



Replica mean field theory for granular media

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Abstract

An infinite range spin-glass-like model for granular systems is introduced and studied through the replica mean field formalism. Equilibrium properties under vibration and gravity are obtained, as well as the phase diagram showing the dependence on gravity, density and vibration. © 1998 Elsevier Science B.V. All rights reserved.

Besides industrial applications, the unusual static and flow properties of granular materials [1,2] offer a challenging problem from the theoretical point of view, and despite the enormous effort that has been devoted in recent years, they are far from being fully understood. At a fixed macroscopic density, a granular system may be in a large number of different microscopic states, that has lead to the introduction of a statistical mechanics description of powders [3,4], replacing the energy by the volume and the temperature by the compactivity. On the other hand, in analogy with the thermal motion in liquids and gases, a granular temperature has also been introduced, which depends on the motions of the particles, in contrast with the compactivity that characterizes a static system.

These systems, composed of many discrete macroscopic particles, present slow relaxations under perturbations (vibrations) that resemble the ones found in frustrated systems like glasses and spin glasses. The analogy among them has been suggested some time ago [1,2] and stressed recently along with the role of geometric frustration [5]. For glass-forming liquids, a simple lattice model has been introduced [6,7] that explicitly takes into account these effects and as the Ising model makes the connection between simple fluids and magnets, this model bridges complex fluids (glasses) and complex magnets (spin glasses). An infinite range version [8,9] has also been studied in the framework of replica theory, yielding a very rich phase diagram. In order to apply this model for granular systems, Nicodemi et al. [10,11] introduced the effects

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of gravity and studied this simple frustrated Ising lattice gas (FILG) in 2D following a diffusion-like Monte-Carlo dynamics while applying a sequence of taps. Among several interesting properties, the system displays a logarithmic relaxation behaviour, also found in real experiments, as well as a localization transition, signalled by a zero diffusion constant, in which the particles get trapped in local cages. This transition point seems to correspond to the Reynolds (or dilatancy) transition observed in real systems.

Here we introduce a variant of this model [12] considering L layers of N sites, each site in the ℓ th layer being connected with all sites in the $\ell - 1$ and $\ell + 1$ layers, but not with sites in the same layer. Each site may be occupied by a particle ($n_i = 0, 1$) having an internal degree of freedom ($S_i = \pm 1$) that feels the steric effects set as quenched, gaussian distributed lattice bonds with $\overline{J_{ij}} = 0$ and $\overline{J_{ij}^2} = J/N$. Also, each layer has its own chemical potential satisfying $\mu_{\ell+1} > \mu_\ell$ (counting from top to bottom) that accounts for the effect of gravity and $\mu_\ell = g\ell$ in order to have a constant force. Thus, we consider the following Hamiltonian:

$$\mathcal{H} = - \sum_{i < j} \sum_{\ell=1}^{L-1} (J_{ij}^\ell S_i^\ell S_j^{\ell+1} + K/N) n_i^\ell n_j^{\ell+1} - \sum_{\ell=1}^{L-1} \mu_\ell \sum_i n_i^\ell. \quad (1)$$

The parameter K may tune the repulsive/attractive interaction between particles [8,9] but here we do not consider those effects ($K = -1$) [6–9].

In evaluating the free energy, only states with a given density ρ are taken into account. Assuming replica symmetry ($J = 1$):

$$\begin{aligned} f = & \frac{\beta}{4} \sum_\ell q_\ell q_{\ell+1} - \frac{1}{2} \left(\frac{\beta}{2} - 1 \right) \sum_\ell d_\ell d_{\ell+1} - \sum_\ell (\mu_0 + \mu_\ell) d_\ell - \frac{\beta}{2} \sum_\ell r_\ell q_\ell \\ & + \beta \sum_\ell t_\ell d_\ell - \frac{L}{\beta} \ln 2 + \mu_0 \rho L - \frac{1}{\beta} \sum_\ell \int \mathcal{D}z \ln \{ 1 + \cosh(\beta \sqrt{r_\ell z}) e^{-\Xi_\ell} \}. \end{aligned} \quad (2)$$

The order parameters are $q_{ab}^\ell = \langle S^{a\ell} n^{a\ell} S^{b\ell} n^{b\ell} \rangle$ and $d_a^\ell = \langle n^{a\ell} \rangle$ while μ_0 accounts for the constraint $\rho = L^{-1} \sum_\ell d_\ell$ and

$$\Xi_\ell = \frac{\beta^2}{4} (q_{\ell+1} + q_{\ell-1}) - \frac{\beta}{2} \left(\frac{\beta}{2} - 1 \right) (d_{\ell+1} + d_{\ell-1}) - \beta (\mu_\ell + \mu_0). \quad (3)$$

