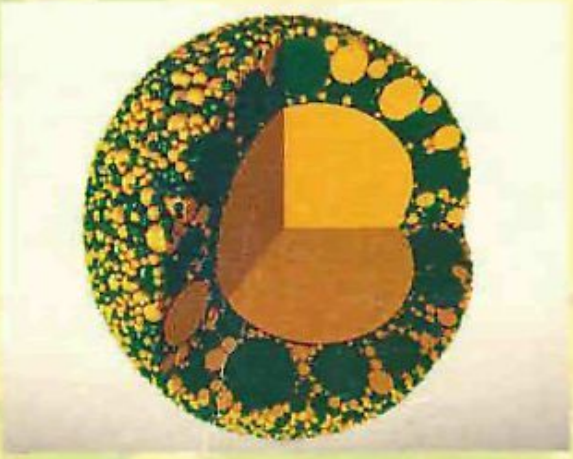
I-st BELGIAN-UKRAINIAN MINI-SYMPOSIUM

Selected Topics of Soft Matter Physics:

Granular Materials



Odessa, September 5-7, 2012

BOOK OF EXTENDED ABSTRACTS

UNIVERSITY OF LIEGE, GRASP, LIEGE, BELGIUM

KU LEUVEN, LEUVEN, BELGIUM

ODESSA STATE ENVIRONMENTAL UNIVERSITY, ODESSA, UKRAINE

Under the patronage of the Royal Embassy of the Kingdom of Belgium in Ukraine

ORGANIZING COMMITTEE

Chair O.Gerasymov

Co-Chairs: N.Vandewalle, J.Indekeu

LOCAL ORGANIZING COMMITTEE

Prof. O.Gerasymov
Dr. N.Khudyntsev
A.Spivak
M.Somov

Edited by

Prof. O.Gerasymov

Welcome address to the book of abstracts

Granular materials are ubiquitous in nature and extensively utilized in many processes in chemical/pharmaceutical, civil, mechanical and mining industries. Granular matter is the second most manipulated material in man's industries and labs. Therefore, understanding the fundamental principles governing granular matter is a research activity of increasing interest.

There is an immense need to understand how particle properties and interactions affect the bulk scale behavior and how process operations determine product characteristics. The ability to predict such links is vital for mitigating natural hazards and for optimizing industrial processes. It is my pleasure to outline that the intensive study of the variety of the physical properties of granular materials is carried on in the closest collaboration between Belgian and Ukrainian physicist. It is important to maintain and develop this activity which has deep historic roots in the engineering industry and which is now fulfilled by solid perspectives in such fundamental science as physics.

The present book of abstracts of the Conference "Selected Topics of Soft Matter Physics: Granular materials" chaired by Professor Oleg Gerasymov, Commander of the Order of the Crown of Belgium, and hosted by Odessa State University of Environment, brings together original papers in a field which belongs to the frontiers of research in this intriguing scientific direction.

I hope that the outlined results not only confirm the fundamental research level of the participants from the attending Universities and Labs, but have also opened new challenges and perspectives for this intensively developing branch of science. I too would like to stress that an intensive and fruitful collaboration between Belgian and Ukrainian scientists adequately support the ideas of development of human capital and mobility of the members of the great scientific community, which are among the most important issues for all mankind and figure among the priorities of the mission of the Embassy of Belgium in Ukraine.

Jana Zikmundova, Ambassador of His Royal Highness the King of the Belgians in Ukraine

Foreword

Since two decades now, the diversity of characters of the behavior of granular materials has been generally described by phenomenological models built upon the framework of the methods invited from the liquid state and solid state theories. This approach has led to observable successes: (i) for modeling the behavior of granular materials, even in the case of a their great complexity (like magnetized and wet granular materials), and their implementation into confined element codes; and (ii) for modeling the behavior of structures and their dynamic properties.

However, the above phenomenological interdisciplinary approach has reached some limits, for instance for granular mobility and compaction (jamming), when it becomes obvious that for complex loading paths a continually increasing number of ad-hoc parameters required.

In such a situation, first, a new intensive experiments are strongly required, and then, probably, new approaches are necessary like for instance - dissipative micromechanics within which the question of constructing realistic constitutive relations for such a materials with only a few physical parameters can be addressed.

Homogenization techniques (linking the particle scale to the representative element volume one) and localization operators (for the inverse change of scales) can now be successfully applied to modeling of granular materials, where the local interaction law between the particles can mostly be described in a very simple way. For instance, an inter-granular Hertz forces is just sufficient to simulate qualitatively the main transport properties of mechanical momentum inputted into the granular media. Interestingly, numerical studies based on discrete element methods coming from molecular dynamics lend support to analytical an experimental approaches. Indeed for granular materials as well as for some other isomorphic materials (like colloids, dusty plasma), the complexity of their behavior, as observed in the experiments, is generally just due to the compaction of great number of particles confined into some space and not to the complexity of the interaction law between them.

The present book of Abstracts include the papers presented for Belgian-Ukrainian Mini-Symposium on Physics of Soft Matter with a focus on Granular Materials which is organized by the leaders of scientific groups from the Universities of Liege (Ulg), Leuven (KU Leuven) and Odessa (OSEnU) mainly directed on outlining the results of intensive scientific collaboration between Ukrainian and Belgian physicists in the area of studying of the complex (granular) systems and related new functional materials. The research are partially carried on within the framework of the Programs supported by FNRS (Belgium), NATO, ULg University Council (GRASP Laboratory).

The presented papers focused on experimental investigations and theoretical modeling of such systems, studying the links between their local structure and dynamic properties, kinetics of compaction, momentum/energy transmission. Among the areas of interest are: discussing the analogies between the observed physical

properties of g.m. and the behavior of complex statistical systems; developing the relevant models for the micro-mechanical systems which shows a reminiscence to statistical physics objects, like gases, liquids or solids. An attractive future of the included materials is the discussion of fundamentals and perspectives of applications of the discovered specific properties of granular materials in modern industries.

I would like to express utmost gratitude to: H.E.Ambassador of the Kingdom of Belgium in Ukraine, Mrs.J.Zikmundova, Rector of Odessa State Environmental University, Professor S.Stepanenko, Co-Chairs of the Conference- Professor N.Vandewalle and Professor J.Indekeu for having given the opportunity of organizing this meeting that has inspired this book.

I too I hope that this thematic issue will constitute an exciting and stimulating source for ongoing collaborative and fructuous works!

Oleg Gerasymov Conference Chair,
Professor, Dr.Sci., Head of the Department of General and Theoretical Physics, Odessa State Environmental University
Commander of the Order of the Crown of Belgium

Contents

Dry and wet granular materials

N.Vandewalle, S.Dorbolo, J.E.Fiscina, F.Ludewig, G.Lumay

GRASP, Institut de Physique B5a, Université de Liège, B4000 Liège, Belgium.

