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MEAN-FIELD ENERGY OF ELEMENTARY GRAIN ARRANGEMENTS IN WET GRANULAR ENSEMBLES

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Abstract. The energy of elementary grain arrangements in wet granular system is analyzed within the Mean Field Approximation. For an ensemble of vibrating grain it is calculated how the mean free energy of a grain depends on its surface curvature and porosity.

Introduction

Granular materials have a lot of unusual physical properties particulary under the influence of humidity. It is known that many mechanical properties of a granulate change if some liquid is added [1, 2]. For example, even small amount of interstitial liquid adds an attractive force to the system and then, increase its stability. It is calculated that amount of wetting liquid in granular systems has an influence on capillary energy. In this article it is determined the relation between free energy and the curvature and porosity of grain surface and supplied the energy gain by the system due to vibration process.

To energy of elementary grain arrangements is analysed in the framework of so-called Mean-Field Approximation (MFA) which is a kind of approximation frequently applied to many-body systems with interactions. The main idea of MFA is to replace all interactions to any one body with an average or effective interaction of the system which is interacted each particle.

1. Formulation of the problem

Within the MFA approach to energy of granular ensemble fluctuations of physical quantities are neglected with regard to location of a system node. In case of non-spherical grains it is examined how surface shape and its porosity of a grain affect an energy of capillary adhesion. Results of MFA analysis are very interesting because they allow ones to search relationship between the vibration of grains and capilary adhesion. In detail it is looked into a case of grains on the square lattice. According to the discussion in [3, 4] it has been assumed that a grain, which is

located in a lattice point, is allowed to take of two possible orientations. For simplicity it is possible mutual arrangements of grains are labelled as:

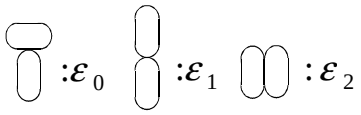


Fig. 1 Three possible energetically different arrangements of non-spherical grains in granular system.

Capillary bonds in configurations presented in Figure 1 correspond to energies: $\varepsilon_2 = \varepsilon_0 + \Delta$ and $\varepsilon_1 = \varepsilon_0 + \delta$, where quantities δ, Δ characterize the energy level spacing. As a level of energy reference it is established the quantity: $E_0 = 2\varepsilon_0 + \varepsilon_2 + \varepsilon_1 = 4\varepsilon_0 + \delta + \Delta$. Using symmetry operations, from a set of 32 possible arrangements of 5 grains on the square lattice, it is received a set of 9 different elementary configurations which transform into themselves at change of orientations of single grains. These configurations are presented in Table 1 where each configurations is graphically presented with corresponding energy and statistical weight factors of Gibbs distribution.

There are three triplet energy levels which correspond to grain assemblage which: $\{E_1, E_2, E_4\}$, $\{E_3, E_5, E_8\}$, $\{E_6, E_7, E_9\}$. Using quantities E_0, Δ and δ these energies take the following formulas:

$$\begin{aligned} E_1 = E_2 = E_4 &= E_0 - \Delta, \\ E_3 = E_5 = E_8 &= E_0, \\ E_6 = E_7 = E_9 &= E_0 + \Delta. \end{aligned} \tag{1}$$

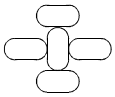
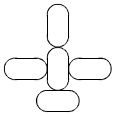
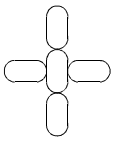
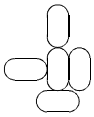
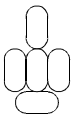
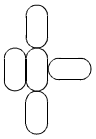
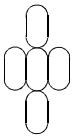
The partition function of the system under consideration has the following form:

$$Z = \sum_{\{E_i\}} \exp[-E_i / T_g] = \exp[-\beta E_0] \cdot [1 + 2\cosh(\beta\delta)][1 + 2\cosh(\beta\Delta)] \tag{2}$$

where T_g is grain temperature and $\beta = 1/T_g$.

Table 1.

