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Irreversible spherical model and its stationary entropy production rate

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Abstract

The nonequilibrium stationary state of an irreversible spherical model is investigated on hypercubic lattices. The model is defined by Langevin equations similar to the reversible case, but with asymmetric transition rates. In spite of being irreversible, we have succeeded in finding an explicit form for the stationary probability distribution, which turns out to be of the Boltzmann–Gibbs type. This enables one to evaluate the exact form of the entropy production rate at the stationary state, which is non-zero if the dynamical rules of the transition rates are asymmetric.

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1. Introduction

The spherical model was introduced by Kac [1] as a modification of the Ising model in which discrete spin variables are replaced by continuous ones, but subjected to the spherical constraint, which is a condition that ensures the thermodynamic properties of this system for any temperature. The critical behaviour of this model was first analysed by Berlin and Kac [2], and the exact solution can be found in any dimension d. The model displays a continuous phase transition for $d > 2$, with non-classical critical behaviour for $2 < d < 4$ and mean field properties for $d > 4$. The rich critical behaviour [3], together with the establishment of many exact results, has made the spherical model a good laboratory for statistical mechanics methods.

Being defined in a static way by the Boltzmann–Gibbs probability distribution, the spherical model has no dynamics. However, a dynamics can be assigned to the model by the introduction of a set of Langevin equations [4], which will rule the time evolution of the spin variables now transformed into stochastic variables. The Langevin equations have additive white noise and the deterministic parts are linear in the stochastic variables [5, 6].

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These variables, as in the static case, are associated with the sites of a regular lattice and, in addition, they are subject to the spherical constraint. The stationary probability distribution of the associated Fokker–Planck equation turns out to be the Boltzmann–Gibbs probability distribution of the spherical model.

The time-dependent behaviour of the dynamic spherical model defined by the Langevin equation has been examined in a series of papers [7–9]. In these works, the relaxation to the thermodynamic equilibrium was investigated through two-point functions (autocorrelation and response function), which enables one to quantify a distance of the system from the equilibrium state [10]. This approach is based on an extension of the fluctuation–dissipation theorem to non-equilibrium states [11, 12]. We remark that the nonequilibrium situations analysed in these papers, in which the system relaxes to the equilibrium, should be distinguished from the ones that concern us here, namely the situation in which the system finds itself in a nonequilibrium stationary state.

The deterministic part of the Langevin equations, which we call force, may be understood as the gradient of the Hamiltonian defining the spherical model. In other words, the force is conservative. Since the Hamiltonian is a quadratic form, the force is linear in the stochastic variables so that the linear coefficients make up a symmetric matrix. In this paper, we consider Langevin equations for which the forces are still linear, but the coefficients lose the symmetric property becoming nonconservative. The set of Langevin equations with these nonconservative linear forces, together with the spherical constraint, defines the irreversible spherical model. We show here that, in spite of the irreversibility, the stationary probability distribution can be written as being of the Boltzmann–Gibbs type. The description of the stationary distribution by a Boltzmann–Gibbs-type function has already been found in models with Ising spin variables that lack detailed balance [13–17].

In the stationary state, the system is no longer in the state of thermodynamic equilibrium because the forces are nonconservative. In this case, there will be a continuous production of entropy. The second purpose of this paper is to calculate the production of entropy in the stationary state, which, as we shall see, can be done exactly. The entropy production rate for systems described by a set of Langevin equations, or by the associated Fokker–Planck equation, can be obtained from an expression introduced by Tomé [18], and also considered by van den Broeck [19], which was derived from an expression advanced by Schnakenberg [20] for systems described by a master equation. The critical behaviour of the entropy production rate is shown to be similar to that of the energy of the equilibrium spherical model.