How a large number of spherical objects fill a volume is one of the most persistent puzzles in mathematics and science. The packing fraction of a dense granular assembly is defined as the ratio between the volume of all grains and the volume of the container. When identical spherical grains are gently poured into a tube, a packing fraction around 0.59-0.64 is obtained. The latter value is called the Random Close Packing (RCP) fraction. Small mechanical sollicitations of the random assembly induces local rearrangements of the grains, thus increasing the packing fraction. A crystal of grains with a packing fraction around 0.74 is however far to be reached. Indeed, numerous studies proved that the compaction dynamics of a «dry» packing submitted to a series of taps is extremely slow and similar to relaxation mechanisms in glassy systems (see Figure 1).

We conducted experiments of compaction for «wet» granular assemblies [1]. A wet granular material consists in a dry system with the addition of a small amount of liquid, the latter being located at the contact of the grains. The cohesion, due to capillary bridges between neighboring grains, is tuned using different liquids having specific surface tension values. The compaction dynamics of a cohesive packing obeys an inverse logarithmic law, like most dry random packings (see Figure 1). However, the characteristic relaxation time grows strongly with cohesion. A model, based on free volume kinetic equations and the presence of a capillary energy barrier, is able to reproduce quantitatively the experimental curves.

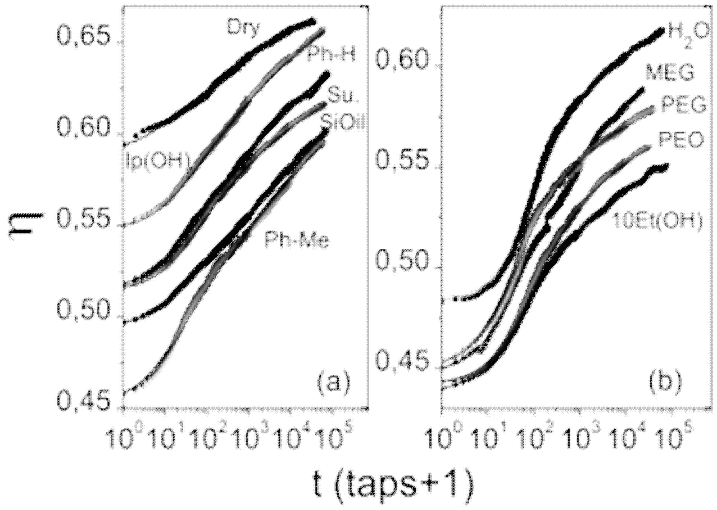


Figure 1 - Typical compaction curves for dry and wet granular materials in a semi-log scale. The slow compaction dynamics is emphasized. The curves have been fitted with an inverse log behaviour in order to extract the characteristic time tau of compaction, see Figure 2.

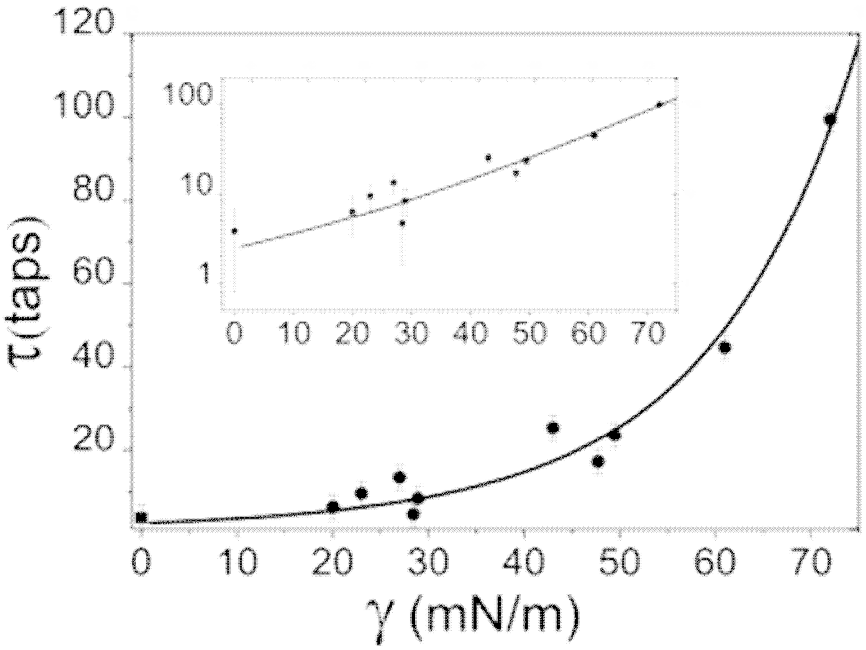


Figure 2 - The characteristic time for compaction tau, as a function of the surface tension of the liquid wetting the system. The characteristic time is seen to increase dramatically with surface tension. This effect is captured by a model which fits the data (continuous curve).

Although experimentalists suspect some effect of the Relative Humidity (RH) on the physical properties of granular materials, almost no author reports the value of RH besides his data. This missing information is however crucial. In order to quantify the effect of RH, we performed a series of compaction experiments under controled RH [2]. Even large glass beads (diameter 1 mm) have been used, a significant effect of RH is observed on the compaction dynamics. Dry air implies triboelectricity. Moisture implies nucleation of liquid bridges. Cohesion becomes therefore important for low and large RH values. An optimum, reducing cohesion, is found around RH=45%.

Compaction curves are fitted by stretched exponentials, which are seen to be deeply affected by the moisture content. A kinetic model (see Figure 3), taking into account both triboelectric and capillary effects, is in excellent agreement with our results. It confirms the existence of an optimal condition at RH=45\% for minimizing cohesive interactions between glass beads. As a consequence, RH represents a relevant parameter that should be reported for every experimental work on a slowly driven dense random packing.

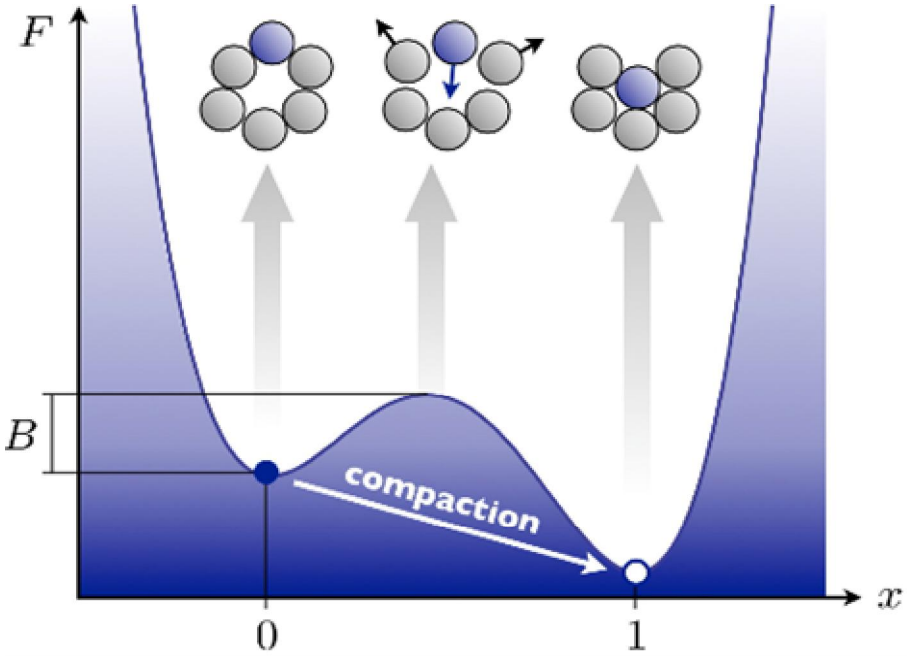


Figure 3 - Sketch of a local configuration of grains which evolves towards a denser arrangement. This can be achieved by the cooperative displacement of grains requiring some energy. An energy barried (B) should therefore be considered in models.

