 36 1285
[19] de Mendonça J R G and de Oliveira M J 1998 J. Stat. Phys. 92 651
[20] de Oliveira M J 1999 Phys. Rev. E 60 2563
[21] Mamada H and Takano F 1968 J. Phys. Soc. Japan 25 675
[22] Tomé T and de Oliveira M J 1989 Phys. Rev. A 40 6643