2. Spherical model

The spherical model [2, 3] is defined as follows. On a d-dimensional hypercubic lattice, with N sites and periodic boundary conditions, a continuous spin variable $\sigma_{\mathbf{r}}$ is attached to each site $\mathbf{r}$ of the lattice. The usual nearest-neighbour interaction Hamiltonian is written as

$$\mathcal{H}(\sigma) = -\sum_{\mathbf{r}}\sum_{\mathbf{e}} J_{\mathbf{e}}\sigma_{\mathbf{r}}\sigma_{\mathbf{r}+\mathbf{e}} + \mu\sum_{\mathbf{r}}\sigma_{\mathbf{r}}^2, \tag{1}$$

where the summation in $\mathbf{e}$ is over the d orthogonal unit vectors that define the d-dimensional hypercubic lattice. In a cubic lattice, for instance, these unit vectors are $\mathbf{e}_1 = (1, 0, 0)$, $\mathbf{e}_2 = (0, 1, 0)$ and $\mathbf{e}_3 = (0, 0, 1)$. We consider the anisotropic case in which the interactions are distinct for distinct directions. The symbol σ stands for the set of configurations $\{\sigma_{\mathbf{r}}\}$ of the spins and $J_{\mathbf{e}}$ and μ are the parameters.

The probability distribution of configuration σ is given by

$$P(\sigma) = \frac{1}{Z}\mathrm{e}^{-\beta\mathcal{H}(\sigma)}, \tag{2}$$

where $\beta = 1/k_B T$, with k_B being the Boltzmann constant and T the temperature. The parameter μ is not free, but should be chosen such that

$$\sum_r \langle \sigma_r^2 \rangle = N, \tag{3}$$

which is called the (mean) spherical constraint [21, 22].

The dynamics of the (mean) spherical model may be formulated through the Langevin equation

$$\frac{\mathrm{d}\sigma_{\mathbf{r}}}{\mathrm{d}t} = f_{\mathbf{r}}(\sigma) + \eta_{\mathbf{r}}(t), \tag{4}$$

where the force $f_{\mathbf{r}}(\sigma)$ is given by

$$f_{\mathbf{r}}(\sigma) = -\frac{\partial}{\partial \sigma_{\mathbf{r}}} \mathcal{H}(\sigma) \tag{5}$$

or

$$f_{\mathbf{r}}(\sigma) = \sum_{\mathbf{e}} J_{\mathbf{e}}(\sigma_{\mathbf{r}+\mathbf{e}} + \sigma_{\mathbf{r}-\mathbf{e}}) - 2\mu\sigma_{\mathbf{r}}. \tag{6}$$

As usual, the noise term $\eta_{\mathbf{r}}(t)$ has the properties

$$\langle \eta_{\mathbf{r}}(t) \rangle = 0 \qquad \text{and} \qquad \langle \eta_{\mathbf{r}}(t)\eta_{\mathbf{r}'}(t') \rangle = 2\Gamma\delta_{\mathbf{r},\mathbf{r}'}\delta(t-t'), \tag{7}$$

where $\Gamma = k_B T$ and T is identified with the heat-bath temperature.

The time evolution of the probability $P(\sigma, t)$ of state σ at time t is given by the Fokker–Planck equation

$$\frac{\partial P(\sigma, t)}{\partial t} = -\sum_{\mathbf{r}} \frac{\partial}{\partial \sigma_{\mathbf{r}}} \mathcal{J}_{\mathbf{r}}(\sigma, t), \tag{8}$$

where $\mathcal{J}_{\mathbf{r}}(\sigma, t)$ is the probability current, given by

$$\mathcal{J}_{\mathbf{r}}(\sigma, t) = f_{\mathbf{r}}(\sigma)P(\sigma, t) - \Gamma\frac{\partial}{\partial \sigma_{\mathbf{r}}} P(\sigma, t). \tag{9}$$

The probability distribution given by equation (2) is the stationary solution of the Fokker–Planck equation. In fact, in the present case, each probability current at the stationary state,

$$\mathcal{J}_{\mathbf{r}}(\sigma) = f_{\mathbf{r}}(\sigma)P(\sigma) - \Gamma\frac{\partial}{\partial \sigma_{\mathbf{r}}} P(\sigma), \tag{10}$$

vanishes, and we may say that the system is in thermodynamic equilibrium.

