Possible Test of the Thermodynamic Approach to Granular Media

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We study the steady state distribution of the energy of the Sherrington-Kirkpatrick model driven by a tapping mechanism which mimics the mechanically driven dynamics of granular media. The dynamics consists of two phases: a zero temperature relaxation phase which leads the system to a metastable state, then a tapping which excites the system thus reactivating the relaxational dynamics. Numerically, we investigate whether the distribution of the energies of the blocked states obtained agrees with a simple canonical form of the Edwards measure. It is found that this canonical measure is in good agreement with the dynamically measured energy distribution. A possible experimental test of the Edwards measure based on the study here is proposed.

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Complex systems such as granular media possess a large number of metastable or blocked configurations. When a granular medium is shaken, it quickly relaxes into a blocked configuration, a subsequent shake or tap will lead it to another blocked or jammed state, and so on. If the driving mechanism is held constant, one expects the system to enter into a quasiequilibrium stationary state. Various driving mechanisms can be investigated experimentally, such as vertical tapping [1] and horizontal shaking [2]. In granular media and other complex systems such as spin glasses, the entropy of these blocked states is extensive in the system size. Hence, it has been proposed that one may use a thermodynamic measure over blocked states to describe this steady state. The simplest proposition is that the system is characterized by a number of quantities which are fixed on average, and then the measure on the steady state is obtained from the maximum entropy state (on blocked states) with the relevant macroscopic quantities fixed [3]. This simple idea has recently been investigated in a wide range of systems and has been shown to be relatively successful. Various tests of the applicability of these thermodynamic ideas have been carried out and, although some confirmation has been made in more realistic sheared granular systems [4], most work has been carried out on simpler model systems which one hopes capture the basic physics of granular media. The Edwards flat measure has been shown to be of predictive value in some simple one-dimensional lattice models [5,6], but there are clearly examples where the approach fails [7]. However, recently it was shown that more sophisticated versions of the Edwards measure introducing ensembles with several quantities fixed on average can remedy the deficiencies of the basic measure in these cases [8]. Other toy models that have been analyzed are lattice based models with kinetic constraints in higher dimensions [9,10] and also spin glass models [11] where nonthermal driving is used to move the system between blocked states.

Even if it is not expected to be exact, many systems may be described to a good engineering level by these measures. Given the difficulty of the analysis of the highly nonlocal dynamics in these systems, this is an important step toward understanding their steady state regimes. There is no clear ergodicity in these systems and no detailed balance as in usual statistical mechanics. Edwards argued that a system might conceivably explore blocked configurations in a flat manner if the driving involved extensive manipulations, meaning the displacement of a macroscopic number of particles, for example, shaking, stirring, or pouring granular media. An interesting consequence of the applicability of thermodynamic ideas is that one may describe phase transitions in these driven systems [12]. However, even considering the success of the Edwards measure in describing various simple models, evidence in realistic granular media is still lacking. In this Letter, we investigate whether, at a fixed tapping rate (to be defined later), the states explored dynamically obey a form of Boltzmann distribution. The results presented here are quite striking; despite a lack of detailed balance we shall see that a Boltzmann distribution excellently describes the histogram of the energies of the blocked states visited during the tapping. Motivated by these results, we propose a generic and simple experimental test of the Edwards measure, which should be feasible in a wide range of driven granular systems.

As mentioned above, a good theoretical and numerical testing ground for this thermodynamic approach to granular media are spin glasses. The definition of a blocked state in a spin glass simulated on a computer depends, of course, on the local dynamics. Under single spin flip dynamics, a metastable state is one where flipping any single spin increases the energy; it is thus a blocked state under any single spin flip Monte Carlo dynamics. Various spin glass models have been studied to explore the accuracy of the Edwards measure as a function of the relaxational dynamics and the tapping mechanism [11]. Here we shall explore the driven dynamics of the Sherrington-Kirkpatrick (SK) [13] spin glass model defined by the Hamiltonian $H = -\sum_{i<j} J_{ij} S_i S_j$, where the S_i $(1 \leq i \leq N)$ are Ising spins and the interaction J_{ij} are independent Gaussian random variables of zero mean and variance $\overline{J_{ij}^2} = 1/N$.