Grain configurations for square lattice, $p_0 = \exp[-E_0/T_g]$, $p_\Delta = \exp[\Delta/T_g]$, $p_\delta = \exp[\delta/T_g]$

arrangement	energy	statistical weight factor
	$E_1 = E_0 - \Delta - \delta$	$p_0 p_\Delta p_\delta$
	$E_2 = E_0 - \Delta$	$p_0 p_\Delta$
	$E_3 = E_0 - \delta$	$p_0 p_\delta$
	$E_4 = E_0 - \Delta + \delta$	$\frac{p_0 p_\Delta}{p_\delta}$
	$E_5 = E_0$	p_0
	$E_6 = E_0 + \Delta - \delta$	$\frac{p_0 p_\delta}{p_\Delta}$
	$E_7 = E_0 + \Delta$	$\frac{p_0}{p_\Delta}$
	$E_8 = E_0 + \delta$	$\frac{p_0}{p_\delta}$
	$E_9 = E_0 + \Delta + \delta$	$\frac{p_0}{p_\Delta p_\delta}$

Considering the previous expression it is obtained the relation between free energy of the grain system and value of grain temperature and energy of all microscopic realizations of capillary bridges. Free energy on the node $F = -T_g \ln Z$ is given by

$$F = E_0 - T_g(\ln[1+2\cosh(\Delta/T_g)]+\ln[1+2\cosh(\delta/T_g)]) \tag{3}$$

In [3] it is shown that in asperity regime – very small amount of the liquid – capillary energy dependence on minimum radius R of local grain curvature in the area of real contact of two non-spherical grains and on an average height roughness h of surface is given by $\sim\sqrt{hR}$. For non-spherical grains difference $\varepsilon_1 - \varepsilon_0 = \delta = \delta(\sqrt{hR})$ is very small. However it can cause various preferences mutual arrangements of contacted grains. Assuming in Equation (3) only terms up to fourth order in δ it is obtained an formula for free energy of one node:

$$F \approx F_0 - \frac{T_g}{3}(\delta/T_g)^2 + \frac{T_g{}^3}{36}(\delta/T_g)^4 \tag{4}$$

Free energy (4) is presented in Figure 2.

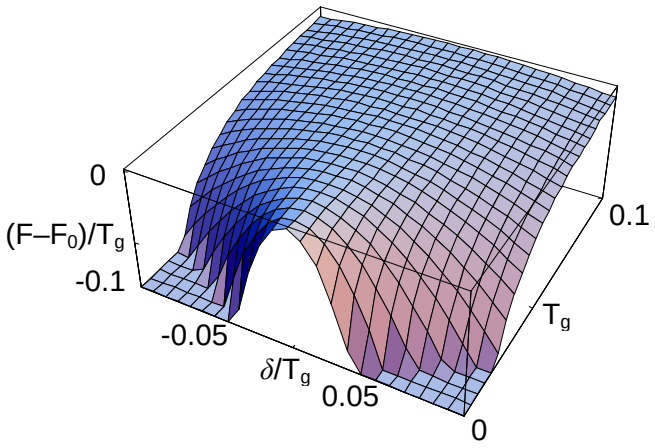


Fig. 2. Illustration relation between free energy and quantity which is characterized fluctuations of curvature and porosity of grain surface δ and delivered energy to the system in vibration process (T_g)

The Equation (4) does not contain a direct connection between local radius of the curvature of grain and vibration amplitude and its frequency, however F is expressed by δ and T_g, and these parameters dependent on grain's surface and

frequency of vibration. Figure 2 illustrates influence fluctuations of radius of grain curvature on free energy of the system. For small values T_g, which correspond to low frequency and small vibration amplitudes is visible a range of values δ whereas fluctuations of grain curvature lower the system energy. This effect is not presented for large T_g.

Conclusions

Computation of energy corresponding to different grain arrangements is time and memory consuming even for small systems. The memory resources and computational time can be significantly lowered if the MFA is applied. However within MFA the only qualitative picture of the energy surface can be constructed.

References

[1] Bocquet L. et al., Physics of humid granular media, C. R. Physique 2002, 3, 207-215.

[2] Fournier Z. et al., Mechanical properties of wet granular materials, J. Phys. Condensed Matter 2005, 17, S477-S502.

[3] Błaszczuk J., Dynamics and statics of packing of granular materials, PhD thesis, Czestochowa, 2005, (in Polish).

[4] Błaszczuk J., Domański Z., The model coupling liquid bridge between ellipsoidal grains, III European Conference on Computational Mechanics Solids, Structures and Coupled Problems in Engineering, C.A. Mota Soares et al (eds.), Lisbon 2006, 8 pages.