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Non-equilibrium stationary state of a two-temperature spin chain

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Abstract

A kinetic one-dimensional Ising model is coupled to two heat baths, such that spins at even (odd) lattice sites experience a temperature T_e (T_o). Spin-flips occur with Glauber-type rates generalized to the case of two temperatures. Driven by the temperature differential, the spin chain settles into a non-equilibrium steady state which corresponds to the stationary solution of a master equation. We construct a perturbation expansion of this master equation in terms of the temperature difference and compute explicitly the first two corrections to the equilibrium Boltzmann distribution. The key result is the emergence of additional spin operators in the steady state, increasing in spatial range and order of spin products. We comment on the violation of detailed balance and entropy production in the steady state.

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1. Introduction

In recent years, considerable interest has focused on non-equilibrium stationary states (NESS) in interacting many-body systems, induced by deterministic or stochastic microscopic dynamics [1, 2]. In the stochastic case, the starting point is typically a master equation, i.e. a continuity equation for the (time-dependent) configurational probabilities. Different models are characterized by their microscopic transition rates. Both equilibrium and non-equilibrium stationary states have time-independent macroscopic observables. However, only in the equilibrium case it is possible to compute these observables without explicit reference to the imposed dynamics, in the framework of Gibbs ensembles. In stark contrast, NESS and their properties depend generically on the details of the dynamic rules. Since a unifying theoretical description of NESS is still lacking, most progress to date is made by studying specific models.

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In some of the simplest models, a NESS is established by driving the system with an external field. A characteristic example is the (fully periodic) Ising lattice gas, subject to a uniform electric field which induces a nonzero particle current [3]. A second class of models involves two temperature baths. These can either be coupled to the system boundaries [4, 5] or act throughout the bulk: in the latter case, each temperature bath controls a (translationally invariant) subset of configurational transitions. For instance, in an Ising lattice gas, particle–hole exchanges along certain spatial axes might be coupled to a higher temperature [6, 7]. Or, in the non-conserved case, spin-flips on a selected sub-lattice might occur at a different temperature [8, 9]. In all of these cases, equilibrium can be recovered upon letting a key parameter vanish, e.g. the strength of the bias or the temperature difference. In this spirit, these models allow us to probe the effect of non-equilibrium perturbations on equilibrium properties, and we may ask to what extent *universal* (i.e., long-wavelength, long-time) features are affected. One finds, generically, that non-equilibrium perturbations are far more relevant, in a renormalization group sense, in systems with conservation laws [7, 10, 11]. In contrast, it can be shown that Ising-like models with *non-conserved* dynamics remain in the universality class of the equilibrium Ising model, even if the usual $\mathbb{Z}_2$-symmetry of the Ising model is broken [12]. While these results are clearly of major theoretical interest, they do not reveal how NESS configurational probabilities differ from their equilibrium counterparts: how, for instance, is the Boltzmann distribution for the equilibrium Ising model modified, when a second, different temperature bath is coupled to some spin-flips or spin-exchanges? Clearly, such modifications must be severe if universal behaviour is to be affected. Yet, even if long-wavelength, long-time properties remain effectively Ising-like, fundamental changes in the configurational probabilities should arise from the breaking of detailed balance.

It is with these motivations, questions and expectations in mind, that we turn to the arguably simplest non-equilibrium Ising-type model, namely, a one-dimensional *interacting* spin chain with spin-flip dynamics. The rates are a simple but nontrivial generalization of the well-studied Glauber [13] rates: spins at odd (even) sites are coupled to a temperature T_o (T_e). In dimensions $d \geqslant 2$, this model [8, 9] exhibits an order–disorder phase transition which should be in the Ising universality class, according to renormalization group arguments [12]. Detailed Monte Carlo simulations in $d = 2$ [9] confirm this expectation. In $d = 1$, an exact solution for the two spin correlation functions has been found [14]. In the following, we seek an analytic expression for the steady state probability distribution, i.e. the solution of the master equation for this model. While we have not been able to find an exact solution, our perturbative analysis provides some insight into how the equilibrium distribution is modified when a (small) temperature difference is present.

As energy is fed into a NESS from one reservoir, it must also be dissipated: in general, a NESS constantly produces 'entropy'. Possible definitions of 'entropy' and 'entropy production' in non-equilibrium systems have been discussed intensely in recent years, from the viewpoints of both stochastic and deterministic dynamics [15, 16]. However, different perspectives have been developed rather independently, so that the relations between them still remain somewhat unclear. Therefore, we find it worthwhile to compare results from different approaches to entropy production, using our model.

We conclude with two comments. First, while some analytic results for steady-state distributions are available, they are confined to two classes of systems: first, $d = 1$ lattice gas models, restricted to excluded volume interactions, such as the asymmetric exclusion process and its relatives [17–19], and second, very special ($d = 1$) spin systems whose master equations are solved by the Ising Boltzmann factor [3, 20]. Second, even though our main emphasis rests on fundamental aspects, we note briefly that two-temperature systems of this type can be established in real systems, and maintained for significant amounts of time.

For example, via nuclear magnetic resonance in an external magnetic field, a lattice of nuclei in a solid can be prepared to have a certain *spin temperature* [21]. Thus, in a crystal with two sub-lattices of different nuclei the temperatures of these sub-lattices can differ.