The tapping mechanism introduced in spin glass models involves two steps: (1) Relaxation: The system evolves under zero temperature Glauber dynamics until it is blocked in a metastable state. (2) The system is tapped with tapping parameter p, that is to say each spin is flipped in parallel with probability p; this is the extensive manipulation as at each tap on average pN spins are flipped. Given a tapping rate p, it is observed that the system reaches a steady state regime with a fixed average energy per spin ϵ [the energy being measured at the end of step (1) above]. If we postulate the canonical form of the Edwards measure for the quasiequilibrium distribution of the driven dynamics (observed on the blocked states), one has the steady state distribution of energy given by

$$\rho_{\mathrm{Edw}}(E) = \frac{N_{\mathrm{MS}}(E)\exp(-\beta E)}{Z}, \tag{1}$$

where $N_{\mathrm{MS}}(E)$ is the number of metastable states of energy E, β is the inverse Edwards temperature, which can be thought of as a Lagrange multiplier fixing the average energy per spin, and $Z = \sum_E N_{\mathrm{MS}}(E)\exp(-\beta E)$ is the canonical partition function. We note that a fully flat measure with fixed energy per spin would be $P_\alpha = \exp(-\beta E_\alpha)/Z$, where E_α is the energy of the blocked state α. In this Letter, we shall investigate only the weaker form of the measure Eq. (1). Such an investigation has been carried out in a model of particle deposition [5], but the originality of the approach of this Letter is that one can partially test Eq. (1) without knowing the Edwards entropy. This is crucial, since it opens up the possibility of looking at a wider range of granular models and even experiments.

The hypothesis Eq. (1) will be tested in the following manner. We fix a bin size for the energies ΔE and by exact enumeration we compute $N_{\mathrm{MS}}(E)$ for a given system and realization of the disorder. The exact enumeration means that we can explore system sizes up to $N = 30$. Then the tapping dynamics is applied to the same system and the dynamical histogram $N_D(E, p)$ of the energy with the same bin size ΔE is computed over 10^6 taps after the system has been tapped 10^6 times to reach the steady state. If the Edwards measure in the form of Eq. (1) is valid, then one should obtain

$$r(E) = \ln\left(\frac{N_D(E, p)}{N_{MS}(E)}\right) = -\beta E + C, \tag{2}$$

where C is a constant which should be independent of E. If Eq. (2) is valid, then an interesting question to ask is what the dependence of β is on (a) the tapping strength p, (b) the size of the system N, and (c) the realization of the disorder. It is interesting to see if the tapping strength p determines a unique temperature in the limit of large system sizes, for systems with the same statistical distribution of couplings, i.e., is β self-averaging? We shall see that the results obtained here for small system sizes suggest that Eq. (2) is obeyed on increasing the system size and that the parameter β becomes independent of the system size and the disorder realization for large systems.

In order to see what happens for larger systems, where the enumeration of metastable states is no longer feasible and where the thermodynamic approach should be expected to work better, one may compare the dynamical distribution $N_D(E, p)$ measured for the steady states at different tapping rates. If the Edwards measure holds, i.e., $N_D(E, p) \propto \rho_{\mathrm{Edw}}(E)$, then for any two tapping strengths p and p' we should find that

$$\begin{aligned} c(p, p', \epsilon) &= \frac{\ln[N_D(E, p)] - \ln[N_D(E, p')]}{N} \\ &= -(\beta(p) - \beta(p'))\epsilon + \frac{1}{N} f(N, p, p'), \end{aligned} \tag{3}$$

where $\epsilon = E/N$ is the energy per spin and $f(N, p, p')$ is independent of E. This constitutes a weak test of the Edwards hypothesis but has the merit of being practicable for large system sizes.