There is a critical temperature where all q_ℓ go to zero. When $g = 0$ (no gravity), $d_\ell = \rho$ ($\forall \ell$) and $T_c = \rho T_c^{SK}$ where T_c^{SK} is the critical temperature of the L -layered SK model [12]. On the other limit, when $g \rightarrow \infty$ (strong gravity), in analogy with the layered SK model, the critical temperature is related to the smallest positive root x^* of a given polynomial, $T_c = 1/\sqrt{2x^*}$, depending on the density ρ . For $0 \leq \rho \leq 1/L$, we have $T_c = 0$ because all particles occupy the lowest layer and do not interact. For $1/L \leq \rho \leq 2/L$, some sites occupy the second lowest layer and the critical temperature is obtained with the root of $P_2(x)$. In general, for $(n-1)/L \leq \rho \leq n/L$, the relevant

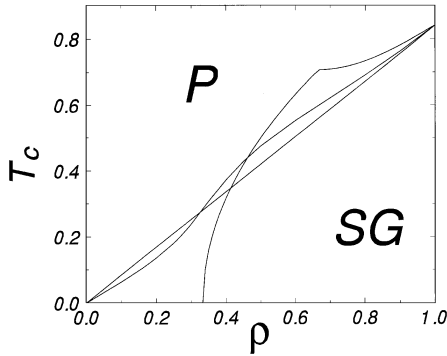


Fig. 1. Phase diagram T versus ρ for $L=3$ and $g=0$ (straight line), 1 and ∞ , showing the disordered phase (P , $q_\ell = 0, \forall \ell$) and a spin-glass-like phase (SG , $q_\ell \neq 0$).

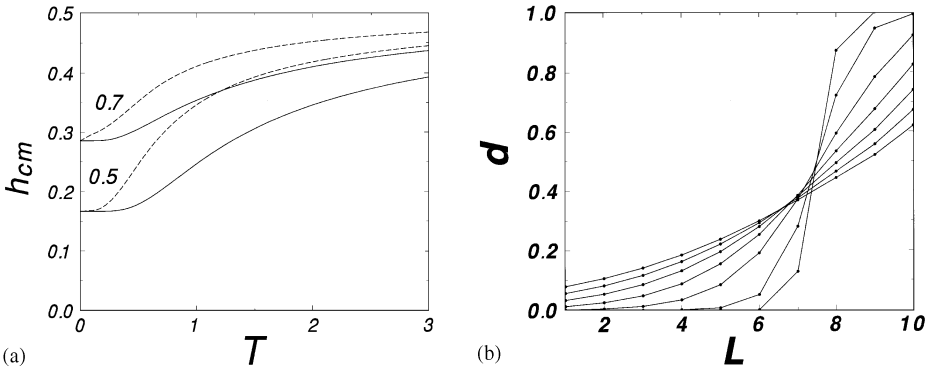


Fig. 2. (a) Height lifting as a function of temperature for $L=3$, $g=1$ (dashed) and $g=2$ (solid) for $\rho=0.5$ and 0.7 . (b) The density profile for $L=10$, $g=1$ and $\rho=0.3$ for several values of temperature: 0.1, 0.5, 1, 1.5, 2, 2.5 and 3.

polynomial is $P_n(x)$. These polynomials are obtained recursively by

$$P_\ell(x) = \frac{P_{\ell-1}(x)}{\delta_{\ell L}(\rho L - L + 1)^2 + (1 - \delta_{\ell L})} - x^2 P_{\ell-2}(x), \tag{4}$$

with $P_0(x) = P_1(x) = 1$. As $L \rightarrow \infty$, $T_c \rightarrow 1$ for all densities. Fig. 1, for $L=3$, shows the critical temperature for both extreme cases, $g=0$ and $g \rightarrow \infty$ and for an intermediate one, $g=1$.

As the granular temperature increases, there is an elevation of the center of mass of the system [13], given by $h'_{CM} = (\rho L)^{-1} \sum_\ell \ell d_\ell$ and this is a function of both temperature and gravity. We further rescale it to have a function in the interval (0 being the bottom) by $h_{CM} = (L - h'_{CM}) / (L - 1)$. Fig. 2a illustrates the height lifting for $L=3$. The density profile, that is, the density as a function of the system height, has been measured both in real experiments [14] as well as in simulations. Experimentally, as the steady state is achieved, independently of the up and down motion

of the heap, the density profile is always preserved. In Fig. 2b this profile is shown for ten layers under $g=1$ and filled up to $\rho=0.3$. Notice that the curves get steeper as the vibration diminishes. It is important to stress that, in analogy with the FILG [8,9], there are two regimes of densities: one is the L-layered SK regime where the particles settle in the lowest possible layers disregarding the geometric effects and the most interesting regime where the steric effects become important and even at $T=0$ there are still vacant sites.

In conclusion, we introduced an infinite range version of a frustrated lattice gas model [5,10,11] for granular systems and applied, for the first time, the replica formalism to these systems. In this mean field version, we are able to study stationary properties, obtaining the vibration, density and gravity-dependent phase diagram as well as information on quantities like the density profile and height lifting.

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