Thermodynamics and statistical mechanics of frozen systems in inherent states

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We discuss a statistical mechanics approach in the manner of Edwards to the "inherent states" (defined as the stable configurations in the potential energy landscape) of glassy systems and granular materials. We show that at stationarity the inherent states are distributed according a generalized Gibbs measure obtained assuming the validity of the principle of maximum entropy, under suitable constraints. In particular, we consider three lattice models (a diluted spin glass, a monodisperse hard-sphere system under gravity, and a hard-sphere binary mixture under gravity) undergoing a schematic "tap dynamics," showing via Monte Carlo calculations that the time averages of macroscopic quantities over the tap dynamics and over such a generalized distribution coincide. We also discuss about the general validity of this approach to nonthermal systems.

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I. INTRODUCTION

There are many complex systems where thermal fluctuations are small enough that the temperature of the external bath, T_{bath}, can be considered zero. Examples are supercooled liquids quenched at zero temperature in metastable states (blocked configurations), called "inherent structures," which correspond to the local minima of the potential energy in the particles configuration space [1–4]. Granular materials [5] at rest are another important example of the system frozen [6] in mechanically stable microstates (blocked configurations), which by analogy with the glass terminology can also be called inherent states.

The issue we consider here, which recently raised considerable interest, is to investigate the possibility to describe these systems by using concepts from statistical mechanics, as Edwards [7] suggested for granular media more than 10 years ago. His assumption was that, by gently shaking the system under the constraint of fixed volume V, the distribution over the mechanically stable (blocked) states would be uniform. This leads to the definition of a configurational entropy, $S=\ln\Omega$, where Ω is the number of mechanically stable states corresponding to the fixed volume V and energy E, and to the concept of compactivity, $X^{-1}=\partial\ln\Omega/\partial V$. In a similar way one can also define a configurational temperature, $T_{conf}^{-1}\equiv\beta_{conf}=\partial\ln\Omega/\partial E$.

Also in glasses, following, for example, the inherent structure approach [1–4], one can define a configurational entropy associated to the number of inherent structures corresponding to a fixed energy E, and consequently the configurational temperature. When the system is frozen at zero temperature in one of its inherent states it does not evolve anymore. However, one can explore the inherent structures space essentially in two ways. One way is by quenching the system over and over from an equilibrium temperature T to zero temperature [1,3,4]. Using this procedure, Sciortino *et al.* [3] found that in a supercooled glass forming liquid, studied by molecular dynamics simulations, the configurational temperature numerically coincides with the equilibrium temperature T, provided that T is low enough.

Another way to visit the inherent structures is by letting the system aging in contact with an almost zero bath temperature, T_{bath}. During the aging process an effective temperature T_{dyn} can be defined via the off-equilibrium extension of the fluctuation-dissipation ratio [8]. It happens that in mean field models [9] this effective temperature coincides with the above configurational temperature. The possibility to introduce an effective temperature for granular media via the extension of the fluctuation-dissipation relation, was suggested in Ref. [10].

The connection between Edwards's approach for granular media and the results in glass theory has been pointed out in Refs. [10–14]. In particular, in Ref. [11] it was shown that, for a class of finite-dimensional systems, in the limit $T_{bath}\to 0$, T_{dyn} coincides in fact with the configurational temperature, predicted by the Edwards hypothesis.

In Refs. [13,14] the inherent states are visited in another way by using a tap dynamics (i.e., a procedure similar to that used in the compaction of real granular materials), where each tap consists in raising the bath temperature to a value T_Γ and, after a lapse of time τ_0, quenching it back to zero. By cyclically repeating the process the system explores the space of the inherent states [13–20]. Once the stationary state is reached one can define a temperature, T_{fd}, via the equilibrium fluctuation-dissipation relation. One can then see that, if Edwards's assumption applies, T_{fd} coincides with the configurational temperature. This has been verified in fact for different finite-dimensional models [13–15]. It was also shown numerically that for low enough T_Γ one has that $T_{fd}=T_{conf}\simeq T_\Gamma$, confirming on lattice models for granular media the result of Ref. [3]. In fact when the duration of each single tap is infinite ($\tau_0\to\infty$), the tap coincides with the way to explore the inherent states implemented in molecular dynamics simulations for Lennard-Jones mixtures [1,3]. However, the method used in Ref. [3] only allows the calculation of T_{conf} when the configurational temperature is low, i.e., where all the different temperatures almost coincide. Many

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other studies confirming Edwards's approach have also been presented [16–18,21].

In this paper we give a comprehensive view of the results obtained in Refs. [13–15] by considering other models and giving more details. In particular we study here three schematic lattice models for glassy systems and granular media, i.e., a diluted spin glass, a monodisperse hard-sphere system under gravity and a hard-sphere binary mixture under gravity. In particular, in the diluted spin glass and in the monodisperse hard-sphere system under gravity, the asymptotic states reached by the system are found to be described only by the configurational temperature. Whereas in the hard-sphere binary mixture under gravity the asymptotic states are found to be described by two thermodynamic parameters [22], coinciding with the two configurational temperatures that characterize the distribution among the inherent states when the principle of maximum entropy is satisfied under the constraint that the energies of the two species are independently fixed. In Ref. [15] a description of the segregation observed in the binary system in terms of these two temperatures is also given.

In Secs. II A and II B, the frustrated lattice gas model and the results of its study with the tap dynamics are, respectively, presented. In Sec. II D, the same results are obtained at higher density where the system at small temperature reaches a quasistationary state in which one-time quantities decay as the logarithm of time. In Sec. II C Edwards's hypothesis is formulated using the principle of maximum entropy. The results obtained in the monodisperse hard-sphere system under gravity are shown in Sec. III. In Sec. IV the statistical mechanics approach is extended to the hard-sphere binary mixture under gravity, where two thermodynamic parameters are necessary to describe the asymptotic states reached by the system. Finally, in the Conclusions we draw a picture of the statistical mechanics approach to systems found in inherent states, as emerges from our extensive investigation.