A final test is to use the analytic, but annealed, calculation of the average number of metastable states at fixed energy, $\overline{N_{\mathrm{MS}}(\epsilon)}$ (the overline indicates the disorder average over realizations), which gives in the thermodynamic limit $\overline{N_{\mathrm{MS}}(\epsilon)} \approx \exp[N S_{\mathrm{MS}}^a(\epsilon)]$, where [14,15]

$$S_{\mathrm{MS}}^a(\epsilon) = \min_z \left\{ \frac{1}{2} z^2 - E^2 + \ln\left[1 - \mathrm{erf}\left(\frac{z + 2E}{\sqrt{2}}\right)\right]\right\} \tag{4}$$

is the annealed entropy per spin of metastable states of energy ϵ per spin. If the Edwards measure holds, then we should find that

$$\frac{\ln[N_D(\epsilon, p)] - \ln[\overline{N_{\mathrm{MS}}(\epsilon)}]}{N} = -\beta(p)\epsilon + C. \tag{5}$$

We further expect that the dynamical entropy per spin $S_D(\epsilon, p) = \ln[N_D(\epsilon, p)]/N$ and the entropy of metastable states per spin $S_{\mathrm{MS}}(\epsilon) = \ln[N_{\mathrm{MS}}(\epsilon, p)]/N$ are self-averaging and, thus, Eq. (5) may be written for large N as $r(\epsilon) = \overline{S_D(\epsilon, p)} - \overline{S_{\mathrm{MS}}(\epsilon)} = -\beta(p)\epsilon + C$. Unfortunately, no exact calculation for $\overline{S_{\mathrm{MS}}(\epsilon)}$ exists; however, it is known that $S_{\mathrm{MS}}^a(\epsilon) = \overline{S_{\mathrm{MS}}(\epsilon)}$ for $\epsilon_c > -0.672$ [15]. Furthermore, this annealed approximation seems to be good, though not exact, to even lower energies as confirmed by a replica symmetric calculation [16]. Hence, at energies above ϵ_c, $r_a(\epsilon) = \overline{S_D(\epsilon, p)} - S_{\mathrm{MS}}^a(\epsilon) = -\beta(p)\epsilon + C$, which should also work well approximately at energies below, but not too far from, ϵ_c. We remark here that by Jensen's inequality $S_{\mathrm{MS}}^a(\epsilon) \geq S_{\mathrm{MS}}(\epsilon)$.

We now discuss the results of these numerical tests. Systems between size 15 and 30 were analyzed. The numerically measured value of $r(E)$ was computed from the static metastable state energy histogram and the histogram obtained by tapping the system 10^6 times. This was done for values of p: 0.1, 0.2, 0.3, 0.4, and 0.5. Increasing the number of taps did not change the dynamical histogram so we can be sure that we are measuring the steady state (this is natural given the small system sizes). It is possible that with very low tapping rates the time to reach the steady state even for a system of 30 spins becomes large. As an example, the results for $p = 0.3$ are shown in Fig. 1. We see that for small system sizes the points of the numerically measured $r(E)$ are scattered about the straight line fit predicted by Eq. (2). However, as the system size is increased the straight line fit appears excellent. The deviations from the straight line fit also appear to be nonsystematic. Similarly good fits are also obtained for all the tapping rates studied. In the case of the SK model, a Boltzmann distribution of the energies of the metastable states visited in the steady state regime appears to depend simply on having a large enough system size. It is generally believed that the Edwards measure should be more accurate in gently driven systems; here the weak form characterized by Eq. (2) seems equally valid at all tapping rates. We also note that the slope of the straight lines appears to be saturating to a constant value of $\beta(p)$ on increasing N, suggesting that in the thermodynamic limit the Edwards temperature is fully characterized by the tapping rate p.