3. Irreversible spherical model

In order to induce an irreversibility, and inspired by the Langevin equation (4), we introduce the irreversible dynamics by

$$\frac{\mathrm{d}\sigma_r}{\mathrm{d}t} = f_{\mathbf{r}}(\sigma) + \eta_{\mathbf{r}}(t), \tag{11}$$

where the forces are now given by

$$f_{\mathbf{r}}(\sigma) = \sum_{\mathbf{e}} (J_{\mathbf{e}}\sigma_{\mathbf{r}+\mathbf{e}} + J_{-\mathbf{e}}\sigma_{\mathbf{r}-\mathbf{e}}) - 2\mu\sigma_{\mathbf{r}}, \tag{12}$$

and cannot be derived from a Hamiltonian anymore unless $J_{\mathbf{e}} = J_{-\mathbf{e}}$ for all $\mathbf{e}$. The parameters $J_{\mathbf{e}}$ and $J_{-\mathbf{e}}$, in this context, should be understood as the strengths of the transition rates of the Markovian process defined by the Langevin equation, and not as an exchange integral entering the Hamiltonian as in the reversible case. Note that, as before, μ is not free but is a time-dependent parameter that should be chosen so that constraint (3) is fulfilled.

The Fokker–Planck equation has the same form as before,

$$\frac{\partial P(\sigma,t)}{\partial t} = -\sum_{\mathbf{r}} \frac{\partial}{\partial \sigma_{\mathbf{r}}} \mathcal{J}_{\mathbf{r}}(\sigma,t) = -\sum_{\mathbf{r}} \frac{\partial}{\partial \sigma_{\mathbf{r}}} \left[f_{\mathbf{r}}(\sigma) P(\sigma,t) - \Gamma \frac{\partial}{\partial \sigma_{\mathbf{r}}} P(\sigma,t) \right], \tag{13}$$

but now the forces $f_{\mathbf{r}}(\sigma)$ are nonconservative and given by (12). In the stationary state, the probability current

$$\mathcal{J}_{\mathbf{r}}(\sigma) = f_{\mathbf{r}}(\sigma) P(\sigma) - \Gamma \frac{\partial}{\partial \sigma_{\mathbf{r}}} P(\sigma) \tag{14}$$

does not vanish anymore, although the stationarity condition

$$\sum_{\mathbf{r}} \frac{\partial}{\partial \sigma_{\mathbf{r}}} \mathcal{J}_{\mathbf{r}}(\sigma) = 0 \tag{15}$$

is fulfilled for the stationary probability distribution $P(\sigma)$.

The stationary probability distribution $P(\sigma)$ is obtained by assuming a form similar to (2), namely

$$P(\sigma) = C\mathrm{e}^{\Psi(\sigma)} \qquad \text{with} \qquad \Psi(\sigma) = \sum_{\mathbf{r}} \sum_{\mathbf{e}} B_{\mathbf{e}} \sigma_{\mathbf{r}} \sigma_{\mathbf{r}+\mathbf{e}} - A \sum_{\mathbf{r}} \sigma_{\mathbf{r}}^2, \tag{16}$$

where the summation is over the nearest-neighbour pairs and A and $\{B_{\mathbf{e}}\}$ are parameters to be found. We start by writing the stationary Fokker–Planck equation (15) in the form

$$\sum_{\mathbf{r}} g_{\mathbf{r}}(\sigma) = 0, \tag{17}$$

where

$$g_{\mathbf{r}}(\sigma) = \frac{\partial f_{\mathbf{r}}}{\partial \sigma_{\mathbf{r}}} + f_{\mathbf{r}} \frac{\partial \Psi}{\partial \sigma_{\mathbf{r}}} - \Gamma \frac{\partial^2 \Psi}{\partial \sigma_{\mathbf{r}}^2} - \Gamma \left(\frac{\partial \Psi}{\partial \sigma_{\mathbf{r}}} \right)^2, \tag{18}$$

which was obtained after dividing the stationary equation (15) by $P(\sigma)$. The substitution of $\Psi(\sigma)$, given by (16), and $f_{\mathbf{r}}(\sigma)$, given by (12), into (18) shows that $g(\sigma)$ is a quadratic form in the variable $\sigma_{\mathbf{r}}$ plus a constant. This constant is $2(\mu - \Gamma A)$, and should vanish. We conclude, therefore, that