II. THE FRUSTRATED LATTICE GAS MODEL

A. The model

Recently a lattice model has been introduced to describe glass formers [24–26] and, in the presence of gravity, granular materials [19,27,28]. The Hamiltonian of the model is

$$-H=J\sum_{\langle ij\rangle}(\epsilon_{ij}S_iS_j-1)n_in_j+\mu\sum_i n_i, \tag{1}$$

where the sum $\Sigma_{\langle ij\rangle}$ is over nearest neighbor sites, $S_i=\pm1$ are Ising spins, $n_i=0,1$ are occupation variables, μ is the particle chemical potential, and ϵ_{ij} are quenched and random variables, equal to ±1 with equal probability. This model reproduces the Ising spin glass in the limit $\mu\to\infty$ (i.e., when all sites are occupied, $n_i\equiv1$).

In the other limit, $J\to\infty$, the model describes a frustrated lattice gas with properties recalling those of a "frustrated" liquid. In fact the first term of Hamiltonian (1) implies that two nearest neighbor sites can be freely occupied only if their spin variables satisfy the interaction, that is, if $\epsilon_{ij}S_iS_j=1$, otherwise they feel a strong repulsion. To make the connection with a liquid, we note that the internal degree of freedom, S_i, may represent, for example, the internal orientation of a nonspherical particle. Two particles can be nearest neighbors only if the relative orientation is appropriate, otherwise they have to move apart. Since in a frustrated loop the spins cannot satisfy all interactions, in this model particle configurations in which a frustrated loop is fully occupied are not allowed. The frustrated loops in the model are the same as the spin glass model and correspond in the liquid to those loops that, due to geometrical hindrance, cannot be fully occupied by the particles. In three dimensions (3D) [26,29], the model has a maximum density $\rho_{\max}\simeq0.68$, and a transition at $\rho_c\simeq0.62$ where the nonlinear spin susceptibility diverges.

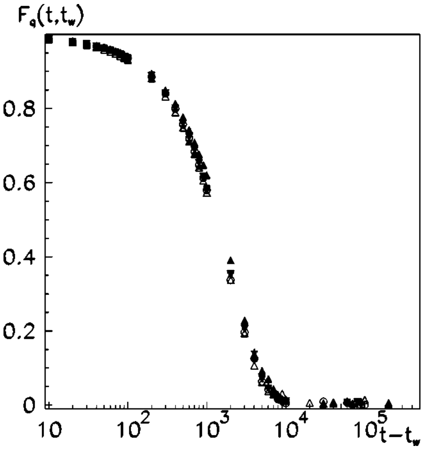

FIG. 1. The self-scattering two-time function $F_q(t,t_w)=\Sigma_i e^{\vec{q}\cdot[\vec{r}_i(t)-\vec{r}_i(t_w)]}/\rho L^3$, with $q=\pi/4$, as a function of $t-t_w$ (for $t_w=10^4$, 2×10^4, 5×10^4, 8×10^4, 10^5) in the frustrated lattice gas model for density $\rho=0.65$, during the tap dynamics, with tap amplitude $T_\Gamma=0.3$ J and tap duration $\tau_0=1$ MCS. The function $F_q(t,t_w)$ only depends on $t-t_w$, showing that the system has reached stationarity.

In the present paper, the 3D cubic frustrated lattice gas model with J finite is considered. The value of particle density, $\rho=\Sigma_i n_i/L^3$ (L is the lattice linear size), is fixed, and a Monte Carlo tap dynamics, which allows the system to explore its inherent states, is applied. During the dynamics, the system cyclically evolves for a time τ_0 (the tap duration [30]) at a finite value of the bath temperature, T_Γ (the tap amplitude), and afterwards it is suddenly frozen at zero temperature in one of its inherent states (at zero temperature the system does not evolve anymore if the energy cannot be decreased by one single-particle movement). After each tap, when the system is at rest, we record the quantities of interest. The time t considered is therefore discrete and coincides with the number of taps.

B. The results obtained under the tap dynamics

We first consider the case $\rho=0.65$ [31]. At this value of the density the system under the tap dynamics reaches a stationary state for each value of T_Γ (and τ_0) considered. In Figs. 1 and 2 [32], the self-scattering two-time function

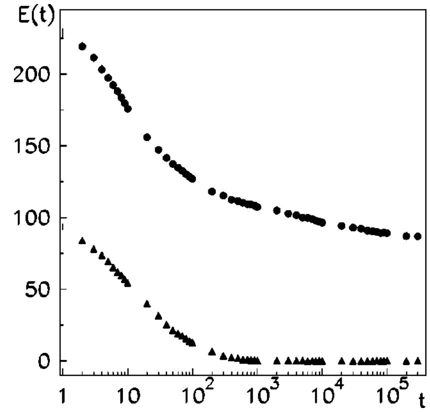

FIG. 2. Energy $E(t)$ of the inherent states as a function of the tap number t, in the frustrated lattice gas model during the tap dynamics with tap amplitude $T_\Gamma = 0.3$ J and tap duration $\tau_0 = 1$ MCS. The lower curve, corresponding to a density of particles $\rho = 0.65$, exponentially saturates to its asymptotic value, whereas the upper curve, corresponding to $\rho = 0.75$, shows a logarithmic relaxation at long times.

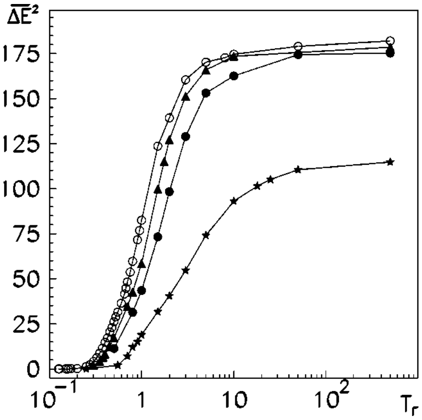

FIG. 4. The time average of energy fluctuations, $\overline{\Delta E^2}$, recorded in the stationary regime as a function of the tap amplitude, T_Γ (in units of J), in the frustrated lattice gas model for $\rho = 0.65$. The four different curves correspond to different values of the tap duration, $\tau_0 = 1,\ 5,\ 10,\ \infty$ MCS (from bottom to top). This shows again that T_Γ is not a right thermodynamic parameter.

