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2001 J. Phys. A: Math. Gen. 34 L213

(http://iopscience.iop.org/0305-4470/34/14/101)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) L213–L220 www.iop.org/Journals/ja PII: S0305-4470(01)22114-3

LETTER TO THE EDITOR

Tapping thermodynamics of the one-dimensional Ising model

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Received 14 February 2001

Abstract

We analyse the steady-state regime of a one-dimensional Ising model under a tapping dynamics recently introduced by analogy with the dynamics of mechanically perturbed granular media. The idea that the steady-state regime may be described by a flat measure over metastable states of fixed energy is tested by comparing various steady-state time-averaged quantities in extensive numerical simulations with the corresponding ensemble averages computed analytically with this flat measure. The agreement between the two averages is excellent in all the cases examined, showing that a static approach is capable of predicting certain measurable properties of the steady-state regime.

PACS numbers: 0520, 7510N, 8105R

1. Introduction

In complex systems such as granular media the energy available due to thermal fluctuations is not sufficient to cause particle rearrangement, hence in the absence of external perturbations the system is trapped in a metastable state. A granular medium may be shaken mechanically and experiments reveal a steady-state regime defined by an asymptotic compactivity [1]. The non-trivial behaviour of these systems, such as slow relaxation dynamics and hysteresis effects, arises from the fact that such systems have an extensive entropy of metastable or blocked states. A vertically tapped system of hard spheres tends to a random close packing [1], whereas a horizontally shaken system crystallizes [2]; the stationary states obtained in these systems are not theoretically understood at present. Edwards [3] has proposed that one may construct a thermodynamics over metastable states in the same way as Boltzmann and Gibbs developed over microstates; his hypothesis is that the equilibrium measure over these states, in gently tapped systems, is flat over all blocked states satisfying the relevant macroscopic constraints. Recently this scenario has been put to the test in [4], where the authors examine a form of tapping dynamics on two systems having an extensive entropy of metastable or blocked configurations, the Kob–Anderson model [5] and the random field Ising model in three dimensions. They then compared the time-averaged quantities obtained in the late-time aging regime with those generated by a flat Edwards measure numerically calculated over blocked configurations of the

0305-4470/01/140213+08$30.00

system. While the Edwards measure worked well for the Kob–Anderson model it was shown to be incorrect for the random field Ising model in three dimensions. Hence, though it is not generically true, there appear to be systems where the flat measure works. The development of a thermodynamics for such systems is important to understand the behaviour of granular media, powders and glasses, and has far-reaching fundamental physical and practical applications. Let us add that method of simulated annealing, where an analogy with classical thermodynamics is used for optimization problems, is one of the most robust general methods of optimization used in science and industry; it is possible that tapping type algorithms are more efficient in certain circumstances (see e.g. [6]) and thus the general theory we are searching for should clearly have applications well beyond physics.

Recently tapping dynamics has been introduced on simple spin systems in order to draw analogies with the physics of granular media. These spin systems are spin glasses and ferromagnets on random thin graphs [7, 8] and the three-spin model with ferromagnetic coupling on random hypergraphs [9]. In the p-spin spherical model a tapping-like dynamics has been recently introduced using a time-dependent oscillating magnetic field [10]. Simulations on hard-sphere systems with a similar tapping mechanism were also carried out in [11]. A tapping dynamics on a one-dimensional lattice model with facilitated dynamics has been studied in [12], in the limit of very weak tapping. The general picture emerging from these studies and the experiment [1] is that the compactivity of the system is increased as the tapping strength (the amplitude of the external perturbation) is reduced. However, in the horizontal shaking experiments [2] this is not the case. The main reason for choosing the spin systems studied in [7–9] is that they have an extensive entropy of metastable states [9, 13, 14]; that is to say, the total number of metastable states N_{MS} is given by