$$A = \frac{\mu}{\Gamma}. \tag{19}$$

Using this result, $g_{\mathbf{r}}(\sigma)$ becomes the quadratic form

$$\begin{aligned} g_r(\sigma) = {} & \sum_{\mathbf{e}} B_{\mathbf{e}} \left(c_{\mathbf{e}}\, \sigma_{\mathbf{r}+\mathbf{e}}^2 + c_{-\mathbf{e}}\, \sigma_{\mathbf{r}-\mathbf{e}}^2 \right) - 2A \sum_{\mathbf{e}} \sigma_{\mathbf{r}} (c_{\mathbf{e}}\, \sigma_{\mathbf{r}+\mathbf{e}} + c_{-\mathbf{e}}\, \sigma_{\mathbf{r}-\mathbf{e}}) \\ & + \sum_{\mathbf{e}} B_{\mathbf{e}} (c_{\mathbf{e}} + c_{-\mathbf{e}}) \sigma_{\mathbf{r}-\mathbf{e}} \sigma_{\mathbf{r}+\mathbf{e}} + \sum_{\substack{\mathbf{e},\mathbf{e}' \\ \mathbf{e} \perp \mathbf{e}'}} B_{\mathbf{e}} (c_{\mathbf{e}}\, \sigma_{\mathbf{r}+\mathbf{e}} + c_{-\mathbf{e}}\, \sigma_{\mathbf{r}-\mathbf{e}})(\sigma_{\mathbf{r}+\mathbf{e}'} + \sigma_{\mathbf{r}-\mathbf{e}'}), \end{aligned} \tag{20}$$

where

$$c_{\mathbf{e}} = J_{\mathbf{e}} - \Gamma B_{\mathbf{e}} \qquad \text{and} \qquad c_{-\mathbf{e}} = J_{-\mathbf{e}} - \Gamma B_{\mathbf{e}}. \tag{21}$$

The trivial solution of (17) is obtained by setting $c_{\mathbf{e}} = 0$ and $c_{-\mathbf{e}} = 0$, which gives $J_{\mathbf{e}} = \Gamma B_{\mathbf{e}} = J_{-\mathbf{e}}$, leading us back to the reversible model. To obtain a nontrivial solution, we substitute expression (20) into (17) and rewrite it in the form

$$\begin{aligned} & \sum_{\mathbf{r}} \sum_{\mathbf{e}} B_{\mathbf{e}} (c_{\mathbf{e}} + c_{-\mathbf{e}}) \sigma_{\mathbf{r}}^2 - 2A \sum_{\mathbf{r}} \sum_{\mathbf{e}} (c_{\mathbf{e}} + c_{-\mathbf{e}}) \sigma_{\mathbf{r}} \sigma_{\mathbf{r}+\mathbf{e}} + \sum_{\mathbf{r}} \sum_{\mathbf{e}} B_{\mathbf{e}} (c_{\mathbf{e}} + c_{-\mathbf{e}}) \sigma_{\mathbf{r}-\mathbf{e}} \sigma_{\mathbf{r}+\mathbf{e}} \\ & \qquad + \sum_{\mathbf{r}} \sum_{\substack{\mathbf{e},\mathbf{e}' \\ \mathbf{e} \perp \mathbf{e}'}} B_{\mathbf{e}} (c_{\mathbf{e}} + c_{-\mathbf{e}}) (\sigma_{\mathbf{r}+\mathbf{e}} + \sigma_{\mathbf{r}-\mathbf{e}}) \sigma_{\mathbf{r}+\mathbf{e}'} = 0, \end{aligned} \tag{22}$$

which is solved by setting $c_{\mathbf{e}} + c_{-\mathbf{e}} = 0$, leading to the condition

$$B_{\mathbf{e}} = \frac{1}{2\Gamma}(J_{\mathbf{e}} + J_{-\mathbf{e}}). \tag{23}$$

Therefore, the irreversible model defined by equations (11) and (12), which embodies the parameters $J_{\mathbf{e}}$, $J_{-\mathbf{e}}$ and μ, has a stationary state of the Boltzmann–Gibbs type given by (16) with the parameters $\{B_{\mathbf{e}}\}$ and A given by (19) and (23). It is worthwhile to note that a totally asymmetric dynamics is obtained by setting $J_{-\mathbf{e}} = 0$, in which case $B_{\mathbf{e}} = J_{\mathbf{e}}/2\Gamma$, a result valid in any dimension. The totally asymmetric dynamics has been shown to exist in systems with Ising spin variables in one and two dimensions [13, 15].