$F_q(t,t_w) = \Sigma_i e^{\vec{q}\cdot[\vec{r}_i(t) - \vec{r}_i(t_w)]}/\rho L^3$ and the energy $E(t)$ of the inherent states, obtained for $T_\Gamma = 0.3$ J and $\tau_0 = 1$ MCS, are shown. The curves $F_q(t,t_w)$, for different t_w, collapse onto a single master function, when they are plotted as functions of $t - t_w$, and the energy $E(t)$ reaches its time independent asymptotic value, showing that the system has reached a stationary state (our data are averaged up to 32 noise realizations; $L = 8$ and $q = \pi/4$).

During the tap dynamics, in the stationary state, the time average of the energy $\overline{E}$, and its fluctuations $\overline{\Delta E^2}$ are calculated. In Figs. 3 and 4, $\overline{E}$ and $\overline{\Delta E^2}$ are shown as functions the tap amplitude T_Γ (for several values of the tap duration, τ_0). Apparently, T_Γ is not the right thermodynamic parameter, since sequences of taps, with same T_Γ and different τ_0, give different values of $\overline{E}$ and $\overline{\Delta E^2}$. On the other hand, if the stationary states are indeed characterized by a *single* thermodynamic parameter β_{fd}, the curves corresponding to different tap sequences (i.e., different T_Γ and τ_0) should collapse onto a single master function when $\overline{\Delta E^2}$ is parametrically plotted as function of $\overline{E}$. This data collapse is in fact found and shown in Fig. 5. This is a prediction that can be easily checked in real granular materials (where one can consider the density, which is easier to measure than the energy).

The thermodynamic parameter β_{fd} is defined apart from an integration constant β_0, through the usual equilibrium fluctuation-dissipation relation:

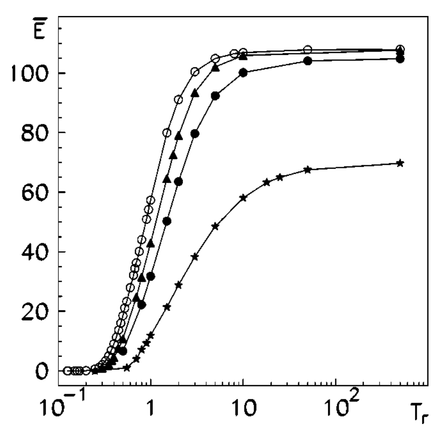

FIG. 3. The time average of the energy $\overline{E}$ recorded in the stationary regime as a function of the tap amplitude T_Γ (in units of J), in the frustrated lattice gas model for $\rho = 0.65$. The four different curves correspond to different values of the tap duration, $\tau_0 = 1,\ 5,\ 10,\ \infty$ MCS (from bottom to top). This shows that T_Γ is not a right thermodynamic parameter, since sequences of taps with different τ_0 give different values for the system observables.

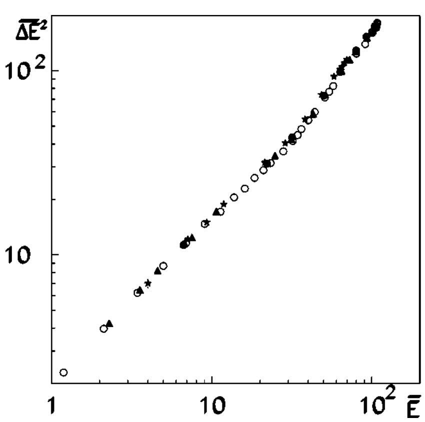

FIG. 5. The time averages of energy fluctuations, $\overline{\Delta E^2}$, when plotted as functions of the time average of energy, $\overline{E}$, collapse onto a single master function, for all the different values of tap amplitude and duration, T_Γ and τ_0, plotted in Fig. 3. This shows that the system stationary states are indeed characterized by a *single* thermodynamic parameter, since the curves corresponding to different tap sequences (i.e., different T_Γ and τ_0) collapse on a "universal" function, when $\overline{\Delta E^2}$ is parametrically plotted as a function of $\overline{E}$.

$$-\frac{\partial \overline{E}}{\partial \beta_{fd}} = \overline{\Delta E^2}. \tag{2}$$

By integrating Eq. (2), $\beta_{fd} - \beta_0$ can be expressed as a function of $\overline{E}$ or (for a fixed value of τ_0) of β_Γ: $\beta_{fd} - \beta_0 \equiv g(\beta_\Gamma)$. The constant β_0 is determined as explained in detail in the Appendix.

C. The Edwards averages

In Sec. II B we have found that the fluctuations of the energy in the stationary state depend only on the energy $\overline{E}$, and not on the past history. If all macroscopic quantities depend only on the energy $\overline{E}$, or on its conjugate thermodynamic parameter β_{fd}, the stationary state can be genuinely considered a "thermodynamic state." In this case one can attempt to construct an equilibrium statistical mechanics, as originally suggested by Edwards [7].

More precisely, one can try to find from basic general principles what is the probability distribution P_r of finding, in the stationary regime, the system in the inherent state r of energy E_r (see Ref. [13]). We assume that the distribution is given by the principle of maximum entropy, $S = -\Sigma_r P_r \ln P_r$, under the condition that the average energy is fixed: $E = \Sigma_r P_r E_r$. Thus, we have to maximize the following functional: $I[P_r] = -\Sigma_r P_r \ln P_r - \beta_{conf}(E - \Sigma_r P_r E_r)$. Here β_{conf} is a Lagrange multiplier determined by the constraint on the energy and takes the name of "inverse configurational temperature." This procedure leads to the Gibbs result:

$$P_r = \frac{e^{-\beta_{conf} E_r}}{Z}, \tag{3}$$

where $Z = \Sigma_r e^{-\beta_{conf} E_r}$. Using standard statistical mechanics, it is easy to show that, in the thermodynamic limit, the entropy S and β_{conf} are also given by

$$S = \ln \Omega(E), \quad \beta_{conf} = \frac{\partial \ln \Omega}{\partial E}, \tag{4}$$

where $\Omega(E)$ is the number of inherent states corresponding to energy E.