$$N_{\mathrm{MS}} \sim \exp(N s_{\mathrm{Edw}}) \tag{1}$$

where s_{Edw} is the total Edwards entropy per spin [3]. The definition of a metastable state depends on the dynamics of the system, where we will define a metastable state to be a configuration where no single spin flip reduces the energy of the system. In this Letter we will examine the validity of the hypothesis of Edwards for the one-dimensional ferromagnet under the tapping dynamics of [7, 8]. If one implements a zero-temperature single-spin-flip dynamics such that only single spin flips lowering the energy are permitted, this system has an extensive Edwards entropy and becomes stuck in metastable states. The dynamics is made to evolve via tapping, that is to say each spin is flipped in parallel with probability $p \in (0, 1/2]$. The system is tapped after it becomes blocked in a metastable state and after the tap it relaxes again under zero temperature or falling dynamics (by analogy with granular material in a gravitational field). Here the quantity corresponding to the compactivity is the energy. If one makes an analogy with granular media, this dynamics corresponds to a rapid relaxation dynamics between taps, meaning that the tapping is characterized only by its strength, p, and not by an additional timescale. This dynamics is therefore, in a sense, the simplest case of realistic tapping. The Glauber dynamics of the one-dimensional Ising model can be solved analytically [15] (at all temperatures); however, the falling dynamics defined here (in between taps) does not seem amenable to analytic solution.

The tapping dynamics for this system leads after a sufficiently large number of taps to a steady-state energy $E(p)$, which is constant. This value of $E(p)$ can be determined by a mean-field theory [7, 8], which we suspect to be exact as it reproduces certain exact results obtained combinatorially and also is in perfect agreement with the numerical simulations. Here we present numerical simulations under tapping dynamics to measure quantities such as correlation functions, distribution of domain lengths and energy fluctuations (corresponding to a specific heat) and confront the results with exact calculations using the Edwards measure.

By the Edwards hypothesis we assume that the stationary measure on the tapped systems is

$$\langle \mathrm{O} \rangle_{\mathrm{Edw}} = \frac{\sum_{\mathcal{C}} \mathrm{O} \exp\left(-\beta(p) H[\mathcal{C}]\right)}{Z} \tag{2}$$

where $\{\mathcal{C}\}$ is the ensemble of metastable configurations and

$$Z = \int \mathrm{d}E \, N_{\mathrm{MS}}(E) \exp(-\beta(p) N E) \tag{3}$$

as suggested in [3] and recently in [16]. Here $N_{\mathrm{MS}}(E)$ is the number of metastable states with energy per spin E and $\beta(p)$ is a Lagrange multiplier fixing the energy of the system, which can also be thought of as a canonical temperature arising from the tapping. Defining the Edwards entropy at internal energy E, $s_{\mathrm{Edw}}(E) = \ln(N_{\mathrm{MS}}(E))/N$, we find that the relation determining $\beta(p)$ (the inverse Edwards temperature) is

$$\beta(p) = \left. \frac{\partial s_{\mathrm{Edw}}(E)}{\partial E} \right|_{E(p)}. \tag{4}$$

It was shown in [7, 8] that $E(p)$ is a monotonically decreasing function of p and from the definition (4) and the calculation of $s_{\mathrm{Edw}}(E)$ carried out in [13] one may calculate the corresponding $\beta(p)$ as a function of p, which is continuous and monotonically decreasing. Hence p plays the role of an effective temperature which fixes the internal energy of the steady state.

This does not prove that the Edwards measure is correct for this system (the hypothesis of Edwards does not tell us how to calculate $\beta(p)$); one now has to see whether the measure (2) can be used to compute quantities in the steady-state regime. In this Letter we calculate using the Edwards measure:

- The internal energy fluctuation per spin $c = (\langle \mathcal{E}^2 \rangle - \langle \mathcal{E} \rangle^2)/N$ where $\mathcal{E}$ is the total internal energy, and consequently $\langle \mathcal{E} \rangle = NE$.
- The correlation functions $C(r) = \langle S_i S_{i+r} \rangle$ and $D(r) = \langle S_i S_{i+1} S_{i+r} S_{i+r+1} \rangle$.
- The distribution of domain sizes.

The results are then compared with extensive numerical simulations.