This paper is organized as follows. We begin by introducing our model and its master equation. The following section describes our perturbative approach towards finding the stationary distribution. We then compute the two leading orders, aiming to highlight some generic properties of the perturbation series. We next turn to the discussion of two more general questions, namely, first, how spin-flips violate the detailed balance condition, and second, whether different definitions for the entropy production rate lead to the same results for our model. We conclude with an outlook and some open questions.

2. The model

Our model is defined on a one-dimensional spin chain of length N (with N even). Each site i carries a spin variable, σ_i, which can take the values ± 1. We impose periodic boundary conditions, so that $\sigma_{N+1} = \sigma_1$. Spins at even (odd) lattice sites are coupled to a heat bath at temperature T_e (T_o). Thus, a configuration $\{\sigma\} = \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ evolves into a new configuration by flipping a randomly selected spin, e.g. spin σ_i, with a rate [14]

$$w_i(\sigma_i \to -\sigma_i) = 1 - \frac{\gamma_i}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1}) \tag{1}$$

where

$$\gamma_i = \begin{cases} \gamma_e = \tanh(2J/k_B T_e) & i \text{ even} \\ \gamma_o = \tanh(2J/k_B T_o) & i \text{ odd.} \end{cases} \tag{2}$$

Here, J denotes a nearest neighbour exchange coupling between spins. From now on, we use dimensionless units for inverse temperature, i.e. $\beta_e \equiv J/(k_B T_e)$ etc. The rates respect the usual $\mathbb{Z}_2$-symmetry of the Ising model. The full stochastic dynamics of the system can be cast in terms of a master equation for the time-dependent configurational probability $p(\{\sigma\}; t)$

$$\partial_t p(\{\sigma\}; t) = \sum_{i=1}^{N} \left[-w_i(\sigma_i \to -\sigma_i) p(\{\sigma\}; t) + w_i(-\sigma_i \to \sigma_i) p\left(\left\{\sigma^{[i]}\right\}; t\right)\right]. \tag{3}$$

Here $\left\{\sigma^{[i]}\right\}$ differs from $\{\sigma\}$ by a flip of the ith spin. A trivial time scale has been set to unity.

An alternate description of our spin chain is the usual defect (domain wall) picture. A unique defect configuration $\{\alpha\}$ is associated with a pair of spin configurations, namely $\{\sigma\}$ and its image under $\mathbb{Z}_2$, $\{-\sigma\}$. The defects are located on the *dual* lattice (i.e., the bonds), with $\alpha_i = 0\,(1)$ if $\sigma_i\sigma_{i+1} = 1\,(-1)$. A spin flip $\sigma_i \to -\sigma_i$ in the spin chain $\{\sigma\}$ can give rise to three different types of processes in the defect state $\{\alpha\}$ depending on the three neighbouring spins $\{\sigma_{i-1}, \sigma_i, \sigma_{i+1}\}$: (a) if $\sigma_{i-1} = -\sigma_i = \sigma_{i+1}$, two adjacent defects annihilate each other, with rate $1+\gamma_e$ if i is even ($1+\gamma_o$ if i is odd); (b) if $\sigma_{i-1} = \sigma_i = \sigma_{i+1}$, two adjacent defects are generated simultaneously, with rate $1 - \gamma_e$ if i is even ($1 - \gamma_o$ if i is odd); and (c) if $\sigma_{i-1} = -\sigma_{i+1}$, a defect diffuses to a neighbouring lattice site, with rate 1.

Clearly, for uniform temperature $T \equiv T_e = T_o$, this model reduces to the well-known Glauber dynamics [13], with homogeneous rates $\bar{w}(\sigma_i \to -\sigma_i)$. The associated steady-state solution is just the Boltzmann distribution

$$\lim_{t\to\infty} p(\{\sigma\}; t) = \frac{1}{Z}\exp(-H/k_B T) \equiv \frac{1}{Z} q_o(\{\sigma\}) \tag{4}$$

where H is the Ising Hamiltonian for a spin chain

$$H(\{\sigma\}) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \tag{5}$$

and Z is the (canonical) partition function. Clearly, $H(\{\sigma\})$ just counts the number of defects, $n(\{\sigma\}) \equiv \sum_{i=1}^{N} \alpha_i$, in configuration $\{\sigma\}$ via $J^{-1}H(\{\sigma\}) = 2n(\{\sigma\}) - N$. The equilibrium distribution $q_0(\{\sigma\})/Z$ will serve as the unperturbed reference solution for our perturbative analysis, to be outlined below. For later reference, we note that detailed balance holds in the equilibrium case, i.e.

$$\bar{w}(\sigma_i \to -\sigma_i) q_0(\{\sigma\}) = \bar{w}(-\sigma_i \to \sigma_i) q_0\left(\left\{\sigma^{[i]}\right\}\right) \tag{6}$$

for any spin-flip.

Returning to the case of two temperatures, it is easy to note that the (time continuous) Markov process, characterized by equation (3) is ergodic, since every configuration $\{\sigma\}$ can be reached after a finite time from every other configuration $\{\sigma'\}$. Hence, any initial condition will converge, for $t \to \infty$, to the unique stationary solution, $q(\{\sigma\})$. The determination of $q(\{\sigma\})$ is our goal here. Being the full configurational probability distribution, it contains *all* information about the system in its non-equilibrium steady state.