Perspectives are given in terms of applications. Grain shapes [3] and various experimental conditions are discussed.

References :

[1] J.E.Fiscina, G.Lumay, F.Ludewig and N.Vandewalle, Phys. Rev. Lett. 105, 048001 (2010)

[2] N.Vandewalle, G.Lumay, F.Ludewig, J.E.Fiscina, Phys. Rev. E 85, 031309 (2012)

[3] F.Ludewig and N.Vandewalle, Phys. Rev. E 85, 051307 (2012)

Structure and energy transport properties of granular materials

O.Gerasymov

Department of General and Theoretical Physics,
Odessa State Environmental University,Odessa, Ukraine

Granular materials are large assemblies of solid macroscopic particles . It is commonly believed that the realization that some methods from liquid or solid state theories under the appropriate circumstances could be useful in understanding of structure and the behavior which observed in granular materials. Yet despite this seeming simplicity, a granular material behaves differently from any of the other familiar forms of matter – solids, liquids, or gases. Attempts toward understanding and controlling both static and dynamic properties of granular materials are of highest interest to many fields of physics (both theoretical and experimental), applied sciences and engineering. We are focused here in understanding of the ways of description of the local structures of granular materials and the crossover between the macroscopic behavior of granular materials and their microstructures. The transport properties of granular systems with respect to mechanical momentum transportation will be also outlined.

The present state of the theory of physical processes which occurs with the granular materials when subjected to gentle internal perturbations of a different types mainly based on the intuitive concepts of the isomorphic character of the physical processes which occurs in g.m. and in typical gases, liquids and solids.

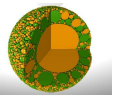
To study the local structure of g.m., inspite of typical condensed matter objects, like liquids or solids, not enough to know the positions of the centers of grains which permit to reconstruct their space arrangements.

Even being at rest g.m. has a complex topology of interparticle space (free volume) which contribute to formation of a local order in form of coexistence of the clusters of a different symmetries within the appropriate scales.

When being weakly shaken, the conglomeration of beads shows a complex dynamic behavior which characterized by transitions between the different symmetries in local arrangements of the grains within a certain scaled-domains.

Besides the grain shape whole, dimension of the system and boundary conditions important role in the complex dynamic behavior of g.m. plays the effects of inelastic intergrain collisions, the presence of intergrain media (vacuum, water, another species, etc.) and magnetization.

Complex structure of g.m. make impossible their description in terms of one structural parameter only. In what follows we are going to show the possible way to introduce the statistical-like measure for a local order in g.m. which leads to respective kinetics of the processes with a transformation of local structure of a different types [1].



Note, that also the modern concepts of local structure of the condensed phases of matter include a diversity of models, which has mostly intuitive (ad hoc) origin. The majority of such approaches has a quite solid background i.e. there are based on idea that order is convenient, to complete information about a crystalline structure can be encoded in a very compact way by retaining only the information about a single fundamental cell plus some translational symmetry operations.

Let restrict our analysis by considering of the discrete set $\{G_i\}$ $(i = 0,1,2,...)$ of points with coordinates $\vec{r}^{(i)}$ representing the centers of particles (grains), which surround the central one located in the origin of the coordinate frame.

We will follow along the common paradigm which tends to definition of the geometrical structure of $\{G_i\}$ can be determined by comparing $\{G_i\}$ with alternative set of points $\{\Gamma_i\}$ which form a collection of familiar ideal (ordered) structure patterns (say, fcc, hcp, etc.).

This collection $\{\Gamma_i\}$ can be chosen from alternative phenomenological sources of information about the local construction of the selected units. One need to note, that there is a limited direct information for example about the local structure of typical liquids.

Contrary, in case of granular materials, especially in 2D case, the local structure and their transformations are observable almost by the naked eyes. Furthermore, the problem of a local structure analysis reduced to their direct observation and classification with respect to a set of the ordered domains of a given (crystallographic) symmetries. The mapping of the structure realizes by means of scaled superimpositions of resemblance of figures and looks like structured in meso- and even in the macro- scales many-particle systems.

After madden upper constructions each state of the ensembles of grains which stroboscopically observed can be quantitatively interpreted as fluctuation i.e. as a deviation from the given set of $\{\Gamma_i\}$.

In another words one can see the local structure as a excitation of one of the selected s.c. “ideal” ordered state.

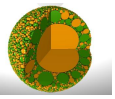
In the phase space those picture looks like division into domains each represented the deformed state of one of the pattern $\{\Gamma_i\}$.

Formal quantitative description along the outlined vide supra approach can be make by means of introducing the relevant local order parameter .

Consider the structure of the selected group consisting of a finite number of particles. The structure of such an object is uniquely determined by the set of the coordinates of its constituent particles (grains) or by the finite set of algebraically independent invariants.

Selecting the appropriate central particle let direct the vectors $\{\vec{r}^{(\alpha)}\}$ centered in this grain to the particles in their neighborhood limited by the certain scale r_0.

The role of r_0 could play the radii of coordinate shells (spheres) or experimentally observed domains which has some distinguish crystallographic ordering. Formally, the set $\{\vec{r}^{(\alpha)}\}$ is already the order parameter which describe the structural order.



Strictly speaking $\{\vec{r}^{(\alpha)}\}$ is a strongly fluctuating value in gases. For the crystals it has the same value for every vortices.

In the case of granular perturbed materials one can adopt the typical in the physics of condensed matter conception: the fluctuations of $\{\vec{r}^{(\alpha)}\}$ are weak enough.

And moreover the weak fluctuations are prescript both for the length and for the relative angles between the vectors from the set $\{\vec{r}^{(\alpha)}\}$.

For the description of structure in a larger scales more convenient are tensor values which can be constructed as follows:

$$T^{(t)}_{\alpha_1\ldots\alpha_l} = \sum_{(a)} \omega\left(\vec{r}^{(a)}\right) t^{(a)}_{\alpha_1\ldots\alpha_l} \quad , \tag{1}$$

and

$$T^{(0)}_{lm} = \sum \tilde{\omega}\left(\vec{r}^{(a)}\right) t_{lm} \quad , \tag{2}$$

where

$$t^{(a)}_{\alpha_1\ldots\alpha_l} = \overline{\vec{r}^{(a)}_{\alpha_1}\ldots\vec{r}^{(a)}_{\alpha_l}} \quad , \tag{3}$$

and $\vec{r}^{(a)}_{\alpha_1}\ldots\vec{r}^{(a)}_{\alpha_l}$ is a Cartesian tensor,

$$t^{(a)}_{lm} = Y_{lm}\left(\Omega^{(a)}\right) \quad , \tag{4}$$

$\Omega^{(a)} = \{\varphi^{(a)}, \vartheta^{(a)}\}$ denotes the polar and azimutal angles that correspond the direction $\vec{r}^{(a)} \Big/ \left|\vec{r}^{(a)}\right|$.