4. Entropy production rate

The variation of entropy S of a system with time can be split into two parts as

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \Pi - \Phi, \tag{24}$$

where Π is the entropy production rate and Φ is the entropy flux from the system to the environment. Following [18], we will now obtain a more explicit formula for Π and Φ. From the definition of entropy,

$$S(t) = -\int \mathrm{d}\sigma P(\sigma, t) \ln P(\sigma, t), \tag{25}$$

its time derivative can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} S(t) = -\int \mathrm{d}\sigma \sum_{\mathbf{r}} \mathcal{J}_{\mathbf{r}}(\sigma, t) \frac{\partial}{\partial \sigma_{\mathbf{r}}} \ln P(\sigma, t) \tag{26}$$

after using (8) and integrating by parts. Combining this last equation with the definition of probability current (9), we have

$$\frac{\mathrm{d}}{\mathrm{d}t} S(t) = \frac{1}{\Gamma} \sum_{\mathbf{r}} \int \mathrm{d}\sigma \left\{ \frac{[\mathcal{J}_{\mathbf{r}}(\sigma, t)]^2}{P(\sigma, t)} - \mathcal{J}_{\mathbf{r}}(\sigma, t) f_{\mathbf{r}}(\sigma) \right\}. \tag{27}$$

Comparing this equation with (24), and since the first term is non-negative, we associate it with the entropy production,

$$\Pi(t) = \frac{1}{\Gamma} \sum_{\mathbf{r}} \int \mathrm{d}\sigma \frac{[\mathcal{J}_{\mathbf{r}}(\sigma, t)]^2}{P(\sigma, t)}, \tag{28}$$

and we obtain the expression

$$\Phi(t) = \frac{1}{\Gamma} \sum_{\mathbf{r}} \int \mathrm{d}\sigma \mathcal{J}_{\mathbf{r}}(\sigma, t) f_{\mathbf{r}}(\sigma) \tag{29}$$

for the entropy flux, which can have both signs. In the stationary state, one has $\Pi = \Phi$, and we can use either expression (28) or (29) to calculate the entropy production rate.

From now on, we restrict ourselves to the simple case in which $J_{\mathbf{e}}$ and $J_{-\mathbf{e}}$ are independent of $\mathbf{e}$, that is,

$$J_{\mathbf{e}} = J \qquad \text{and} \qquad J_{-\mathbf{e}} = J', \tag{30}$$

but $J \neq J'$, and the parameter $B_{\mathbf{e}} = B$ being independent of $\mathbf{e}$, which leads to

$$B = \frac{J + J'}{2\Gamma}. \tag{31}$$

Using the results of the previous section in expression (28), the entropy production rate per site $\Pi^* = \Pi/N$ can be evaluated as

$$\Pi^* = \frac{\mathrm{d}}{2\Gamma}\,(q_0 - q_2)\,(J - J')^2, \tag{32}$$

where q_0 and q_2 are defined by

$$q_0 = \left\langle \sigma_{\mathbf{r}}^2 \right\rangle \qquad \text{and} \qquad q_2 = \langle \sigma_{\mathbf{r}-\mathbf{e}}\sigma_{\mathbf{r}+\mathbf{e}} \rangle, \tag{33}$$

with $\mathbf{e}$ being any one of the unit vectors. Note that Π^* vanishes when the reversibility condition $J = J'$ is satisfied, as expected.

Using the stationary probability distribution (16), we obtain the following results for q_0 and q_2:

$$\begin{aligned} q_0 &= \frac{1}{2}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\frac{\mathrm{d}^d k}{(2\pi)^d}\,\frac{1}{A + 2B\sum_{i=1}^{d}\cos k_i} \\ &= \frac{1}{2}\int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{-At}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\frac{\mathrm{d}^d k}{(2\pi)^d}\,\mathrm{e}^{-2Bt\sum_{i=1}^{d}\cos k_i} \\ &= \frac{1}{4B}\int_0^{\infty}\mathrm{d}\xi\,\mathrm{e}^{-\frac{A}{2B}\xi}\,[I_0(\xi)]^d\,, \end{aligned} \tag{34}$$

where the identity $x^{-1} = \int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{-tx}$ (for $x > 0$) was used, and the integral representation of the modified Bessel function of first kind of order n, I_n, was invoked. By a similar procedure, it is also possible to evaluate q_2 as

$$q_2 = \frac{1}{4B}\int_0^{\infty}\mathrm{d}\xi\,\mathrm{e}^{-\frac{A}{2B}\xi}\,[I_0(\xi)]^{d-1}\,I_2(\xi). \tag{35}$$