If the distribution in the stationary state coincides with Eq. (3), the time average of the energy, $\overline{E}(\beta_{fd})$, recorded during the taps sequences, must coincide with the ensemble average $\langle E \rangle(\beta_{conf})$ over the distribution Eq. (3). In order to check that we have independently calculated the average $\langle E \rangle$ as a function of β_{conf}, we have simulated the model Eq. (1) imposing that the only accessible states are the inherent states, as done in Ref. [11]. The only difference is that in the present paper the Edwards averages are done in the canonical ensemble, whereas in Ref. [11] these are done in the microcanonical ensemble. In particular we have constructed a Hamiltonian, $\mathcal{H}'(\{S_i, n_i\}) = \mathcal{H}(\{S_i, n_i\}) + \delta(\{S_i, n_i\})$, by adding a term to Eq. (1), $\delta(\{S_i, n_i\})$, which is zero, if the configuration is an inherent state, and infinite, otherwise. The canonical distribution for this Hamiltonian gives a weight $e^{-\beta_{conf}\mathcal{H}'}$, which coincides with the weight in the distribution of Eq. (3) for each accessible configuration. Using the standard Monte Carlo simulations, we have calculated $\langle E \rangle \times (\beta_{conf})$. Figure 6 outlines a very good agreement between $\langle E \rangle(\beta_{conf})$ and $\overline{E}(\beta_{fd})$ (notice that there are no adjustable parameters).

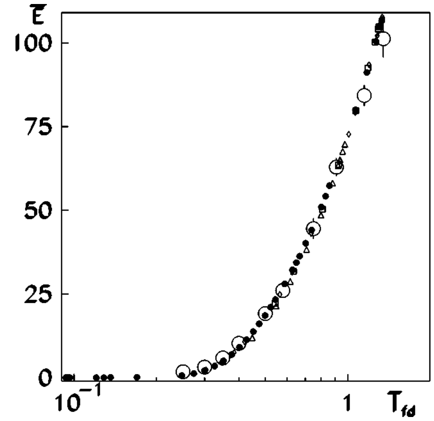

FIG. 6. The time average $\overline{E}$ calculated in the stationary regime of the tap dynamics and the ensemble average over the Edwards distribution Eq. (3), $\langle E \rangle$ (the black empty circles), are plotted, respectively, as functions of T_{fd} and T_{conf} (in units of J), in the frustrated lattice gas model, at $\rho = 0.65$. The two independently calculated sets of points show a very good agreement, outlining the success of Edwards's approach to describe the system macroscopic properties.

Note that the maximum energy reached by the system under the tap dynamics, $E_{max}(\tau_0) \equiv \overline{E}(T_\Gamma \to \infty, \tau_0)$, is less than the maximum energy of the inherent states, $\langle E \rangle(T_{conf} \to \infty)$, for every value of τ_0 considered. Such a prediction, which may have important practical consequences (e.g., in powder, technologies), is consistent with some experimental observations on tapped granular materials [33], where the system density was shown to approach asymptotically a plateau value apparently higher than the minimal possible packing density (obtained, for instance, by just pouring grains in the container) even for very large tap amplitudes.

Using Eq. (4), we have finally evaluated the configurational entropy as $S(E) - S_0 = \int_0^E \beta_{conf}(E') dE'$ (where the unknown non-negative constant $S_0 \equiv S(E=0)$ is the entropy at $T_{conf} = 0$). In Fig. 7, the configurational entropy $S - S_0$ is plotted as a function of T_{conf}. We have also evaluated the integral $S'(E) - S'_0 \equiv \int_0^E \beta_{fd}(E') dE'$. In Fig. 7, $S' - S'_0$ is plotted as a function of T_{fd} and it is compared with the configurational entropy. The agreement is again very good.

D. Quasistationary case

We have also studied the frustrated lattice gas model for $\rho = 0.75$. Differently from the previous case, for small enough values of the tap amplitude T_Γ, the system does not reach a stationary state during our observation time. In Fig. 2, the energy $E(t)$ of the inherent states obtained for $T_\Gamma = 0.3$ J and $\tau_0 = 1$ MCS is shown. $E(t)$ now changes in time and the system is not in a stationary state; however, $E(t)$ at long times decays very slowly [34]. In this regime the time

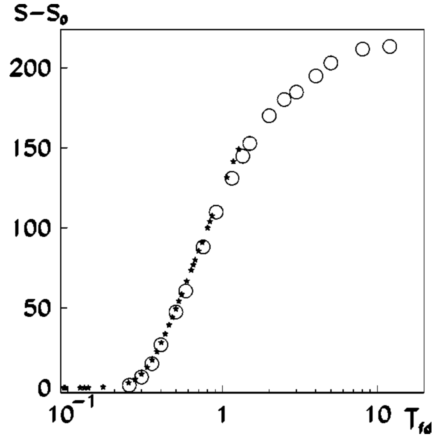

FIG. 7. The configurational entropy $S-S_0$ (the black empty circles in the figure) as a function of T_{conf} (in units of J), compared with $S'(E)-S'_0 \equiv \int_0^E \beta_{fd}(E')dE'$ plotted as a function of T_{fd} (in units of J), in the frustrated lattice gas model for $\rho = 0.65$. The unknown non-negative constant S_0 is the entropy at $T_{conf}=0$.

averages are computed over a time interval such that the energy is practically constant [in the case of Fig. 2, the time average is performed over the time interval $(3\times 10^5, 3\times 10^5+10^4)$]. Performing the same procedure described in the stationary case, a collapse of data is again found (see Fig. 8).

