ENERGY SPECTRUM OF FRUSTRATED GRANULAR MATERIALS

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Abstract. We study the statistical properties of low lying energy states for some special models of two dimensional frustrated granular materials.

1. Introduction

Granular media has attracted much attention. There is much current interest in developing a better understanding of behaviour of systems such as powder and sands, and model systems of metal and glass beads. Granular materials are characterized by variety of different properties [1,2], which in many cases play important roles in industrial applications [3]. To this aim attempts have recently been made to introduce concepts from statistical mechanics, and profound relations with the physics of frustrated and disordered models as spin glasses have been outlined [4,5]. As in spin glasses, granular media also experience the effects of frustration, which is due to quenched disorder in the interactions between the spins, which leads to the existence of subtle correlations [6]. Frustration in granular media, often refered to as "geometric" frustration is generated by the strict constraints imposed by the hard core repulsion of neighbouring grains and the subsequent interlocking which leads to non-local cooperative macroscopic rearrangements and to many possible different packing configurations [2,7,8].
Geometrical frustration [6] is physically originated in granular systems by the actual shapes and arrangements of particles which give rise to multitude of possible microscopic states for fixed macroscopic parameters.

2. The model

The model we study here arose on the basis of Ising model invented to describe phase transitions magnetism. In the model each site can be either occupied or empty. Only nearest neighbours sites interact.
The discrete model system [6,9-11] consists of particles on square lattice tilted by 45°. The two different kinds of bonds represent wavy and straight line, which are characterized by quenched random numbers $\varepsilon_{ij} = \pm 1$ (Fig. 1).

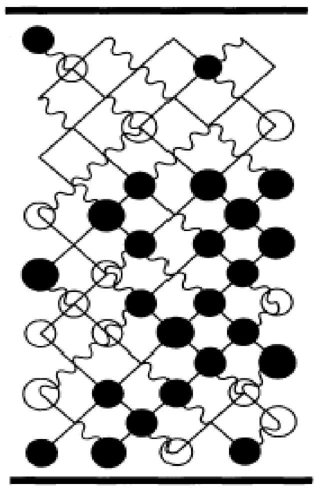

Fig. 1. Schematic picture of the lattice model considered here [6]

Filled (empty) circles are present particles with spin $S_i = +1$ $(S_i = -1)$. As in a lattice gas, an occupancy variable n_i is associated to each vertex i: if a particle is present on i then $n_i = 1$ else $n_i = 0$. The particles which cannot overlap, carry an internal degree of freedom $S_i = \pm 1$ and must satisfy the "geometrical" condition that whenever two (*i* and *j*) are neighbouring, their "spin" has to verify the relation

$$\varepsilon_{ij} S_i S_j = 1 \tag{1}$$

i.e they have to fit the local geometry of the packing. When the density of particles is high enough they can feel the frustration that has been imposed by the choice of the quenched ε_{ij}. As a consequence, in resemblance to frustrated percolation [12], particles can never close a frustrated loop in the lattice leaving always some empty sites.

The model introduced is suited to be described in a standard Hamiltonian formalism, based on following definition:

$$E = -I \sum_{\langle ij \rangle} \left(\varepsilon_{ij} S_i S_j - 1 \right) n_i n_j \tag{2}$$

where $S_i = \pm 1$ are spin variables, $n_i = 0,1$ occupancy variables and $\varepsilon_{ij} = \pm 1$ quenched interactions associated to the bonds of the lattice. This model is based on spin glasses. A crucial concept in spin glasses is frustration. A loop is frustrated when the spins cannot satisfy all pairs of interactions along the loop. It easy to verify that a loop is frustrated if and only if the product of the signs of the interactions ε_{ij} along the loop equals –1.

3. Numerical calculation

Simulations of the model with a low density (only a half nodes are filled by two kinds of particles, the same amount, the rest nodes are empty) described above are performed on the square and triangular lattices without and with periodic boundary conditions. It was studied a lot of lattices, in which changed amount of nodes from 25 to 5000 and boundary conditions. Figure 2 show diagrams distribution of minimum energy. It is seen that distribution of minimum energy is depended on geometrical structures and boundary conditions.

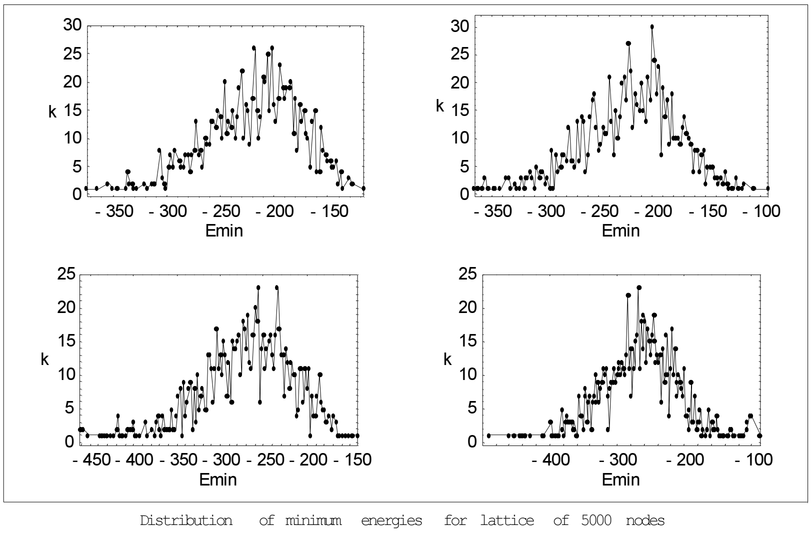

Fig. 2. Distribution of minimum energy the lattice is consisted of 5000 nodes where Emin-minimum energy of the lattice, k - amount of minimum energy Emin: a) square lattice without periodic boundary conditions, b) square lattice with periodic boundary conditions, c) triangular lattice without periodic boundary conditions, d) triangular lattice with periodic boundary conditions