2. Calculations using the Edwards measure

The Hamiltonian we consider is that for the usual one-dimensional ferromagnet with periodic boundary conditions

$$H = -\sum_{i=1}^{N} S_i S_{i+1}. \tag{5}$$

The partition function for the system is then given by

$$Z = \mathrm{Tr} \prod_{i=1}^{N} \exp(\beta S_i S_{i+1}) \theta(S_{i-1} S_i + S_i S_{i+1}) \tag{6}$$

where the function $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x \geqslant 0$ enforces the metastability (each spin is stable or marginally stable in its local field). Performing a local change of variables to new Ising spins $\sigma_i = S_i S_{i+1}$ we obtain

$$Z = \mathrm{Tr} \prod_{i=1}^{N} \exp(\beta \sigma_i) \theta(\sigma_i + \sigma_{i+1}). \tag{7}$$

Hence we find that $Z = \mathrm{Tr}\, T^N$ where T is the transfer matrix

$$T = \begin{pmatrix} a & 1 \\ 1 & 0 \end{pmatrix} \tag{8}$$

with $a = \exp(\beta)$. From this we find that

$$E = \frac{a}{\sqrt{a^2+4}} \tag{9}$$

which simply determines β. The fluctuations in the free energy are then seen to be given by

$$c = -E(1-E^2). \tag{10}$$

The determination of the correlation function $D(r)$ is simple as, in terms of the spins σ_i, one has $D(r) = \langle \sigma_i \sigma_{i+r} \rangle$. Using the Edwards measure one obtains

$$D(r) = \frac{\mathrm{Tr}\, \hat{\sigma} T^r \hat{\sigma} T^{N-r}}{Z} \tag{11}$$

where $\hat{\sigma}$ is the matrix

$$\hat{\sigma} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{12}$$

In the large-N limit one finds

$$D(r) = \left(\langle t_0|\hat{\sigma}|t_0\rangle\right)^2 + \left(\frac{t_1}{t_0}\right)^r \left(\langle t_1|\hat{\sigma}|t_1\rangle\right)^2 \tag{13}$$

where $t_0 = (a + \sqrt{a^2+4})/2$ is the maximal eigenvalue of T and $t_1 = -1/t_0$ the remaining one, $|t_0\rangle$ and $|t_1\rangle$ denoting the respective normalized eigenvectors. Expressing everything in terms of the energy per spin E we find that the connected part of $D(r)$ is given by

$$D_c(r) = (1-E^2)\left(\frac{E+1}{E-1}\right)^r. \tag{14}$$

In the same way, one can calculate the two-point correlation function, finding

$$C(r) = C_c(r) = \frac{\mathrm{Tr}\, (\hat{\sigma} T)^r T^{N-r}}{Z}. \tag{15}$$

The matrix $\hat{\sigma} T$ can be trivially diagonalized: $\hat{\sigma} T = P D P^{-1}$, with

$$P = \begin{pmatrix} u & 1 \\ 1 & u \end{pmatrix} \qquad \text{and} \qquad D = \begin{pmatrix} u & 0 \\ 0 & 1/u \end{pmatrix} \tag{16}$$

with $u = (a + \sqrt{a^2-4})/2$. This yields

$$C(r) = A\left(\frac{u}{t_0}\right)^r + (1-A)\left(\frac{1}{u t_0}\right)^r \tag{17}$$

with

$$A = \frac{u^2 t_0^2 - 1}{(u^2-1)(t_0^2+1)}. \tag{18}$$

Defining by $P(r)$ the probability that a given domain has length r, it is easy to see that this is given by

$$P(r) = \frac{\langle \delta_{\sigma_1,-1}\delta_{\sigma_2,1}\cdots\delta_{\sigma_r,1}\delta_{\sigma_r,1}\delta_{\sigma_{r+1},-1}\rangle}{\langle \delta_{\sigma_1,-1}\rangle}. \tag{19}$$

We find that

$$P(r) = \frac{1}{t_0^2}\left(\frac{a}{t_0}\right)^{r-2} \qquad r \geqslant 2$$
$$= 0 \qquad r < 2. \tag{20}$$

Simplifying this yields

$$P(r) = \left(\frac{1+E}{1-E}\right)\left(\frac{-2E}{1-E}\right)^{r-2} = a(E)\exp\left(-b(E)r\right) \qquad r \geqslant 2$$
$$= 0 \qquad r < 2. \tag{21}$$

Hence, the distribution of domain sizes is geometric for $n > 2$, the fact that $P(1) = 0$ is a consequence of metastability as a domain of length 1 would be a single spin surrounded by two antiparallel neighbours, which is unstable.