We have again evaluated the configurational entropy $S(E)-S_0 = \int_{E_{min}}^E \beta_{conf}(E')dE'$ [where the unknown non-negative constant $S_0 \equiv S(E_{min})$ is the entropy at $T_{conf}=0$ and E_{min} is the minimum value of energy obtained [35]). In Fig. 9, the configurational entropy $S-S_0$ is plotted as a function of T_{conf}. We have also evaluated the integral $S'(E) - S'_0 \equiv \int_0^E \beta_{fd}(E')dE'$. In Fig. 9, $S'-S'_0$ is plotted as a function of T_{fd} and it is compared with the configurational entropy. The agreement is again very good.

We cannot exclude that the agreement here found even for low energy may be due to the fact that the system, which is

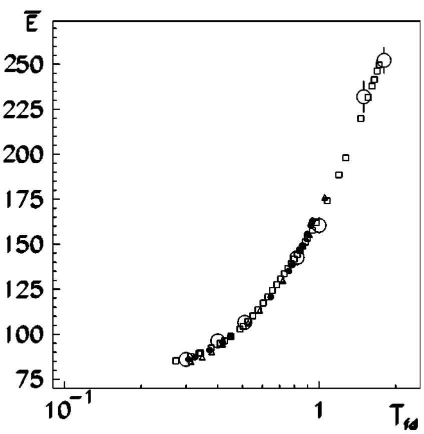

FIG. 8. The time average $\overline{E}$ and the ensemble average over the distribution Eq. (3), $\langle E\rangle$ (the black empty circles), plotted, respectively, as functions of T_{fd} and T_{conf} (in units of J), in the frustrated lattice gas model, at $\rho=0.75$. As well as at $\rho=0.65$, there is a very good agreement between the two independently calculated sets of points.

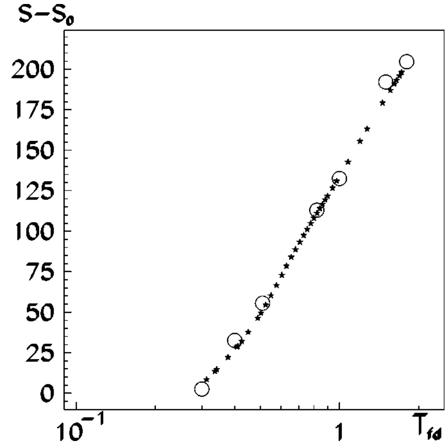

FIG. 9. The configurational entropy $S-S_0$ (the black empty circles in the figure) as a function of T_{conf} (in units of J), compared with $S'(E)-S'_0 \equiv \int_0^E \beta_{fd}(E')dE'$ plotted as a function of T_{fd} (in units of J), in the frustrated lattice gas model for $\rho=0.75$. The unknown non-negative constant S_0 is the entropy at $T_{conf}=0$.

not in a stationary state, is however very close to stationarity.

III. A MONODISPERSE HARD-SPHERE SYSTEM UNDER GRAVITY

As a model more appropriate for granular media, we have also studied a system of monodisperse hard sphere (with diameter $a_0=1$) under gravity, where the centers of mass of grains are constrained to move on the sites of a cubic lattice (see upper inset in Fig. 11). The Hamiltonian of the system is

$$\mathcal{H} = \mathcal{H}_{hc}(\{n_i\}) + gm\sum_i n_i z_i, \tag{5}$$

where the height of site i is z_i, $g=1$ is the gravity acceleration, $m=1$ is the grains mass, n_i is the usual occupancy variable, and $\mathcal{H}_{hc}(\{n_i\})$ is the hard-core term preventing the

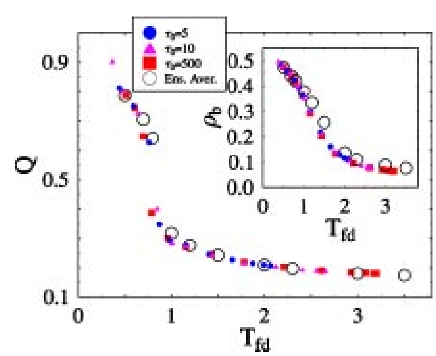

FIG. 10. The density self-overlap function Q and (upper inset) the system density on the bottom layer, ρ_b, plotted as functions of T_{fd} (in units mga_0), compared with the ensemble averages over the distribution Eq. (3) (the black empty circles), plotted as a function of T_{conf} (in units mga_0), in the 3D monodisperse hard-sphere system under gravity. Also, for this system, there is a very good agreement between the independently calculated time averages over the tap dynamics and the statistical mechanics ensemble averages in the manner of Edwards.

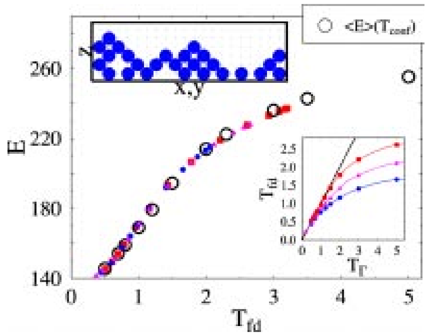

FIG. 11. Main frame: The time average $\overline{E}$ and the ensemble average over the distribution Eq. (3), $\langle E \rangle$ (the black empty circles), plotted, respectively, as functions of T_{fd} and T_{conf} (in units mga_0), in the 3D monodisperse hard-sphere system under gravity described in the text (and schematically depicted in the upper inset). Time averages over the tap dynamics and Edwards's ensemble averages then coincide. Lower inset: The temperature $T_{fd} \equiv \beta_{fd}^{-1}$ defined by Eq. (2) as a function of T_Γ (in units mga_0) for $\tau_0 = 500$, 10, 5 MCS (from top to bottom). The straight line is the function $T_{fd} = T_\Gamma$.