In (3), (4) $\omega\left(\vec{r}^{(a)}\right)$ and $\tilde{\omega}\left(\vec{r}^{(a)}\right)$ are the weight functions which defines the probabilities of the contributions to $T^{(t)}_{\alpha_1\ldots\alpha_l}$ from different coordination shells, and to $T^{(0)}_{lm}$ from the different orientation configurations, respectively.

The tensors $T^{(t)}_{\alpha_1\ldots\alpha_l}$ and $T^{(0)}_{lm}$ can be treated as translational and orientation components of the global order parameter which characterize the considered system. And moreover, $t^{(a)}_{\alpha_1\ldots\alpha_l}$ and $T_{\alpha_1\ldots\alpha_l}$ are the linear combinations of $t^{(a)}_{lm}$ and T_{lm}, respectively. Tensors $T_{\alpha_1\ldots\alpha_l}$ belongs to the basis of the 3D rotational symmetry group O_3. Translational and orientation order parameters given by Eq. (1), (2) adopt the construction of $2(l-1)$ independent (structural) invariants $\{\Psi^{(k)}_l\}$, $l = 0,1,\ldots 2(l-1)$.

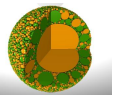
Furthermore, the structural invariants characterize the relative positions of all the particles of the structure.

Note, that the value $T^{(0)}$ gives us the averaged over V_0 density of the number of particles. The value

$$T^{(2)}_{ij} = \tilde{T}^{(2)}_{ij} - \frac{1}{3}\delta_{ij}\tilde{T}^{(2)}_{ii} \tag{5}$$

is density of quadrupole moments.

The values $T^{(4)}_{\lambda_1\lambda_2\lambda_3\lambda_4}$ and $T^{(5)}_{\lambda_1\lambda_2\lambda_3\lambda_4}$ describes the ordered states in the systems of a given crystallographic symmetries.



The definitions given by Eq.(1)-(4) has been constructed under the assuming that all the particles-grains are equivalent to each other. If this condition do not kept one has to determine a relevant set of tensor values ${}^{\kappa}T^{(n)}$ for every component κ ($\kappa = 1,2,...$).

The intensive experimental investigations of the structure of granular materials shows that in most cases within the items coexists both ordered and disordered domains. Passing the external perturbations this domains posses a plenty of transformations which can be described as a transitions between a set of quasi-stationary state.

The $2(l-1)$ independent invariants $\{\Psi_l^k\}$ constructed from the order parameters given by (1), (2) create a structural invariants in the phase space $\{\Psi_l^k\}$. These structural invariants characterize the relative positions of the grains (without taking into account its orientation in space).

Taking into account the sensitivity of structural invariants to the scale-hierarchy of the fluctuations and concluding that the high-rank invariants for the structural analysis with respect to the low-rank ones we expect that for each value of l exist a characteristic scale ξ_l of the grain displacement which corresponds to the selected deviation of $\{\Psi_l^k\}$. The semi-quantitative scenario of the fluctuations of the structural invariants escorted by decreasing of ξ_l with increasing l till the border when ξ become comparable with a relevant ξ_l. Under this condition the respective invariant $\{\Psi_l^k\}$ fluctuates so strongly that system is able to move to another states.

For instance, if we have studied a given 3D cluster with corresponds to fcc and hcp and icosahedrons symmetries as possible structured domains. Each cluster include 1 central a 12 “inner outer” granules equidistantly distributed from the central one. The expected scenario of evolution looks as follows. Initially, each of 12 particles which belong to the considered domain are randomly displaced on to the surface of a sphere with radii ξ positioned around the central grain.

Along the line discussed upper one can introduce two order parameters, namely, the space order-parameter R_{lm} defined as

$$R_{lm} = \frac{1}{N}\sum_a Y_{lm}\left(\Omega^{(a)}\right)\left|\vec{r}^{(a)}\right|^l, \tag{6}$$

and the orientation order-parameter Q_{lm}:

$$Q_{lm} = \frac{1}{N}\sum_a Y_{lm}\left(\Omega^{(a)}\right). \tag{7}$$

The relevant structural invariants has to be studied are:

$$R_l^2 = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}\left|R_{lm}\right|^2, \tag{8}$$

$$Q_l^2 = \frac{2\pi}{2l+1}\sum_{m=-l}^{l}\left|Q_{lm}\right|^2, \tag{9}$$

where Y_{lm} are spherical harmonics and the angle $\Omega^a \equiv \left\{\varphi^{(a)}, \vartheta^{(a)}\right\}$ fix the direction $\frac{\vec{r}^{(a)}}{\left|\vec{r}^{(a)}\right|}$.

The no- fluctuating group of grains $\left(R_l = Q_l\right)$ are characterized by the values collected in Tab.1

	Q_1	Q_2	Q_3	Q_4	Q_5	Q_6	Q_7	Q_8	Q_9	Q_{10}
fcc	0	0	0	0.1909	0	0.5745	0	0.4039	0	0.0129
hcp	0	0	0.0761	0.0972	0.2516	0.4848	0.3108	0.3170	0.1379	0.0102
ics	0	0	0	0	0	0.6633	0	0	0	0.3629

Table 1. Structure invariants $\{Q_i\}$

Analysis of data presented in Tab.1 show that indeed, invariant Q_6 is lager then others for all selected symmetries of crystallic ordering ,namely : fcc, hcp and ics. Obtained results permit us to construct the relevant order parameters which show the relaxation character of the behavior in the vicinity of ordered state with a given symmetry.

Note that the statistics of independent fluctuations of grain positions expressed in terms of probability density of fluctuations of the invariants is different from the those one which occurs due thermal fluctuations in the molecular systems(where correlations are present due to inter-particle interaction).

The physical problem of transport of the impulse impacted from the boundaries into inhomogeneous nonlinear 1D system of beads have been intensively studied by many authors. We consider the general problem of the impulse propagation in gravitationally preloaded granular chain. We show that the equation of motion for the propagating momentum, formulated in form of difference-differential equation for the appropriate boundary conditions adopt analytical solution expressed in terms of the Bessel functions of an integer order. In the continuum limit of the governing equation we found a new analytical solution which is written down in form of traveling wave type of propagating mode. The solution of equation of motion for the momentum in continuum limit which we found has a resonance character which can be interpreted as a Fano-like resonances [2] and occur due to interaction between intrinsic localized- and traveling-like modes (which therefore has to be existed in a weakly inhomogeneous limit). The relevant dispersive relation showed a particular dependence from the position coordinate. This modes are weakly dispersive for large wavelengths. We show that normal mode solutions which also satisfy the governing equation has a resonance character too when taking into account all the frequency modes, but with a different power of resonance. Obtained results fulfilled the theoretical basis of studying the energy/momentum transport in weakly inhomogeneous granular materials .