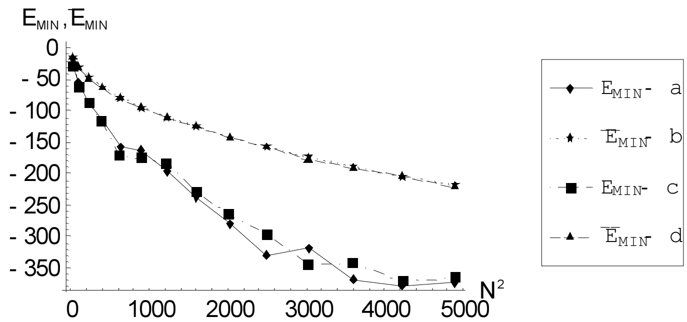

Fig. 3. Energy and mean value of energy depending on size of square lattice: a),b) without periodic boundary conditions, c),d) with periodic boundary conditions

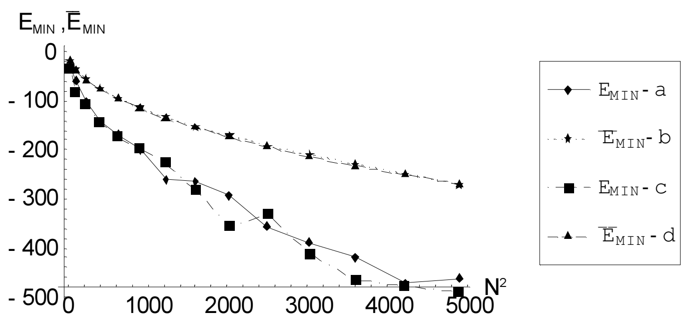

Fig. 4. Energy and mean value of energy depending on size of triangular lattice: a),b) without periodic boundary conditions, c),d) with periodic boundary conditions

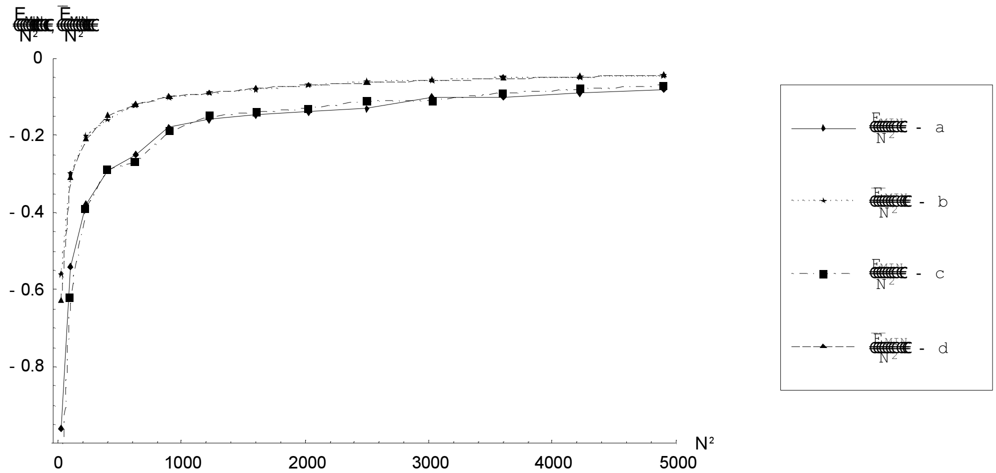

Fig. 5. Minimum energy of the lattice per amount of nodes: a),b) the square lattice without periodic boundary conditions, c),d) the square lattice with periodic boundary conditions

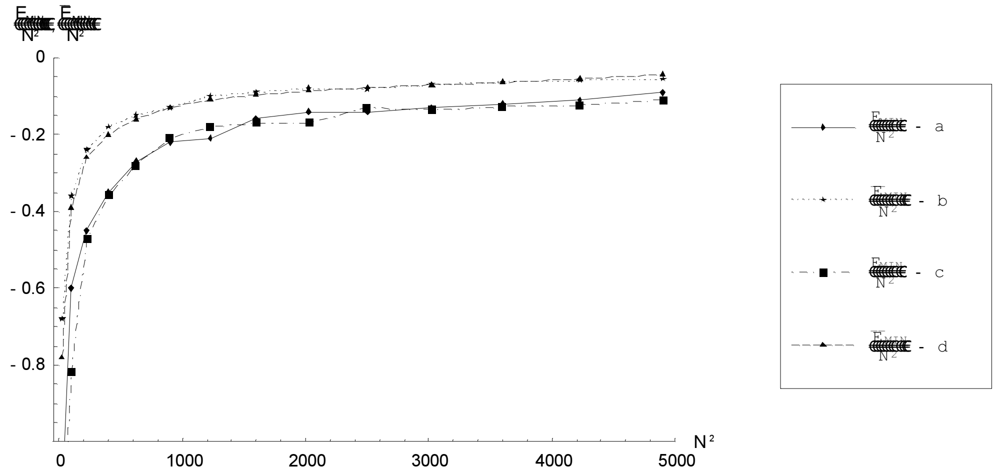

Fig. 6. Minimum energy of the lattice per amount of nodes: a),b) the triangular lattice without periodic boundary conditions, c),d) the triangular lattice with periodic boundary conditions

Conclusions

In this paper we have analysed the influence of a quenched disorder given by a random quenched strength of site - site interaction on the low lying energy states. We have computed the lowest energy levels for the lattices with triangular and square symmetries with and without the boundary conditions.

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