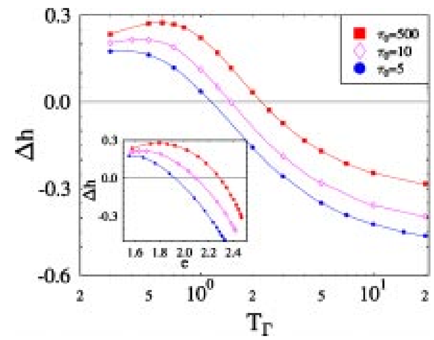

FIG. 12. Main frame: The difference of the average heights of small and large grains, $\Delta h = h_1 - h_2$, measured at stationarity in the binary hard-spheres mixture under gravity, is plotted as a function of tap amplitude T_Γ (in units mga_0). The three sets of points correspond to the shown tap durations τ_0. At high T_Γ larger grains are found above the smaller, i.e, $\Delta h < 0$, as in the Brazil nut effect (BNE). Below a $T_\Gamma^*(\tau_0)$ the opposite is found (reverse Brazil nut effect, RBNE). Inset: The Δh data of the main frame are plotted as a function of the corresponding average energy *e*. The three sets of data do not collapse onto a single master function, showing that a single macroscopic observable, such as *e*, does not characterize the system status.

overlapping of nearest neighbor grains [the analogy with Eq. (1) can be appreciated by writing down $\mathcal{H}_{hc}$: it can be written as $\mathcal{H}_{hc}(\{n_i\}) = J \Sigma_{\langle ij \rangle} n_i n_j$, where the limit $J \to \infty$ is taken].

We have considered a system of $N = 240$ particles, and performed a tap dynamics that allows the system to explore its inherent states. We have considered three different values of the tap duration, $\tau_0 = 500$, 10, 5 MCS. In this case, we again obtain that the asymptotic states reached by the system can be described by a single thermodynamic parameter β_{fd} evaluated by the integration of Eq. (2). We have moreover calculated the system density on the bottom layer, ρ_b, and the density self-overlap function Q, and verified that, when plotted as a function of β_{fd}, they scale on a single master function (see Fig. 10).

As described in Sec. II C, we have calculated the Edwards averages as functions of β_{conf}. As we can see in Fig. 11, we obtain a very good agreement between $\langle E \rangle(\beta_{conf})$ and $\overline{E}(\beta_{fd})$. The same agreement is found for the other quoted observables, ρ_b and Q (see Fig. 10).

IV. A HARD-SPHERE BINARY MIXTURE UNDER GRAVITY

Finally we consider a hard-sphere binary system made of two species 1 (small) and 2 (large) with grain diameters a_0 and $\sqrt{2}a_0$, under gravity on a cubic lattice of spacing $a_0 = 1$. We set the units such that the two kinds of grains have masses $m_1 = 1$ and $m_2 = 2$, and the gravity acceleration is $g = 1$. The hard-core potential $\mathcal{H}_{hc}$ is such that two large nearest neighbor particles cannot overlap. This implies that only couples of small particles can be nearest neighbors on the lattice. The overall system Hamiltonian is

$$\mathcal{H} = \mathcal{H}_{hc} + m_1 g H_1 + m_2 g H_2, \tag{6}$$

where $H_1 = \Sigma_i^{(1)} z_i$ and $H_2 = \Sigma_i^{(2)} z_i$, the height of site i is z_i and the two sums are over all particles of species 1 and 2, respectively. In the above units, the gravitational energies in a given configuration are thus $E_1 = H_1$ and $E_2 = 2H_2$.

Grains are confined to a box of linear size L between hard walls and periodic boundary conditions in the horizontal directions. $N_1 = 120$ grains of type 1 and $N_2 = 40$ grains of type 2 are initially prepared in a random loose stable pack. Under the tap dynamics, the system approaches a stationary state for each value of the tap parameters T_Γ and τ_0. In Fig.12, we plot as a function of T_Γ (for several values of τ_0) the asymptotic value of the *vertical* segregation parameter, i.e., the difference of the average heights of the small and large grains at stationarity, $\Delta h(T_\Gamma, \tau_0) \equiv h_1 - h_2$. Here h_1 and h_2 are the averages of H_1/N_1 and H_2/N_2 over the tap dynamics in the stationary state. (An interpretation, in terms of the approach here presented, of the size segregation phenomenon here found and experimentally observed in a hard-spheres binary mixture under gravity is given in Ref. [15]).

The results given in the main panel of Fig. 12 apparently show that T_Γ is not a right thermodynamic parameter, since sequences of taps with different τ_0 give different values for the system observables. However, if the stationary states corresponding to different tap dynamics (i.e., different T_Γ and τ_0) are indeed characterized by a single thermodynamic parameter, the curves of Fig. 12 should collapse onto a universal master function when $\Delta h(T_\Gamma, \tau_0)$ is parametrically plotted as a function of another macroscopic observable such as the average energy, $e(T_\Gamma, \tau_0) = (E_1 + E_2)/N$ (N is the total number of particles). This collapse of data is clearly not observed here, as is apparent in the inset of Fig. 12. We show, instead, that two macroscopic quantities may be sufficient to characterize uniquely the stationary state of the system. These two quantities are, for instance, the energy *e* and the height difference Δh. Of course, since $e = ah_1 + 2bh_2$

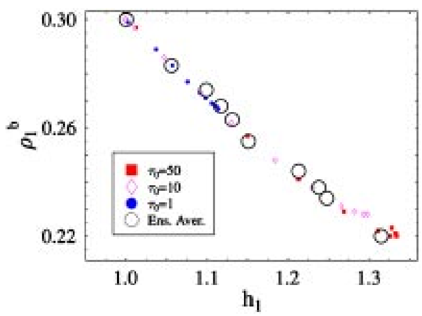

FIG. 13. The average density of small grains on the box bottom layer, ρ_1^b, measured at stationarity as a function of the height of small particles, h_1, in the binary hard-spheres mixture under gravity. Data corresponding to different T_Γ and τ_0 approximately scale on a single master function. The empty circles are the corresponding values obtained by ensemble average with the two temperatures Gibbs measure proposed in the text.