The parameter μ should ensure the spherical constraint, which is simply $\langle\sigma_{\mathbf{r}}^2\rangle = 1$ or $q_0 = 1$. Setting the right-hand side of equation (34) equal to 1, one has B as an implicit function of A. If we define $\theta = 1/B = 2\Gamma/(J + J')$, the production of entropy per site becomes

$$\Pi^* = \frac{\mathrm{d}}{\theta}\,(1 - q_2)\,J^*, \tag{36}$$

where

$$J^* = \frac{(J - J')^2}{J + J'}. \tag{37}$$

Note that the quantity Π^*/J^* is a function of θ only, and a graph $\Pi^*/J^* \times \theta$ is plotted in figure 1 for dimensions $d = 1, 2, 3$. In one dimension, an analytical expression is available and is given by

$$\frac{\Pi^*}{J^*} = \frac{1}{8}(\sqrt{16 + \theta^2} - \theta). \tag{38}$$

When $\theta \to 0$, the quantity Π^*/J^* approaches a constant c_d (in d dimensions), which is given by

$$c_d = \begin{cases} \dfrac{1}{2}, d = 1 \\[2ex] 1 - \dfrac{2}{\pi}, d = 2 \\[2ex] \dfrac{d}{4}\displaystyle\int_{\mathrm{BZ}}\frac{1 - \cos 2k_1}{d - \sum_{i=1}^{d}\cos k_i}\,\frac{\mathrm{d}^d k}{(2\pi)^d}, d \geqslant 3, \end{cases} \tag{39}$$

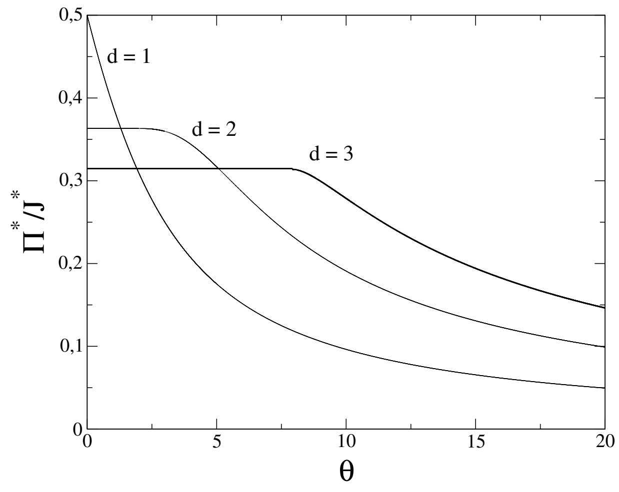

Figure 1. Plot of Π^*/J^* as a function of θ in $d = 1$, $d = 2$ and $d = 3$.

where the integration above is over the Brillouin zone (BZ). For $d = 3$, we obtain $c_3 = 0.314\,762\ldots$. Note that in $d \geqslant 3$, the quantity Π^*/J^* equals the constant c_d in the ferromagnetic phase, $\theta \leqslant \theta_c$, where θ_c is given by

$$\frac{1}{\theta_c} = \frac{1}{4}\int_{\mathrm{BZ}} \frac{1}{d - \sum_{i=1}^{d} \cos k_i} \frac{\mathrm{d}^d k}{(2\pi)^d}. \tag{40}$$

For $d = 3$, we obtain $\theta_c = 7.913\,552\ldots$.

5. Conclusion

In this paper, we have investigated a system in a nonequilibrium stationary state. The (mean) spherical model is a suitable laboratory where many exact results are available, and we have succeeded in finding an exact form for the probability distribution, despite the fact that the system is not in equilibrium state (as testified by the non-zero value of the entropy production). It is worthwhile to mention that the probability distribution found is of the Boltzmann–Gibbs type. The knowledge of this particular form allowed us to explicitly evaluate the stationary entropy production. The origin of the nonequilibrium behaviour in our work, which is responsible for the non-zero entropy production, goes back to the unbalanced transition rate to the opposite direction, $J_{\mathbf{e}} \neq J_{-\mathbf{e}}$ (for any $\mathbf{e}$). If, on the other hand, the condition $J_{\mathbf{e}} = J_{-\mathbf{e}}$ is satisfied for any $\mathbf{e}$, the stationary entropy production vanishes.

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