References

[1] O.I.Gerasymov, Dopov. Nac. akad. nauk Ukr. N11 (2010) p.59.
[2] O.I.Gerasymov, N.Vandewalle, Dopov. Nac. akad. nauk Ukr. N8 (2012) p.67.

The bouncing ball: additional degrees of freedom

S. Dorbolo, F. Pacheco, G. Lumay, F. Ludewig, and N. Vandewalle

GRASP, Département de Physique B5
Université de Liège, Belgium

The bouncing ball on a vibrating surface is among the simplest systems that exhibit chaotic features. A particular case has been visited and revisited in numerous notebook. For the bouncing mode, the control parameter is the maximum normalized acceleration of the plate **G**. On the other hand, there is only one parameter for the ball. This parameter is the coefficient of restitution of the ball which is given by the ratio between the speed after and before the impact. To characterize the mode, the time between two successive contacts and the phase of the contact are sufficient. This problem involves non linear behaviors such as period doubling, orbits, and transition to chaos, that are still far from being exhaustively investigated. This communication presents some experiments in which degrees of freedom are progressively added to the bouncing item.

First, let us consider objects made of two centimetrical beads linked by a rigid rod. This object, coined dimer, is also allowed to bounce. However the coefficient of restitution cannot be as easily determined as in the case of a ball. In Fig. 1, we compare the coefficient of restitution for a ball (in red) and for a dimer. The objects are released from a given height h. We can see that the coefficient of restitution is very different when the dimer is released horizontally or vertically on the plate. The problem turns to be very complicated when the dimer and the plate make an angle. Rotation must be taken into account and the re-distribution of the energy between translational and rotational mode is far of being simple. However, a systematical study of the bouncing allowed to evidence stable bouncing mode and self-propulsion modes.

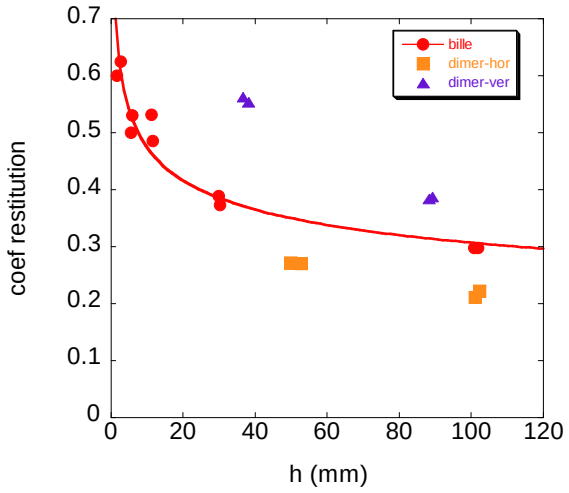


Fig.1: Comparison between the coefficient of restitution for a ball and a dimer which are released either horizontally or vertically on a fixed plate from a height h.

Secondly, we considered trimer. In this case, three beads are linked by rods so as to make an equilateral triangle. In so doing, two additional degrees of freedom are introduced. The coefficient of restitution becomes very complex and strongly depends on the configuration of the trimer before the shock. On the other hand, we can notice that the coefficient of restitution is the lowest when the trimer is released horizontally, namely when the three beads hit the plate at the same moment. Again, a systematical study of the bouncing mode conducts us to find an order in the bifurcation diagrams. In Fig. 2, we present the bifurcation diagram for a bouncing ball, dimer and trimer. The time delay Δt between two successive contacts of the ball, the dimer or the trimer with the plate are presented as a function of the acceleration of the plate (the frequency of the vibration is 25 Hz).

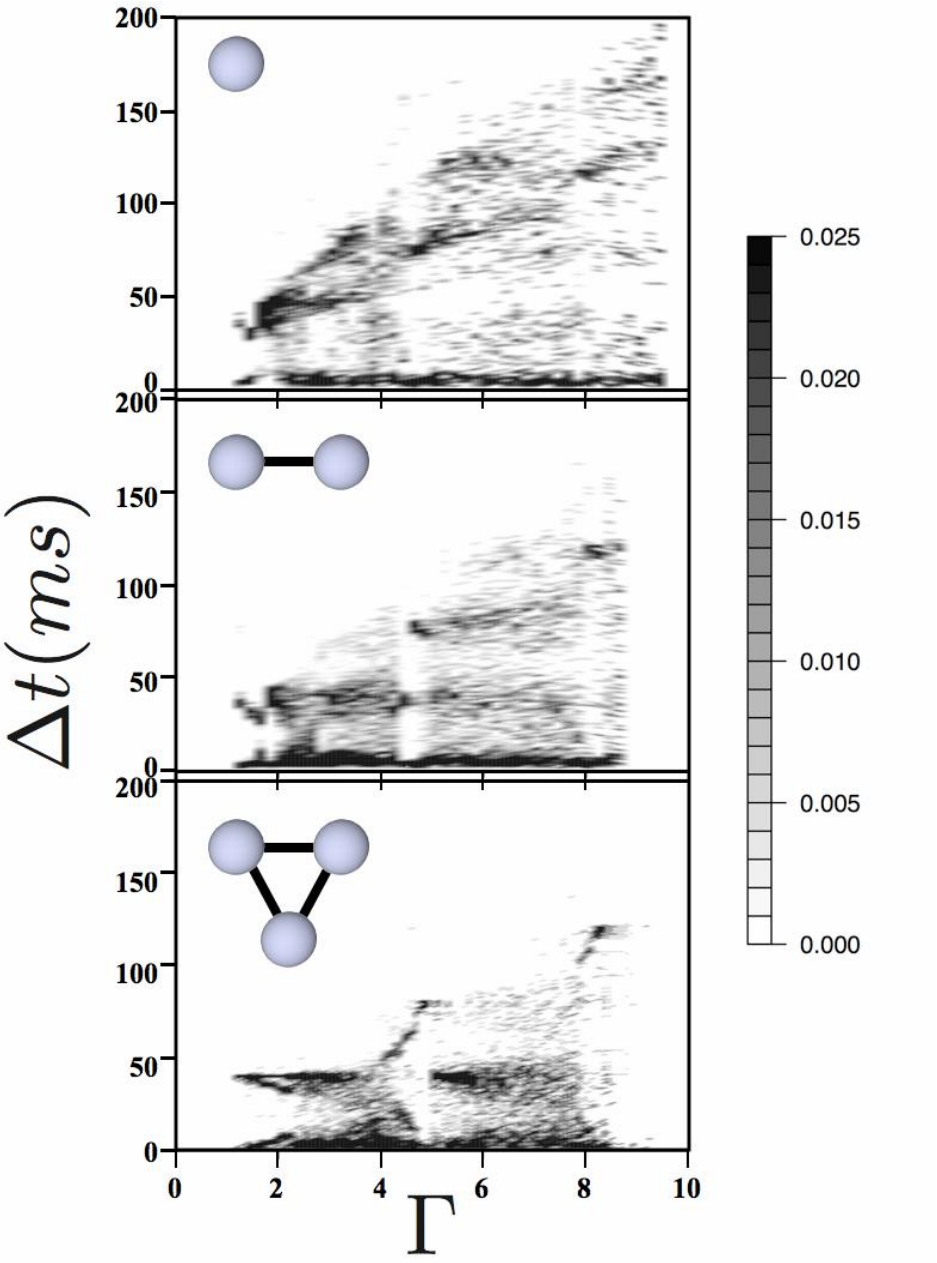


Fig.2: Time delay between two successive contacts of the object with the plate as a function of the reduced acceleration. Darker means more probable time delay. This represents the diagram of bifurcation of a bouncing ball (top), dimer (middle) and trimer (bottom).