3. Comparison with numerical simulations

One can compare the results of numerical simulations of tapping with the above theoretical ones. For a given value of the energy, let us say E, we have tapped the system with a strength p such that in the steady state $E = E(p)$. The value of $E(p)$ can be calculated [7, 8] and we recall that $E(p)$ is maximal for $p = 1/2$, where it takes the value $-1 + \mathrm{e}^{-1}$, and $E(p)$ is monotonically decreasing for $p \in [0, 1/2]$ with $\lim_{p\to 0^+} E(p) = -1$. The system is tapped a sufficiently large number of times, say t_s, to ensure that the average of the internal energy $E(t)$ measured becomes stationary. Once in this steady-state regime, the quantities of interest are measured over a measurement time (number of taps) $t_\mathrm{m} = 10^5$. The systems were of size of 2×10^5 spins and the results were also averaged over N_s realizations. Hence, mathematically, the average value of a quantity A is calculated, as one would in a Monte Carlo simulation of a thermal system, as

$$\langle A \rangle = \frac{1}{N_s}\sum_{i=1}^{N_s}\frac{1}{t_\mathrm{m}}\sum_{t=t_s+1}^{t_s+t_\mathrm{m}} A_i(t). \tag{22}$$

In our simulations we found that, for the number of sites and t_m used here, the results obtained from averaging over several systems were identical to those obtained from measurements over a single system. Hence the results are in the thermodynamic limit and the dependence on the system size vanishes. Consequently the results presented here are from an average over a single system of size 2×10^5 spins. In figure 1, we compare the fluctuation of the energy c calculated using Edwards' measure, as a function of E, against those obtained from the simulations: the agreement is very good. For small values of p the error bars in our measurements are very small and the agreement with equation (10) is excellent. For larger values of p the error bars are large as the statistical fluctuations are larger; however, from figure 1 we see that the value given by equation (10) is within the error bars. The distribution $P(r)$ of domain sizes is shown in figure 2 and has a perfect exponential decay for $r \geqslant 2$. This demonstrates that equation (21) is in perfect agreement with the simulations (as the energy E is fixed) as shown in figure 3.

The correlation functions such as $C(r)$ and $D(r)$ have also been computed numerically. In figure 4 we have plotted the results in comparison with those expected from equations (14) and (17). Here again, the comparison is excellent (note that the agreement is better for low energies, as again the statistical fluctuations due to the tapping are much smaller for low p than for high p).

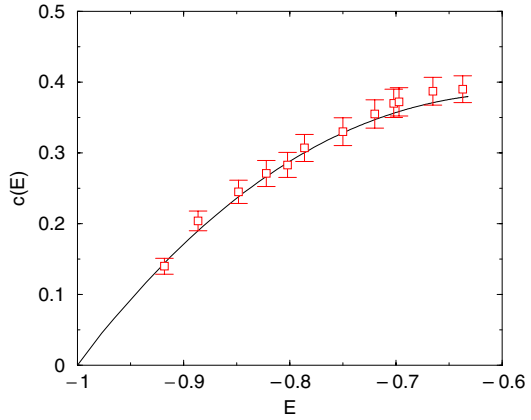

Figure 1. The internal energy fluctuation $c(E)$ versus E. The solid curve corresponds to the value obtained from equation (10) and the symbols are the results obtained from tapping simulations made on 5000 systems of 200 000 spins.

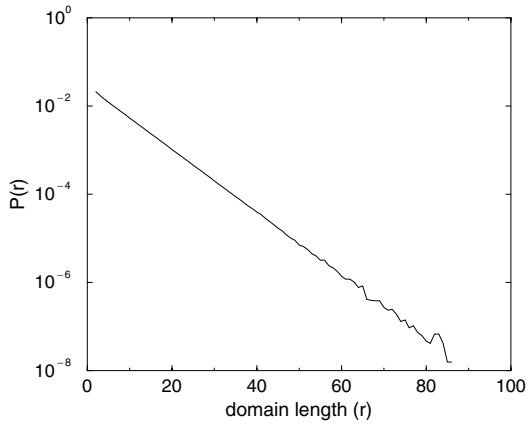

Figure 2. Distribution of domain lengths from tapping simulations for $p = 0.1$. The vertical scale is logarithmic. The slope is $b = 0.165 \pm 0.001$, in excellent agreement with that obtained from equation (21).