Since our NESS violates detailed balance (cf section 4), the determination of $q(\{\sigma\})$ is highly non-trivial. As a starting point, we restrict ourselves to the regime where the two temperatures differ only slightly from each other, so that perturbative methods can be invoked. In particular, we are interested which new spin operators are induced by the coupling to two heat baths. Writing the stationary distribution as

$$q(\{\sigma\}) \equiv \frac{1}{\tilde{Z}} \exp(V(\{\sigma\})) \tag{7}$$

we seek the 'potential' function $V(\{\sigma\})$ in perturbation theory ($\tilde{Z}$ is determined through the normalization condition).

3. Perturbation theory

In order to set up a perturbative treatment of the master equation (3), it is convenient to decompose the flip rates (1) into an equilibrium-like contribution and a non-equilibrium perturbation

$$\begin{aligned} w_i(\sigma_i \to -\sigma_i) &= \left[1 - \frac{\gamma_e + \gamma_o}{4}\sigma_i(\sigma_{i-1} + \sigma_{i+1})\right] + \frac{\gamma_o - \gamma_e}{2}\left[\frac{(-1)^i}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1})\right] \\ &\equiv \bar{w}(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) + \frac{\gamma_o - \gamma_e}{2}\Delta_i(\sigma_{i-1}, \sigma_i, \sigma_{i+1}). \end{aligned} \tag{8}$$

The term in the first [...] bracket, $\bar{w}$, is just the homogeneous Glauber rate at an effective temperature defined via $\tanh(2\bar{\beta}) \equiv \bar{\gamma} \equiv (\gamma_e + \gamma_o)/2$. The second term is explicitly proportional to the 'temperature' *difference*

$$d \equiv \frac{\gamma_o - \gamma_e}{2} \tag{9}$$

and hence captures the non-equilibrium aspect of our dynamics. Thus, d serves as a suitable expansion parameter for a perturbation theory near equilibrium. We note that it is restricted to the interval $0 \leqslant |d| \leqslant 0.5$ where $|d| = 0.5$ corresponds to one temperature being infinite and the other zero.

We seek the stationary solution $q(\{\sigma\})$ of equation (3), namely

$$\begin{aligned} 0 = \sum_{j=1}^{N} \Big[&-(\bar{w}(\sigma_{j-1}, \sigma_j, \sigma_{j+1}) + d\Delta_j(\sigma_{j-1}, \sigma_j, \sigma_{j+1})) q(\{\sigma\}) + (\bar{w}(\sigma_{j-1}, -\sigma_j, \sigma_{j+1}) \\ &+ d\Delta_j(\sigma_{j-1}, -\sigma_j, \sigma_{j+1})) q\left(\left\{\sigma^{[j]}\right\}\right)\Big]. \end{aligned} \tag{10}$$

We assert that $q(\{\sigma\})$ can be written as a perturbation series

$$q(\{\sigma\}) = \tilde{Z}^{-1} q_0(\{\sigma\}) \left(1 + \sum_{n=1}^{\infty} d^n Q_n(\{\sigma\})\right) \tag{11}$$

where $q_0(\{\sigma\}) \equiv \exp\left(\bar{\beta}\sum_i \sigma_i\sigma_{i+1}\right)$ is the Ising potential at inverse temperature $\bar{\beta}$. Actually one can show that this expansion is analytic [22]. Inserting ansatz (11) into equation (10), and ordering terms in powers of d, uniqueness demands that the coefficient accompanying each power d^n, $n = 1, 2, \ldots$ vanishes. The lowest order (d^0) is satisfied by construction. Higher orders are now evaluated recursively: the coefficient of d^n, for $n \geqslant 1$, can be written as the sum of two terms which must cancel, $0 = S_1^{(n)} + S_2^{(n)}$. Here, $S_1^{(n)}$ contains contributions of the form $\Delta_j Q_{n-1}$ and is therefore explicitly calculable with the help of results from the $(n-1)$th order. The second term is generated by applying the equilibrium rates $\bar{w}(\ldots)$ on the unknown Q_n. Even though we cannot invert the Glauber Liouvillean $\bar{w}$ exactly, we can infer the structure of Q_n, based on the knowledge of $S_1^{(n)}$ and the simplicity of $\bar{w}$ (which contains only nearest-neighbour spin operators). Of course, at higher orders, the structure of $S_1^{(n)}$ becomes increasingly complex, so that explicit computations become quite cumbersome. However, at lower orders, this program is quite feasible. In the following, we illustrate the process for the first-order correction, and provide a few pointers for the second order.