From this first numerical study, one may conclude that if the weak form of the Edwards measure holds then it relies on the system being sufficiently large. The results above, however, seem encouraging, especially when one takes into account that the average total number of metastable states in a system of size $N \sim \exp(0.1992N)$ [14], which is only about 400 for a system of size 30.

We now carry out simulations for a system of size 200; here the average number of metastable states is about 2×10^{17}. The bin size is also refined to $0.0025N$. Naively, one would expect the thermodynamics approach to work better in this limit as the phase space of metastable states is much bigger. Also, there are many more states in each energy bin and, hence, it is really the weak form of the Edwards measure that is tested. Shown in Fig. 2 is the numerically computed $c(p, p,' \epsilon)$ from a simulation of the same system tapped at values of p: 0.1, 0.2, 0.3, 0.4, and 0.5. The system was first equilibrated by tapping 5000 times and the dynamical histogram was constructed over 5×10^6 taps. One sees from Fig. 2 that the values of $c(p, p', \epsilon)$ are to a good degree of accuracy on a straight line, as predicted by Eq. (3). The deviations at high energies, where the sampling is lowest, appear nonsystematic.

The energy histograms generated by the precedent simulations were used to compute $r_a(\epsilon)$; the results are shown in Fig. 3. The curves have been shifted vertically for clarity. A straight line fit was performed in the region $\epsilon > \epsilon_c$, and we see that in this region the fit is excellent. In addition, the values obtained from the fits for $\beta(p)$ are compatible with those obtained for the systems of size $N = 30$. The lower energy part of the curves also appears linear down to around $\epsilon = -0.72$. The replica symmetric calculation of [16] also visibly (on the same scale) departs from the annealed calculation near this energy, although we emphasize that this is not an exact calculation but can be expected to be closer to the real result than the annealed one. The lower tapping rates explore the lower

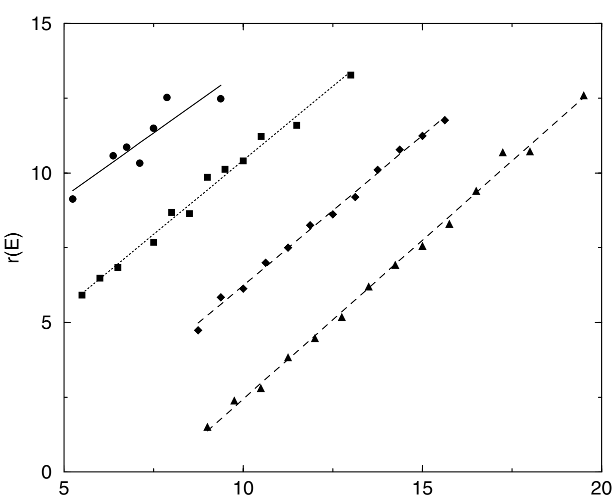

FIG. 1. The computed values of $r(E)$ for the randomized spin flip relaxation at $p = 0.3$ with a bin size of $0.025N$ for system sizes N of 15 (circles), 20 (squares), 25 (diamonds), and 30 (triangles). The straight lines are linear fits to guide the eye.

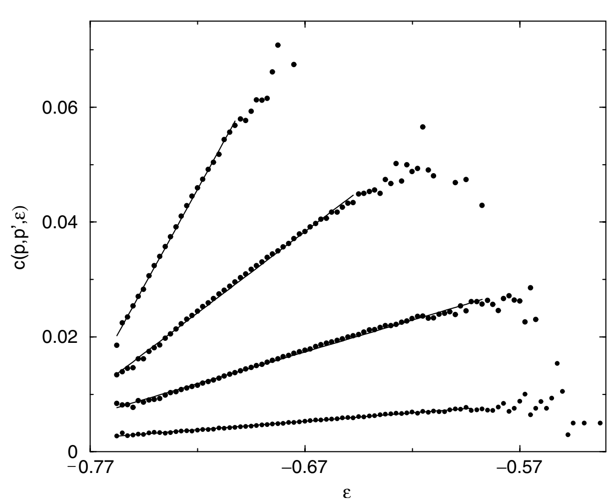

FIG. 2. The numerically computed values of $c(p, p'\epsilon)$ from simulations of a system of size $N = 200$ spins. The curves have been vertically shifted for clarity. Shown in descending order are the results for (p, p'): (0.2,0.1), (0.3,0.2), (0.4,0.3), and (0.5,0.4).