The trimer bouncing also presents particular mode as self-propulsion, rotation and period-3. These modes can also be seen in Fig.2.

Third, we study the bouncing mode of a ballasted ball. In this case, beads (or some sand) were placed inside a hollowed bouncing ball. In so doing, we intend to study the coupling between the bouncing mode and the granular material. In Fig. 3, we show the coupling between the bouncing mode and an oscillon mode is observed.

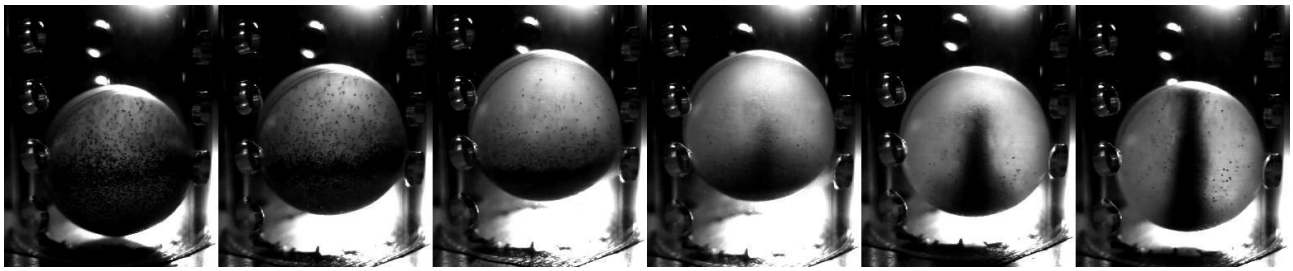


Fig.3: Snapshots of a sand ballasted ping-pong ball. Sand is put inside a hollow ping-pong ball and shaken at 25 Hz. For a given acceleration, a coupling between an oscillon and a period-2 bouncing mode is observed.

Finally, in order to simplify the problem, we study the behavior of a cylindrical container that is vertically shaken. This allow to consider only one dimension. In this context, we studied the bouncing of the empty container, filled with one, two and three beads and finally filled with sand. An example of the diagram of bifurcation can be seen in Fig.4.

According to the result, we may propose some general statement about the relationship between the bouncing and the number of degree of freedom. On the whole, we can conclude with a short-cut expression: complex objects reduce the complexity of the diagram of bifurcation.

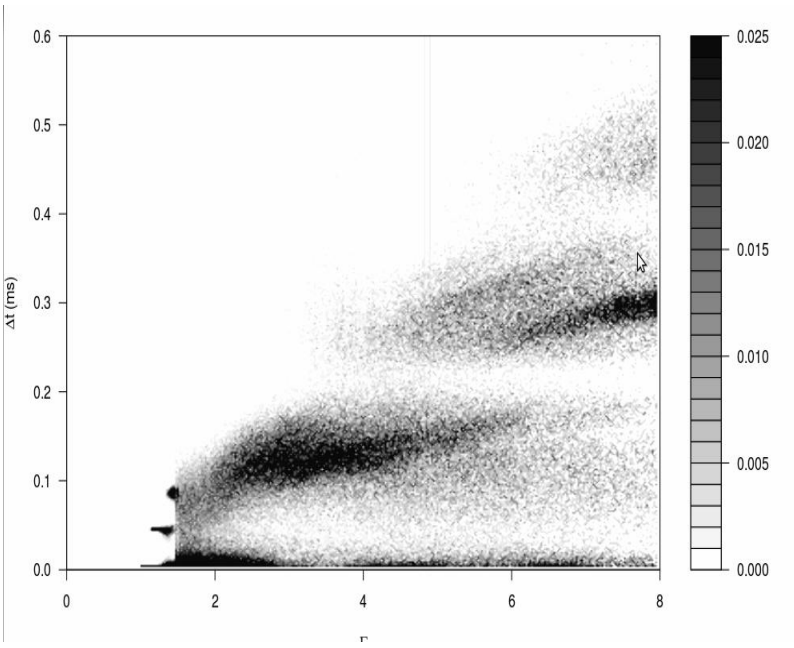


Fig.4: Bifurcation diagram of a bouncing tube containing 2 spheres (the frequency of shaking is 25 Hz)

Electromagnetic Wave Propagation in 1D Model Granular System

O.Gerasymov, N.Khudyntsev

Odessa State Environmental University
Ukraine, Odessa

The study of electromagnetic wave propagation in one-dimensional granular systems is one of the important areas of soft matter physics research [1]. The using of standard methods for finding the optical parameters of the problem (such as the transfer matrix method [2]), is difficult due to violations of translational invariance in these systems caused by the defect, decoration, heterogeneity in external fields and other types of symmetry breaking.

The optical properties of periodic media (structure) are determined by the relevant material parameters – tensors of permittivity $\overline{\overline{A}}(\vec{r})$ and permeability $\overline{\overline{\mu}}(\vec{r})$, which in the case of strictly periodicity in the direction of a dedicated systems (chains) are satisfied by expressions:

$$\begin{aligned}\overline{\overline{E}}(x,y,z) &= \overline{\overline{E}}(x,y,z+d)\\ \overline{\overline{\mu}}(x,y,z) &= \overline{\overline{\mu}}(x,y,z+d)\end{aligned} \qquad (1)$$

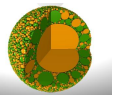
where $d=\sum_{\ell=1}^{G} a_\ell$ – period of the superlattice, G – number of layers (in the unit cell), a_ℓ – layer's thickness ℓ in one-dimensional (topologically ordered) system along the axis Z.

We write the expression for the corresponding tensors $\overline{\overline{A}}$ and $\overline{\overline{\mu}}$ for superlattices with an arbitrary number of layers G in the coordinate representation in the form of a piecewise uninterrupted continuous function in the following the form

$$\begin{pmatrix}\overline{\overline{E}}(Z)\\ \overline{\overline{\mu}}(Z)\end{pmatrix}=\sum_{n,x}\begin{pmatrix}En,\ell\\ \mu n,\ell\end{pmatrix}\left\{\theta\left[Z-(n-1)d-\sum_{0=1}^{\ell}\left(a_{nj}-a_{n\ell}\right)\right]-\theta\left[Z-(n-1)d-\sum a_{nj}\right]\right\}, \qquad (2)$$

where $\theta(Z)$ – Heaviside function, $n=\pm1;\pm2;.....-$ cell number of one-dimensional crystal;
$\ell=1,2,3,....., G$ enumerates the elements of the cell.