At order d, we need to find $Q_1(\{\sigma\})$ such that

$$\begin{aligned}
0 = \sum_{j=1}^{N} &\left[-\Delta_j(\sigma_{j-1}, \sigma_j, \sigma_{j+1}) q_0(\{\sigma\}) + \Delta_j(\sigma_{j-1}, -\sigma_j, \sigma_{j+1}) q_0\left(\left\{\sigma^{[j]}\right\}\right)\right] \\
&+ \sum_{j=1}^{N} \left[-\bar{w}(\sigma_{j-1}, \sigma_j, \sigma_{j+1}) q_0(\{\sigma\}) Q_1(\{\sigma\})\right. \\
&\left.+ \bar{w}(\sigma_{j-1}, -\sigma_j, \sigma_{j+1}) q_0\left(\left\{\sigma^{[j]}\right\}\right) Q_1\left(\left\{\sigma^{[j]}\right\}\right)\right] \\
&= S_1^{(1)} + S_2^{(1)}
\end{aligned} \tag{12}$$

where $S_1^{(1)}$ and $S_2^{(1)}$ represent the first and second sum over j, respectively. We first compute $S_1^{(1)}$:

$$S_1^{(1)} = -q_0(\{\sigma\}) \frac{\sinh(4\bar{\beta})}{2} \sum_{j=1}^{N} (-1)^j \sigma_j \sigma_{j+2} \tag{13}$$

which suggests the following ansatz for $Q_1(\{\sigma\})$:

$$Q_1(\{\sigma\}) = \lambda \sum_{i=1}^{N} (-1)^i \sigma_i \sigma_{i+2} \tag{14}$$

where the (real) parameter λ needs to be determined. Inserting (14) into $S_2^{(1)}$, we obtain

$$S_2^{(1)} = 4\lambda q_0(\{\sigma\}) \sum_{j=1}^{N} (-1)^j \sigma_j \sigma_{j+2}$$

from which we obtain

$$\lambda = -\frac{\sinh(4\bar{\beta})}{8}. \tag{15}$$

Thus, we arrive at the first-order correction to the stationary distribution:

$$q(\{\sigma\}) = \frac{1}{\tilde{Z}} q_0(\{\sigma\}) \left(1 - d\frac{\sinh(4\bar{\beta})}{8} \sum_{i=1}^{N} (-1)^i \sigma_i \sigma_{i+2}\right) + \mathcal{O}(d^2) \tag{16}$$

Hence, in first-order perturbation theory the temperature difference induces an interaction between *next-nearest* neighbours with a sign difference for even/odd pairs. The correction has a simple, intuitive interpretation in the defect picture. If $n_e(\{\sigma\})$ and $n_o(\{\sigma\})$ denote the number of *defect pairs* centred on even or odd sites, respectively, it is easy to note that

$$\frac{1}{4}\sum_{i=1}^{N}(-1)^i\sigma_i\sigma_{i+2} = n_o(\{\sigma\}) - n_e(\{\sigma\})$$

i.e. $Q_1(\{\sigma\})$ is proportional to the *difference* between the number of 'even' and 'odd' defect pairs. For $T_e > T_o$, d is positive, so that, e.g., a spin configuration with a single *even* defect pair acquires a *higher* statistical weight than a configuration with a single *odd* pair. In contrast, those two configurations are degenerate in equilibrium, i.e they have the same weight. Clearly, the high degeneracy of the equilibrium probabilities is reduced by the perturbative correction: now, not only the total number of defects matters, but also how defect pairs are distributed over the two sub-lattices.

Turning to the *second-order* contribution, the calculations, while becoming more involved, proceed in essentially the same manner. Collecting all terms of equation (10) with a factor d^2 the condition for the correction $Q_2(\{\sigma\})$ reads

$$\begin{aligned}0 = \sum_{j=1}^{N}\big[-\Delta_j(\sigma_{j-1},\sigma_j,\sigma_{j+1})q_0(\{\sigma\})Q_1(\{\sigma\}) + \Delta_j(\sigma_{j-1},-\sigma_j,\sigma_{j+1})\\ \times q_0\big(\big\{\sigma^{[j]}\big\}\big)Q_1\left(\big\{\sigma^{[j]}\big\}\right)\big] + \sum_{j=1}^{N}\big[-\bar{w}(\sigma_{j-1},\sigma_j,\sigma_{j+1}))q_0\left(\{\sigma\}\right)Q_2(\{\sigma\})\\ + \bar{w}(\sigma_{j-1},-\sigma_j,\sigma_{j+1})q_0\big(\big\{\sigma^{[j]}\big\}\big)Q_2\big(\big\{\sigma^{[j]}\big\}\big)\big] =: S_1^{(2)} + S_2^{(2)}\end{aligned} \tag{17}$$

where again the two terms $S_1^{(2)}$ and $S_2^{(2)}$ are defined as the first and the second sums over j, respectively. We obtain

$$\begin{aligned}S_1^{(2)} = 4\lambda^2 q_0(\{\sigma\})\left\{\left(\sum_{i=1}^{N}(-1)^i\sigma_i\sigma_{i+2}\right)^2 + 4\sum_{i=1}^{N}[(\sigma_i\sigma_{i+2} + \sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3})\right.\\ \left. - \coth(4\bar{\beta})(\sigma_i\sigma_{i+1} + \sigma_i\sigma_{i+3})]\right\}\end{aligned} \tag{18}$$

with λ given in equation (15). Again, a suitable ansatz, based on the structure of $S_1^{(2)}$, allows us to determine the second-order correction $Q_2(\{\sigma\})$:

$$\begin{aligned}Q_2\left(\{\sigma\}\right) = \frac{\lambda^2}{2}\left\{\left(\sum_{i=1}^{N}(-1)^i\sigma_i\sigma_{i+2}\right)^2 + 4\sum_{i=1}^{N}[(\sigma_i\sigma_{i+2} + \sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3})\right.\\ \left. - \coth(2\bar{\beta})(\sigma_i\sigma_{i+1} + \sigma_i\sigma_{i+3})]\right\}.\end{aligned} \tag{19}$$

Remarkably, we now encounter both *higher-order* spin operators and *next-next-nearest* neighbour interactions.