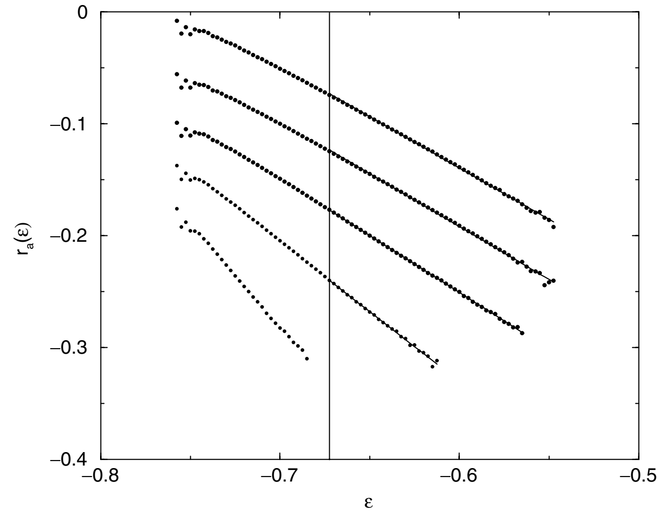

FIG. 3. The calculation of $r_a(\epsilon)$ for a system with $N = 200$ and data taken over 5×10^6 taps. Shown in ascending order are the plots for p: 0.1, 0.2, 0.3, 0.4, and 0.5. The straight line fits are shown in the region $\epsilon > \epsilon_c$ (to the right of the vertical line).

energy regime while the higher rates explore the higher energy regime. The deviations above ϵ_c from the annealed entropy are at the high energy end of the numerical histogram where the sampling is smallest. Though the range of energy over which the plots of Fig. 3 are made seems small (due to the large system size), the fact that one sees straight lines is nontrivial as can be seen by plotting the function $S^a_{\mathrm{MS}}(E)$ over the same range. Over this range, $S^a_{\mathrm{MS}}(E)$ shows a distinct bend.

In summary, we see that the assumption of an effective Boltzmann distribution for the energy of the states explored by tapping dynamics describes extremely well the numerically obtained results. This description seems to work better on increasing the system size for small systems and seems to be valid for larger systems via slightly more indirect tests. Why it works is rather mysterious, and if it is exact it would be an extremely useful method to numerically map out the distribution of metastable states in various spin glass models. The relaxational dynamics used was a random update which uses a lot of computer time for these simulations. A sequential update is much quicker for these simulations, and we have carried out such simulations and found to within very small deviations the same results. If one could prove the applicability of the Edwards measure for these types of dynamics, one would have an extremely powerful method to explore metastable states and inherent states in glassy systems. The standard method employing an auxiliary Hamiltonian [9] is much more time consuming—although classical statistical mechanics tells us that it will give the right result.

In the original proposition of Edwards in the context of granular media, the steady state volume fraction V occupied by a driven granular media is described in the canonical approach by $\rho_{\mathrm{Dyn}}(V) \propto \exp(-\frac{V}{X} + S(V))$, where X is the compactivity and $S(V)$ is the entropy of blocked states occupying volume V. The problem of calculating $S(V)$ in a real system seems formidable; however, it can be calculated in a simple toy model of granular material [17]. However, it should be possible to test the prediction of Eq. (3) experimentally by comparing the histograms of V for systems driven at different driving amplitudes. This would be a crucial, though perhaps difficult due to the large number of data points required, experimental test (though we emphasize again, not a demonstration) of the validity of the Edwards measure.

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