4. Conclusion

We have simulated numerically tapping dynamics on a one-dimensional system and measured fluctuations of the energy, correlation functions and distributions of domain sizes. The values of these quantities expected from a thermodynamics built by using a flat measure over blocked configurations agree very well with our simulation data. The use of the flat measure therefore allows one to accurately predict the two-point correlation function, a particular four-point function $D(r)$ and also a hierarchy of n-point functions (see equation (19)) corresponding to the distribution of domain sizes $P(r)$. In principle further quantities could be investigated but the numerical study would be hampered by statistical fluctuations. The important point here is that the principal quantities open to experimental determination are well predicted from Edwards' measure. A proof of the absolute validity of the use of the flat measure seems difficult: there is no obvious form of detailed balance in the tapping dynamics and

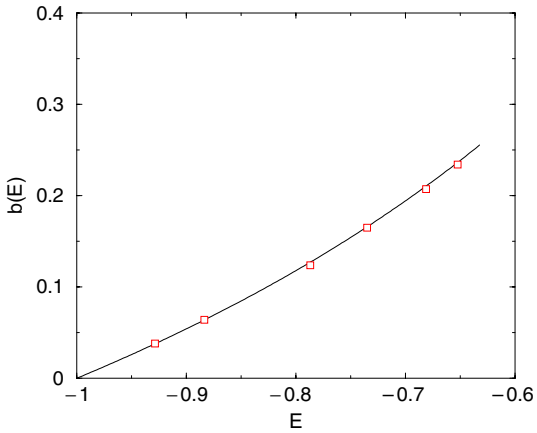

Figure 3. Slope of $\ln(P(r))$, $b(E)$ (as defined by equation (21)), with respect to the energy. The solid curve corresponds to equation (21) and the symbols correspond to the same numerics as figure 1.

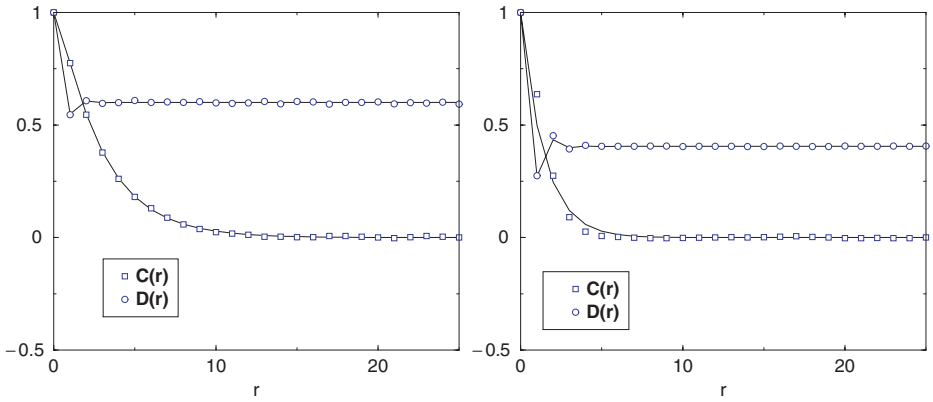

Figure 4. Comparison of the expected $C(r)$ and $D(r)$ from the theoretical calculation with the results from numerical simulations for $E = -0.78$ (left) and $E = -0.63$ (right). The symbols are the results of the tapping experiments and the solid curves correspond to those predicted by equations (14) and (17).

one would need to show that at fixed internal energy per spin the system explores uniformly the metastable states of this energy. Physically this seems quite likely in the limit of small tapping. Here a metastable state can be viewed as a configuration of islolated domain walls. The first-order $O(p)$ effect of tapping creates domain wall diffusion and annihilation upon the encounter of two domain walls as in the zero-temperature Glauber dynamics of the Ising model [15, 17]. In addition within a domain the flipping of two consecutive spins creates a domain of length 2 which then contributes the diffusion/annihilation process mentioned previously; this process is, however, $O(p^2)$. Physically, the steady state is then reached upon the equilibrium between the creation of small domains of this type within larger domains and the annihilation of domains driven by diffusion. Hence, as the steady-state regime is characterized by an average number of domain walls with the annihilation and creation processes mentioned above in equilibrium, it seems plausible that the diffusion generated

by the O(p) tapping enables the system to explore the configurations available in a flat manner.

During this work we have benefited from useful and illuminating discussions with Jorge Kurchan, Satya Majumdar and Erik Sorensen.

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