Clearly, $d^2Q_2(\{\sigma\})$ should be added to the first-order solution, equation (16). It is instructive to write the stationary distribution in exponential form, via $q(\{\sigma\}) \equiv \tilde{Z}^{-1}\exp\left[\sum_{n=0}^{\infty}d^nV_n(\{\sigma\})\right]$, to illustrate the differences from the equilibrium form even more succinctly. To $\mathcal{O}(d^2)$, we obtain

$$V_0(\{\sigma\}) \equiv \bar{\beta}\sum_i \sigma_i\sigma_{i+1} \qquad V_1(\{\sigma\}) \equiv \lambda\sum_i (-1)^i \sigma_i\sigma_{i+2}$$
$$V_2(\{\sigma\}) \equiv 2\lambda^2\sum_i [\sigma_i\sigma_{i+2} + \sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3} - \coth(2\bar{\beta})\,(\sigma_i\sigma_{i+1} + \sigma_i\sigma_{i+3})]. \tag{20}$$

The functions V_k, $k = 0, 1, \ldots$ contain the interaction terms that arise in the kth order of perturbation theory. The system size N enters only through the summation over i. Clearly, the functions V_k respect the basic symmetries of our model: the usual Ising $\mathbb{Z}_2$ invariance and oddness in d under the exchange of even and odd sub-lattices. Of course, V_0 is the Ising Hamiltonian. In stark contrast to the equilibrium case, the stationary distribution $q(\{\sigma\})$ cannot be written as $\exp(-\beta H(\{\sigma\}))$ with an appropriate Hamiltonian $H(\{\sigma\})$, since the potentials V_k possess a complicated dependence on the two inverse temperatures β_e and β_o. We also note that, at least for $k \leqslant 2$, the potentials V_k are sums of spin operators each of which involves only a local 'cluster' $S_k \equiv \{\sigma_i, \sigma_{i+1}, \ldots \sigma_{i+k+1}\}$ of (at most) $k+2$ spins. Hence, it appears that the size of these clusters grows linearly with k but the coupling strength between two spins, σ_i and σ_{i+k+1}, decreases exponentially as d^k. We conjecture that this behaviour lies at the source of the exponential decay which characterizes correlation functions in this model [14, 23].

We conclude this section with some comments on the accuracy of our perturbation theory. The effective expansion parameter, up to and including second order, is λd, so that the mean inverse temperature, $\bar{\beta}$, also plays a role. In particular, the limit $\bar{\beta} \to \infty$ looks troubling at first sight, since $\lambda \propto \sinh(4\bar{\beta})$ (cf equation (15)). However, a more careful analysis shows that $|\lambda d| < 1$ independently of how γ_o and γ_e approach unity, and our perturbation theory remains valid for low mean temperature.

To test its numerical accuracy, we compare our perturbative solution, $q_{\text{pert}}(\{\sigma\})$, with an exact result, $q_{\text{ex}}(\{\sigma\})$, for a short chain of six sites [24]. For such small systems, the zero eigenvector (stationary distribution) of the master equation is easily found. As a quantitative measure, we define

$$\chi \equiv \sqrt{\sum_{\{\sigma\}} (q_{\text{pert}}(\{\sigma\}) - q_{\text{ex}}(\{\sigma\}))^2}. \tag{21}$$

Keeping the mean temperature, i.e. $(\gamma_e + \gamma_o)/2$, fixed, we expect χ to scale as $\chi \sim d^{k+1}$ for $d \to 0$, if we consider $q_{\text{pert.}}$ to kth order. Figure 1 confirms this scaling behaviour for $k = 1$ and $k = 2$ at $(\gamma_e + \gamma_o)/2 = 0.4$ for a large range of d. Remarkably, even for the largest d investigated (0.4), χ remains well below 0.01 indicating that our perturbative solution is an excellent approximation to the exact result. For smaller d, the deviations are even smaller, giving us considerable confidence in our perturbative approach.

In the next two sections, we turn to two general features of our two-temperature spin chain, namely the violation of detailed balance and the concept of entropy production.

4. Violation of detailed balance

Following [25], it is straightforward to show that our dynamics violates detailed balance even without knowing the steady-state distribution. The proof involves closed orbits (loops) in configuration space, $\{\sigma\}_1 \to \{\sigma\}_2 \to \cdots \to \{\sigma\}_k \to \{\sigma\}_1$, of 'length' $k = 1, 2, \ldots$. Each of the configurations in the loop differs from its successor by a single spin-flip. For each closed orbit, we consider the product of the transition rates traversing the loop in the 'forward' and