We assume the existing of disorder in a direction Z, that is due to variations in thickness of the doped layers (in this case $\overline{\overline{A}}_{n\ell}\equiv\overline{\overline{A}}_\ell$). With this approach, the parameters of superlattice, which deviate from the periodical ones, are depended



from configurations, and may be represented by a set of random variables $\{\eta_{n\ell}^{\nu}\}$ satisfying the following conditions: $\eta_{n\ell}^{\nu}=1$ if the layer off sort $\nu(\ell)$ with thickness $a_{\ell}^{\nu(\ell)}$ is included in the $n\ell$- ordered crystalline chain; and $\eta_{n\ell}^{\nu}=0$ – if this condition is violated.

Obviously, we can write

$$a_{n\ell}=\sum_{\nu(\ell)=1}^{r(\ell)}a_{\ell}^{\nu(\ell)}\eta_{n\ell}^{\nu(\ell)}, \tag{3}$$

where $r(\ell)$ – number of sorts of elements (layers) in ℓ- sublattice of $1D$ crystal ordered structure.

We introduce the concept of configuration-averaged values $\langle a_{n\ell}\rangle$ and $\langle d_n\rangle$ under the following rules:

$$\begin{aligned}\langle a_{\grave{o}\,\ell}\rangle &= a_{\ell}\cdot\{\tilde{N}_{\ell}^{\nu(\ell)}\}=\sum_{\nu(\ell)=1}^{r(\ell)}G_{\ell}^{\nu(\ell)}\tilde{N}_{\ell}^{\nu(\ell)}\\ \langle d_n\rangle &\equiv d\{\tilde{N}_{\ell}^{\nu(\ell)}\}=\sum_{\ell=1}^{G}\sum_{\nu(\ell)=1}^{r(\ell)}a_{\ell}^{\nu(\ell)}\tilde{N}_{\ell}^{\nu(\ell)}\end{aligned} \tag{4}$$

In terms of averaged values the typical problem of finding the spectral characteristics of similar systems is reduced to consideration of the analogous problem for perfectly periodic multilayer structure with the layer thickness $a_n\{\tilde{N}_{\ell}^{\nu(\ell)}\}$ and the layer period $d\{\tilde{N}_{\ell}^{\nu(\ell)}\}$.

Conventionally, the approach described above is called a model of virtual topological ordering. In this approximation, for example, parameters such as spectrum, width of the energy gap and the others is determined with the help of standard algorithms by finding such values for a perfectly ordered (periodic) superlattices (layered structures) and transition to the new variables: $a_{n\ell}a_{\ell}\{C_{\ell}^{\nu(\ell)}\}$; $d\to d\{C_{\ell}^{\nu(\ell)}\}$, where $\tilde{N}_{\ell}^{\nu(\ell)}$ – concentration of layers of sort $\nu(\ell)$ with thickness $a_{\ell}^{\nu(\ell)}$ in sublattice $\ell\left(\sum_{\nu(\ell)}\tilde{N}_{\ell}^{\nu(\ell)}=1\right)$.

The proposed model of configurationally averaging permits to restore the translational symmetry which is disturbed after the virtual variations of layer(s) width in $1D$ multi-layer system.

Thus induced translational invariance of $1D$ chain can provide relevant material tensors $\overline{\overline{E}}(Z)$ and $\overline{\overline{\mu}}(Z)$ in the form of Fourier expansions:

$$\begin{pmatrix}\overline{\overline{E}}(Z)\\ \overline{\overline{\mu}}(Z)\end{pmatrix}=\sum_{l}\begin{pmatrix}\overline{\overline{E}}_e\\ \overline{\overline{\mu}}_e\end{pmatrix}\exp\left(-il\frac{2\pi}{d\{C_{\ell}^{\nu(\ell)}\}}Z\right) \tag{5}$$

Using (2) and (5), it is easy to find an expression for the amplitude $\overline{\overline{E}}_e$ and $\overline{\overline{\mu}}_e$:

$$\begin{pmatrix} \overline{\overline{E}}e \\ \overline{\overline{\mu}}e \end{pmatrix} = -\frac{i}{2\pi l}\sum_{\ell}\begin{pmatrix} \overline{\overline{E}}_{nd} \\ \mu_{n\ell} \end{pmatrix}\left\{\begin{array}{l} \exp\left(i\dfrac{2\pi}{d\left\{C_{\ell}^{\nu(\ell)}\right\}}l\sum_{j=1}^{\ell}a_j\left\{C_{\ell}^{\nu(\ell)}\right\}\right)- \\ -\exp\left[i\dfrac{2\pi}{d\left\{C_{\ell}^{\nu(\ell)}y\right\}}l\left(\sum_{j=1}^{\ell}a_j\left\{C_{\ell}^{\nu(\ell)}\right\}-a_{\ell}\left\{C_{\ell}^{\nu(\ell)}y\right\}\right)\right] \end{array}\right\} \tag{6}$$

We now going to write down Maxwell equations for electromagnetic field strengths $(\vec{E},\vec{H})$ in the usual form:

$$\begin{aligned} \vec{\nabla}x\vec{E}(\vec{r},\omega) &= \frac{i\omega}{C}\overline{\overline{\mu}}(Z)\cdot\vec{H}(\vec{r},\omega) \\ \vec{\nabla}xH(\vec{r},\omega) &= -\frac{i\omega}{C}\overline{\overline{E}}(Z)\cdot\vec{E}(\vec{r},\omega) \end{aligned} \tag{7}$$

Applying the Floquet theorem for the periodical structure one can express the values $\vec{E}(\vec{r},\omega)$ and $\vec{H}(\vec{r},\omega)$ as follows

$$\begin{pmatrix} \vec{E}(\vec{r},\omega) \\ \vec{H}(\vec{r},\omega) \end{pmatrix} = \begin{pmatrix} f_k^{(E)}(Z) \\ f_k^{(H)}(Z) \end{pmatrix}\cdot\exp(-i\vec{\chi}\vec{\rho}-ikZ) \tag{8}$$

where $\vec{\rho}=(x,y)$ and $\vec{\chi}$ is an arbitrary planar wave vector lying in the plane $x0y$; $\vec{k}(0,0,k)$ – Bloch vector.