(where $a=N_1/N$ and $b=N_2/N$) and $\Delta h=h_1-h_2$, we can also choose h_1 and h_2 to characterize the stationary state. Namely, we show that any macroscopic quantity A, averaged over the tap dynamics in the stationary state, is only dependent on h_1 and h_2, i.e., $A=A(h_1,h_2)$. We have checked that this is the case for several independent observables, such as the number of contacts between large particles, N_c, the density of small and large particles on the bottom layer, ρ_1^b and ρ_2^b, and others. In particular, as shown in Figs. 13 and 14, we find with good approximation that $N_c \simeq N_c(e)=N_c(ah_1+bh_2)$, $\rho_2^b \simeq \rho_2^b(h_2)$, $\rho_1^b \simeq \rho_1^b(h_1)$. Therefore we need both h_1 and h_2 to characterize unambiguously the state of the system; namely, all the observables assume the same values in a stationary state characterized by the same values of h_1 and h_2, independently on the previous history (i.e., in our case independently on the particular tapping parameters T_Γ and τ_0).

We again find that the stationary state can be genuinely considered as a thermodynamic state. Therefore we can ask what is the probability distribution P_r of finding the system in the inherent state r corresponding to an energy E_{1r} for the small particles and E_{2r} for the large particles. We again assume that the microscopic distribution is given by the principle of maximum entropy $S=-\Sigma_r P_r \ln P_r$, now under the condition that the average energy $E_1=\Sigma_r P_r E_{1r}$ and $E_2=\Sigma_r P_r E_{2r}$ are independently fixed. This can be done by introducing two Lagrange multipliers β_1 and β_2, which are determined by the constraint on E_1 and E_2, and can be, respectively, considered as the "inverse configurational temperature" of species 1 and 2. This procedure leads to the Gibbs result,

$$P_r=\frac{e^{-\beta_1 E_{1r}-\beta_2 E_{2r}}}{Z}, \tag{7}$$

where $Z=\Sigma_r \exp(-\beta_1 E_{1r}-\beta_2 E_{2r})$ and, in the thermodynamic limit, the entropy S is given by

$$S=\ln \Omega(E_1,E_2), \tag{8}$$

and β_1 and β_2:

$$\beta_1=\frac{\partial \ln \Omega(E_1,E_2)}{\partial E_1}, \quad \beta_2=\frac{\partial \ln \Omega(E_1,E_2)}{\partial E_2}. \tag{9}$$

Here $\Omega(E_1,E_2)$ is the number of inherent states corresponding to energy E_1 and E_2. The hypothesis that the ensemble distribution at stationarity is given by Eq. (7) can be tested as follows. We have to check that the time average of any quantity $A(h_1,h_2)$, as recorded during the taps sequences in a stationary state characterized by given values h_1 and h_2, must coincide with the ensemble average $\langle A\rangle(h_1,h_2)$ over the distribution Eq. (7). To this aim, we have calculated the ensemble averages $\langle N_c\rangle$, $\langle \rho_2^b\rangle$, $\langle \rho_1^b\rangle$ for different values of β_1 and β_2; we have expressed parametrically $\langle N_c\rangle$, $\langle \rho_2^b\rangle$, $\langle \rho_1^b\rangle$ as functions of the average of h_1 and h_2, and compared them with the corresponding quantities N_c, ρ_1^b, and ρ_2^b averaged over the tap dynamics. The two sets of data are plotted in Figs. 13 and 14 showing a good agreement (notice, there are no adjustable parameters). In order to calculate the ensemble averages we simulate the model with $\mathcal{H}$ from Eq. (6) where we impose the constraint that the only accessible states are the inherent states, as already described in Sec. II C.

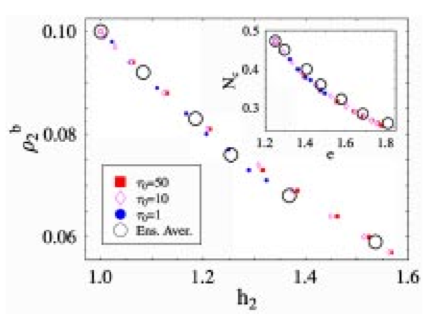

FIG. 14. Main frame: The average density of large grains on the box bottom layer, ρ_2^b, obtained for different T_Γ and τ_0, scale almost on a single master function when plotted as a function of the large grains height, h_2. Upper inset: The average number of contacts between large grains per particle, N_c, obtained for different T_Γ and τ_0, scale on a single master function when plotted as a function of the system energy e.

V. CONCLUSIONS

In conclusion, in the context of models for glasses and granular materials, we have shown that the stationary (or quasi-stationary) state reached by the system subject to a tap dynamics among its inherent states is genuinely a thermodynamic state, which can be well described by Edwards's assumption of a uniform measure, i.e., a probability distribution obtained assuming the validity of the principle of maximum entropy. In particular in the frustrated lattice gas model and in the system of monodisperse hard-spheres under gravity, we have found that the observables recorded during different tap sequences (different amplitude and duration of taps) fall on universal master curves when plotted as a function of a single thermodynamic parameter. These curves turn

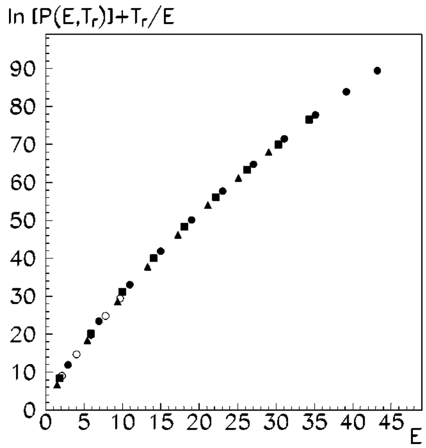

FIG. 15. The curves $\ln[P(E,T_\Gamma)]+E/T_\Gamma$ (apart from a T_Γ-dependent constant) as functions of the energy E in the frustrated lattice gas model for $\rho=0.65$ and $T_\Gamma=0.275$, 0.425, 0.475, 0.525 J.