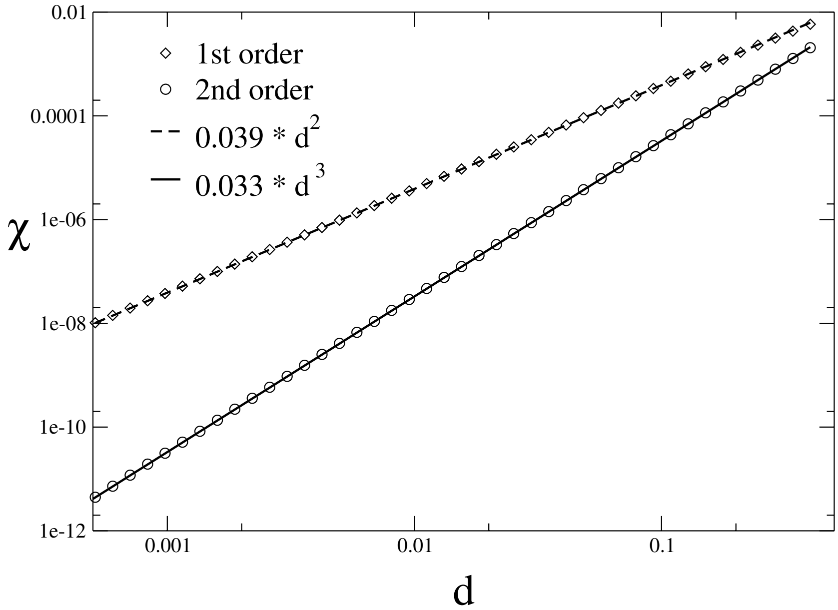

Figure 1. Quantity χ, from equation (21), evaluated for a chain of six sites for first- (diamonds) and second- (circles) order perturbation theory. We plot χ as a function of d, at fixed mean temperature $\bar{\gamma} = 0.4$.

'reverse' directions, namely

$$\Pi_f \equiv w(\{\sigma\}_k \to \{\sigma\}_1) \prod_{j=1}^{k-1} w(\{\sigma\}_j \to \{\sigma\}_{j+1})$$

$$\Pi_r \equiv w(\{\sigma\}_1 \to \{\sigma\}_k) \prod_{j=1}^{k-1} w(\{\sigma\}_{j+1} \to \{\sigma\}_j)$$

respectively. Detailed balance is violated if we can identify a single loop for which $\Pi_f \neq \Pi_r$. For our model, the shortest loop of this type has length 4 and involves four nearest neighbour spins, $\sigma_{i-1}, \ldots \sigma_{i+2}$. We begin with a configuration $\{\sigma\}_1$ in which these four spins are all +1 and i is even. The two central spins play the key role: $\{\sigma\}_2$ has spin $\sigma_i = -1$; $\{\sigma\}_3$ has $\sigma_i = -1$ and $\sigma_{i+1} = -1$; finally, $\{\sigma\}_4$ has $\sigma_{i+1} = -1$. Flipping σ_{i+1} back to +1 restores $\{\sigma\}_1$. In defect language, we first create an even defect pair, then the right defect, followed by the left defect, diffuses right by one lattice site and then the resulting odd defect pair is annihilated: $000 \to 110 \to 101 \to 011 \to 000$. It is easy to compute $\Pi_f = (1 - \gamma_e)(1 + \gamma_o)$ which differs from $\Pi_r = (1 + \gamma_e)(1 - \gamma_o)$. Thus our model does indeed violate detailed balance.

Our (perturbative) steady-state solution sheds further light on this issue, demonstrating which, and how, elementary spin-flips contribute. We focus on the net probability current F between two configurations $\{\sigma\}$ and $\left\{\sigma^{[i]}\right\}$,

$$F\left(\{\sigma\}, \left\{\sigma^{[i]}\right\}\right) \equiv w_i(\sigma_i \to -\sigma_i) q(\{\sigma\}) - w_i(-\sigma_i \to \sigma_i) q\left(\left\{\sigma^{[i]}\right\}\right). \qquad (22)$$

In *zeroth* order of perturbation theory, all F vanish since detailed balance holds. To obtain the leading *non-vanishing* contributions to F, we decompose the rates according to equation (8) and insert the first-order expression for the stationary density. To $\mathcal{O}(d)$, we find

$$F\left(\{\sigma\}, \left\{\sigma^{[i]}\right\}\right) = \tilde{Z}^{-1} d (A_1 + A_2)\, q_0(\{\sigma\}) + \mathcal{O}(d^2)$$

with

$$A_1 \equiv \Delta_i(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) - \Delta_i(\sigma_{i-1}, -\sigma_i, \sigma_{i+1}) \frac{q_0\left(\left\{\sigma^{[i]}\right\}\right)}{q_0(\{\sigma\})}$$
$$A_2 \equiv \bar{w}(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) Q_1(\{\sigma\}) - \bar{w}(\sigma_{i-1}, -\sigma_i, \sigma_{i+1}) \frac{q_0\left(\left\{\sigma^{[i]}\right\}\right)}{q_0(\{\sigma\})} Q_1\left(\left\{\sigma^{[i]}\right\}\right).$$

Here, A_1 reflects the effect of the non-equilibrium rate, Δ, whereas A_2 contains the first-order correction, $Q_1(\{\sigma\})$, to the Ising stationary distribution. Using our definitions and results from the previous section, one finds easily that

$$A_1 = \frac{(-1)^i}{2} \sigma_i(\sigma_{i-1} + \sigma_{i+1})[1 + \exp(-2\bar{\beta}\sigma_i(\sigma_{i-1} + \sigma_{i+1}))] \tag{23}$$

and

$$A_2 = \frac{\sinh(4\bar{\beta})}{2} \left[1 - \frac{\bar{\gamma}}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1})\right] \left\{\left[n_o\left(\left\{\sigma^{[i]}\right\}\right) - n_e\left(\left\{\sigma^{[i]}\right\}\right)\right] - [n_o(\{\sigma\}) - n_e(\{\sigma\})]\right\}. \tag{24}$$

One can show, by considering elementary spin-flips and their effect on the defect representation, that the $\{\ldots\}$ bracket in equation (24) can take only the values ± 1 or 0.