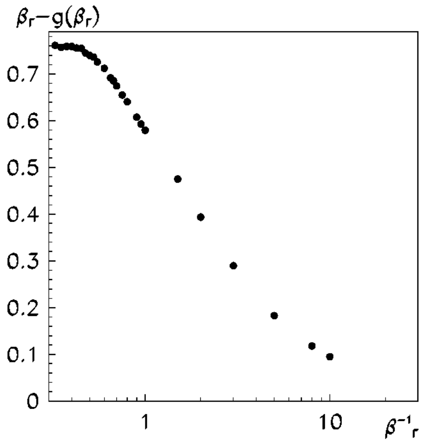

FIG. 16. The curve $\beta_\Gamma-g(\beta_\Gamma)=\beta_\Gamma-[\beta_{fd}(\beta_\Gamma)-\beta_0]$ as a function of β_Γ^{-1} (in units of J) in the frustrated lattice gas model for $\rho=0.65$. The limit $\beta_\Gamma^{-1}\to 0$ of $\beta_\Gamma-g(\beta_\Gamma)$ gives the integration constant β_0.

out to coincide with those predicted, within the described statistical mechanics approach, by the generalized Gibbs distribution of Eq. (3). On the other hand, the results obtained in a system under gravity made of particles of two different sizes show that a single thermodynamic parameter is not enough to describe the macrostates, and two configurational temperatures are instead necessary. In general, for a more complex system one might expect more constraints to be imposed, leading to more than two thermodynamical parameters [15,18,23]. In practice, the criteria to determine *a priori* the required parameters cannot be easily accessible. However, more recently we have extended data regarding the hard-sphere binary mixture for very low energy [36] and found that only one thermodynamical parameter is necessary to describe the stationary state. This seems to be a general feature [14]. If this is the case, a statistical mechanics approach with only one thermodynamical variable may be feasible for low energy.

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APPENDIX: DETERMINATION OF THE INTEGRATION CONSTANT β_0

Adapting to lattice models the procedure of Sciortino *et al.* [3], we have evaluated β_{fd} at small values of T_Γ, for $\tau_0\to\infty$, and consequently the integration constant β_0.

Given an inherent state r of energy E_r we define the basin of attraction, B_r, of such state r as the set of states in the configurational space, which after the quench at $T=0$ are frozen in the inherent state r. Therefore the probability distribution P_r of finding the system in the inherent state r after quenching the system from an equilibrium state at temperature T_Γ, can be written as

$$P_r=\frac{\sum_{r'} e^{-E_{rr'}/T_\Gamma}}{Z_G(T_\Gamma)}, \tag{A1}$$

where $Z_G(T_\Gamma)$ is the partition function of the system in equilibrium at temperature T_Γ and $\Sigma_{r'}$ is the sum over all the states r' belonging to the basin B_r of energy $E_{rr'}$. By putting $E_{rr'}=E_r+\Delta_{rr'}$, the distribution (A1) can be written as

$$P_r=\frac{e^{-(E_r+g_r(T_\Gamma))/T_\Gamma}}{Z_G(T_\Gamma)}, \tag{A2}$$

where $e^{-g_r(T_\Gamma)/T_\Gamma}=\Sigma_{r'}e^{-\Delta_{rr'}/T_\Gamma}$. From Eq. (A2) it follows that the probability of finding the system in any inherent state of energy E, $P(E,T_\Gamma)=\Sigma_r P_r$ (where Σ_r is the sum over all the inherent states r of energy E), is given by

$$P(E,T_\Gamma)=\frac{\Omega(E)e^{-E/T_\Gamma}e^{-f(T_\Gamma,E)/T_\Gamma}}{Z_G(T_\Gamma)}, \tag{A3}$$

where $\Omega(E)$ is the number of inherent states of energy E and

$$e^{-f(T_\Gamma,E)/T_\Gamma}=\frac{\sum_r e^{-g_r(T_\Gamma)/T_\Gamma}}{\Omega(E)}.$$

From Eq. (A3),

$$\ln[P(E,T_\Gamma)]+\frac{E}{T_\Gamma}=-\frac{f(T_\Gamma,E)}{T_\Gamma}+\ln[\Omega(E)]-\ln[Z_G(T_\Gamma)]. \tag{A4}$$

The probability distribution of finding the system in any inherent state of energy E, $P(E,T_\Gamma)$, is measured during the tap dynamics with amplitude $\tau_0 \to \infty$. If $f(T_\Gamma, E)$ has only a weak dependence on E, then it is possible to superimpose the curves, $\ln[P(E,T_\Gamma)]+E/T_\Gamma$, at different T_Γ which overlap in E by adding a T_Γ-dependent constant. This result is obtained for $T_\Gamma \leqslant 0.525$, as shown in Fig. 15, and suggests that in this interval $f(T_\Gamma, E) \simeq f(T_\Gamma)$. If this is the case, from Eq. (A3) it follows

$$P(E,T_\Gamma) \simeq \frac{\Omega(E) e^{-E/T_\Gamma}}{Z(T_\Gamma)}, \tag{A5}$$

where

$$Z(T_\Gamma) = e^{f(T_\Gamma)/T_\Gamma} Z_G(T_\Gamma) = \sum_E \Omega(E) e^{-E/T_\Gamma}. \tag{A6}$$

The last equality stems from the normalization condition on $P(E,T_\Gamma)$.

From Eq. (A5) it follows that at small T_Γ, $\beta_\Gamma \equiv T_\Gamma^{-1}$ satisfies Eq. (2). Therefore at small T_Γ, β_{fd} and β_Γ coincide. The constant β_0 is consequently obtained as the limit, for $T_\Gamma \to 0$, of the function $\beta_\Gamma - g(\beta_\Gamma)$ (see Fig. 16).

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Eq. (1), at $\rho=0.65$, and we have performed an usual Monte Carlo diffusive dynamics of the model. At a starting time, we prepared the system in equilibrium with a very high bath temperature. Afterwards, it is suddenly cooled at a very low T_{bath}, but the system quickly reaches the equilibrium state, and T_{dyn} coincides with T_{bath}.

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