We are now ready to evaluate the relevance of different spin-flips types (cf the discussion following equation (3)) for detailed balance violation. Spin-flips of type (a) and (b) are inverse to one another: where (b) generates a defect pair, (a) annihilates it. To be specific, we let $\{\sigma\} \to \left\{\sigma^{[i]}\right\}$ be a type (b) transition, with $\sigma_{i-1} = \sigma_i = \sigma_{i+1}$ in $\{\sigma\}$. For this configuration, we find

$$\begin{aligned} A_1 &= (-1)^i[1 + \exp(-4\bar{\beta})] \\ A_2 &= \tfrac{1}{2}\left\{\left[n_o\left(\left\{\sigma^{[i]}\right\}\right) - n_e\left(\left\{\sigma^{[i]}\right\}\right)\right] - [n_o(\{\sigma\}) - n_e(\{\sigma\})]\right\}. \end{aligned} \tag{25}$$

Given the constraint on the $\{\ldots\}$ bracket, the inequality $|A_2| < 2|A_1|$ follows. Thus, A_1 determines the *sign* of the probability current. For $T_e > T_o (d > 0)$ we have $F\left(\{\sigma\}, \left\{\sigma^{[i]}\right\}\right) > 0$ if i is even, and negative otherwise: at the hotter (even) sites, defect pairs are more often generated than removed. At the cooler (odd) sites, the situation is reversed. In this manner, spin-flips of types (a) and (b) always contribute to detailed balance violation in the presence of two temperatures.

If the spin-flip $\{\sigma\} \to \left\{\sigma^{[i]}\right\}$ is a type (c) process (i.e., defect diffusion), then its inverse also belongs to this class, and both occur with rate 1. Since $\sigma_{i-1} = -\sigma_{i+1}$ for a type (c) spin flip, A_1 vanishes and only A_2 contributes to the probability current. As a result, a type (c) transition violates detailed balance in first order of d (i.e., generates a nonzero F) only if it changes the difference of odd and even defect pairs. In defect notation, the process $\ldots 0, 1, 1, 0, 0, \ldots \to \ldots 0, 1, 0, 1, 0, \ldots$ violates detailed balance while $\ldots 0, 1, 0, 0, \ldots \to \ldots 0, 0, 1, 0, \ldots$ does not. If the defect pair in the former process is centred on an even site, we will have $F\left(\{\sigma\}, \left\{\sigma^{[i]}\right\}\right) > 0$ for $T_e > T_o$, etc.

Including terms of $\mathcal{O}(d^2)$, we find that *all* type (c) spin-flips now generate non-vanishing probability currents. Thus, currents between pairs of configurations, connected by single spin-flips, are generically nonzero.

5. Entropy production

We finally consider two different approaches to entropy production in our model. The first [14] is very intuitive and tailored to our specific model, by focusing on the energy ('heat') flux from one bath to the other. The second method [16, 26–28] is more general, defining an entropy production for any master equation. In the following, we show that both approaches are equivalent for our model.

We briefly review the first method. As the spin chain is connected to two baths at different temperatures, heat flows from the warmer reservoir into the spin chain and on into the colder one. Since the energy difference of two configurations connected via a single spin-flip at site i is $-2\sigma_i(\sigma_{i-1}+\sigma_{i+1})$, the energy transfer at this site is given by

$$j(i) \equiv \langle -2\sigma_i(\sigma_{i-1}+\sigma_{i+1}) w_i(\sigma_i \to -\sigma_i)\rangle \tag{26}$$

where $\langle\cdot\rangle$ denotes the configurational average with respect to $q(\{\sigma\})$. Standard thermodynamics then suggests defining the entropy production of the whole chain as

$$\dot{S} = \frac{N}{2}\left(\frac{j(2i+1)}{T_o} + \frac{j(2i)}{T_e}\right). \tag{27}$$

Using equation (1) for the rates, $j(i)$ is easily expressed in terms of the *exactly known* [14] two-spin correlation function

$$\langle\sigma_i\sigma_j\rangle = \sqrt{A(i)A(j)}\,\lambda^{|j-i|}$$

with

$$A(i) \equiv \begin{cases} A_e = (\gamma_e+\gamma_o)/(2\gamma_o) & i \text{ even} \\ A_o = (\gamma_e+\gamma_o)/(2\gamma_e) & i \text{ odd} \end{cases} \tag{28}$$

$$\lambda \equiv \frac{1}{\sqrt{\gamma_e\gamma_o}}\left(1-\sqrt{1-\gamma_e\gamma_o}\right).$$

Hence

$$\dot{S} = \frac{N}{2}(\gamma_o-\gamma_e)\left(\frac{1}{T_o}-\frac{1}{T_e}\right) \tag{29}$$

follows exactly for any choice of temperatures. We note that the entropy production is positive whenever the two temperatures differ.

The more general approach [16, 26–28] to entropy production begins with the Gibbs entropy for the full time-dependent probability distribution $p(\{\sigma\},t)$:

$$S_G(t) = -\sum_{\{\sigma\}} p(\{\sigma\},t)\ln p(\{\sigma\},t)\,. \tag{30}$$

For the stationary distribution $q(\{\sigma\})$, the time derivative $\mathrm{d}S_G/\mathrm{d}t$ must vanish. With the help of the master equation, we find $\mathrm{d}S_G/\mathrm{d}t = \dot{\tilde{S}}_1 - \dot{\tilde{S}}_2$ where

$$\begin{aligned}\dot{\tilde{S}}_1 &= \frac{1}{2}\sum_{\{\sigma\}}\sum_{i=1}^{N}\left[w_i(\sigma_i\to-\sigma_i)q(\{\sigma\}) - w_i(-\sigma_i\to\sigma_i)q\left(\left\{\sigma^{[i]}\right\}\right)\right] \\ &\qquad\times\ln\left(\frac{w_i(\sigma_i\to-\sigma_i)q(\{\sigma\})}{w_i(-\sigma_i\to\sigma_i)q\left(\left\{\sigma^{[i]}\right\}\right)}\right) \\ \dot{\tilde{S}}_2 &= \sum_{\{\sigma\}}\sum_{i=1}^{N} q(\{\sigma\})w_i(\sigma_i\to-\sigma_i)\ln\left(\frac{w_i(\sigma_i\to-\sigma_i)}{w_i(-\sigma_i\to\sigma_i)}\right).\end{aligned} \tag{31}$$

The two expressions $\dot{\tilde{S}}_1$ and $\dot{\tilde{S}}_2$ constitute two alternate representations for entropy production. In particular, we recognize the probability current $F\left(\{\sigma\},\left\{\sigma^{[i]}\right\}\right)$ of equation (22) in the expression for $\dot{\tilde{S}}_1$. One easily observes $\dot{\tilde{S}}_1 \geqslant 0$ since each term in the sum is non-negative.

Moreover, $\dot{\mathcal{S}}_1$ vanishes if and only if detailed balance is satisfied. Thus, strictly positive entropy production is equivalent to the violation of detailed balance.

We now evaluate the expression for $\dot{\mathcal{S}}_2$ in equation (31)[2]. Since our model exhibits translation invariance with period 2, we only have to consider one even $(2i)$ and one odd $(2i+1)$ site, so that

$$\dot{\mathcal{S}}_2 = \frac{N}{2} \sum_{\{\sigma\}} \sum_{j\in\{2i,2i+1\}} q(\{\sigma\}) w_j(\sigma_j \to -\sigma_j)[-2\beta_j \sigma_j(\sigma_{j-1} + \sigma_{j+1})]. \qquad (32)$$

Here, we have used the simple relation

$$\frac{w_i(\sigma_i \to -\sigma_i)}{w_i(-\sigma_i \to \sigma_i)} = \exp\left[-2\beta_i \sigma_i(\sigma_{i-1} + \sigma_{i+1})\right]$$

Recalling equation (26), we note immediately that

$$\dot{\mathcal{S}}_2 = \frac{N}{2}\left[\beta_e j(2i) + \beta_o j(2i+1)\right] \qquad (33)$$

which is exactly the expression (27) that was derived from thermodynamics. Thus, we confirm the consistency of the more abstract general expressions (31) and the intuitive thermodynamic approach. While this enhances our confidence in (31), a better understanding in terms of more basic physical principles is still outstanding.

6. Conclusions

To summarize, we have gained some analytical insight into the steady state configurational probabilities of an Ising spin chain driven out of equilibrium by a coupling to two heat baths: subject to different temperatures, spins on even and odd sites are updated according to a generalization of the usual Glauber rates. A perturbative calculation in the temperature difference shows that the stationary distribution for this non-equilibrium model is rather complex, with longer range and higher order spin operators appearing. Clearly, the energy of a configuration no longer determines its statistical weight. Unfortunately, at this stage we can only conjecture the structure of this distribution beyond second order in perturbation theory. It seems likely that, at each order, additional spin operators will have to be introduced. Turning to other characteristics of this non-equilibrium steady state, we could understand in more detail how the presence of two temperatures violates detailed balance. We could also show the equivalence of two unrelated definitions of entropy production, thus providing additional support for the general expression [16, 26–28].

Of course, numerous questions remain open. In particular, we would like to reconcile the apparent proliferation of longer range spin couplings in the configurational probabilities with the observed 'triviality' of long-wavelength properties. At present, we have strong indications [23] that arbitrary spin correlation functions decay exponentially, quite similar to the equilibrium Ising chain. However, the most fundamental question still remains unanswered: are there any *a priori* criteria, beyond simple symmetries, that determine which configurations will appear with equal weights? In equilibrium, the determining quantity is their energy. Far from equilibrium, the key concept is still missing.

[2] We are indebted to J Slawny for this argument.

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