Taking into account written upper , we obtain

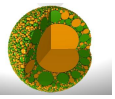
$$\begin{pmatrix} \vec{f}_k^{(\vec{E})}(Z) \\ \vec{f}_k^{(H)}(Z) \end{pmatrix} = \begin{pmatrix} \vec{f}_k^{(E)}\left(Z+d\left\{C_{\ell}^{\nu(\ell)}\right\}\right) \\ \vec{f}_k^{(H)}\left(Z+d\left\{C_{\ell}^{\nu(\ell)}\right\}\right) \end{pmatrix} = \sum_p\begin{pmatrix} \vec{f}_{k,p}^{(E)} \\ \vec{f}_{k,p}^{(H)} \end{pmatrix}\exp\left(-ip\frac{2\pi}{d\left\{C_{\ell}^{\nu(\ell)}\right\}}Z\right) \tag{9}$$

Substitution Eq.(8) into (7) allows us to perform the amplitude of the Fourier transforms of the electromagnetic field $\vec{f}_{k,p}^{(E,H)}$. After trivial manipulations, after use Eq.(7), (8),and accounting Eq.(4), we have:

$$\left[\chi\left(k+p\frac{2\pi}{d\left\{C_{\ell}^{\nu(\ell)}\right\}}\right)\vec{e}_Z\right]x\begin{pmatrix} \vec{f}_{k,p}^{(E)} \\ \vec{f}_{k,p}^{(H)} \end{pmatrix} = \frac{\omega}{c}\begin{pmatrix} -\sum_e\overline{\overline{E}}_e\vec{f}_{k,p-1}^{(E)} \\ \sum_e\overline{\overline{\mu}}_e\vec{f}_{k,p-1}^{(H)} \end{pmatrix}, \tag{10}$$

where $\vec{e}_Z$ – unit vector along the axis z.

The system of equations (10) allows us to perform the normal modes of electromagnetic waves propagating in the constructed "virtually" periodic layered systems, which can be interpreted as one-dimensional models of granular structures.



Now consider the effect of possible variations of the superlattice parameters (for example, the deviation from periodicity which can result from the changing of the layer thickness) in terms of the relevant spectrum transformation.

We restrict ourselves to the analysis of electromagnetic wave propagation in a non-magnetic one-dimensional chain model $\left(\bar{\bar{\mu}} = \bar{\bar{I}}\right)$, where $\bar{\bar{I}}$ – is the identity matrix of the superlattice, configured along a given axis.

We suppose, as it's often assumed when studded the polariton spectra, K are close to its limit (Bragg) values

$$\left| K - \frac{2\pi}{d\left\{C_\ell^{V(\ell)}\right\}} \right| \Rightarrow K \qquad (11)$$
$$cK^2 \to \omega^2 \varepsilon_0$$

In this case, the resonant terms (which correspond to $\vec{f}_{K,p}^{(E,H)} = 0, -1.$)become the main contribution to the equation

$$\left[\vec{\chi}\left(K + \rho \frac{2\pi}{d\left\{C_\ell^{(V)}\right\}} \right) \vec{e}_Z \right] \cdot \begin{pmatrix} \vec{f}_{K,p}^{(E)} \\ f_{K,p}^{(H)} \end{pmatrix} = \frac{\omega}{C} \begin{bmatrix} -\sum_e \bar{\bar{\varepsilon}} e \vec{f}_{K,p-1}^{(E)} \\ \sum_e \bar{\bar{\mu}} e \vec{f}_{K,p-1}^{(H)} \end{bmatrix}$$

The closed system of equations, which were obtained taking into account the made restrictions, leads to the relevant dispersive relation which provide the spectra of the problem:

$$\begin{bmatrix} K^2 - \frac{\omega^2}{c^2}\varepsilon^{(0)} & -\omega^2 \varepsilon^{(1)} \\ -\frac{\omega^2 \varepsilon^{(-1)}}{c^2} & (K^2 - d\left\{C_\ell^{V(\ell)}\right\})^2 - \frac{\omega^2}{c^2}\varepsilon^{(0)} \end{bmatrix} \begin{pmatrix} f_{x,(y),\kappa,0}^{(E)} \\ f_{x(y),K,-1} \end{pmatrix} = 0, \qquad (12)$$

Finally, we have

$$\left(K^2 - \frac{\omega^2}{c^2}\varepsilon^{(0)} \right) \left[\left(K - \frac{2\pi}{d\left\{C_\ell^{V(\ell)}\right\}} \right)^2 - \frac{\omega^2(K)}{c^2}\varepsilon^0 \right] - \left(\frac{\omega^2(K)}{c^2} \left| \varepsilon^{(1)} \right| \right)^2 = 0$$

The roots of the equation (12) determine the behavior of the spectrum. For example, the band $\omega - (K) < \omega < \omega + (K)$ corresponds to the forbidden zone in which the roots of the dispersion equation has the complex form. The corresponding electromagnetic waves are damped. Thus, it is Bragg reflection of electromagnetic waves at frequencies $\omega < \omega - (K)$ and $\omega < \omega + (K)$as the wave propagates along the model of the superlattice.As it was shown in [1],in case of defect zones appear in 1D periodic structures the specific type of singularities(resonances) occur close to boundaries of the band-gapes(Tamm-like resonances). This phenomena can influence

the electromagnetic wave transmission(reflection) mechanism in considered granular chain.This will be the focus of our research plan.

Therefore, we propose a model of virtually ordered quasi-layered structure, which is able to be a model for superlattice with an embedded impurity (defect). With the help of this model, in particular, decorated one-dimensional horizontal granular chain can be described. Based master equations for the components of the electromagnetic field propagating along the axis of symmetry of studied $1D$ system, allowing to calculate the parameters of the model spectrum, are obtained. These results supplement the theoretical tools for parameterization of characteristics of granular materials, in particular, optical circuitry, developed on their basis [3].

References

1. Gerasymov O.I., Scattering of radiation in statistical systems : solved models (Odessa, 1999)
2. J. Ziman, Models of disorder (Moscow, 1982)
3. S. Kasap, H. Ruda, Y. Boucher. Cambridge Illustrated Handbook of Optoelectronics and Photonics (Cambridge, 2009)

Statistical Physics and Interfacial Phenomena in Soft Matter

J. Indekeu

Leuven, KU Leuven

Equilibrium wetting phase transitions and critical phenomena are discussed from a phenomenological point of view. The ubiquitous character of the wetting phase transition is illustrated through its occurrence in a variety of condensed matter systems, ranging from classical fluids to superconductors and Bose-Einstein condensates. The intriguing behaviour of the three-phase contact line and its line tension, at wetting, is an example of a fundamental problem in this field on which much progress has been made.

Excluded volume effects in binary mixtures

Francesco Aliotta

Istituto per I Processi Chimico-Fisici, CNR, Messina, ITALY

Introduction

A largely accepted idea assumes that experimental observation of an excess thermodynamic quantity in binary liquid mixtures can be related with the nature of the inter-molecular interaction between mixture constituents [1-7]. A thermodynamic excess quantity is currently defined as the deviation from the linear dependence from the volume fraction of one of the two species, after the assumption that the linear dependence would correspond to the expected behavior for an ideal mixture which exhibits volume additivity and preserves additivity of all the other extensive thermodynamic parameters.

As an example, ideality implies that if the volume of a mixture, V_{id}, can be described by the relation

$$V_{id} = N_a v_a + N_b v_b \tag{1}$$

where v_a and v_b are the molar volumes of the two components and N_a and N_b their mole number, the ideal adiabatic compressibility, $\beta_{s,id}$, can be obtained differentiating eq. 1

$$\beta_{s,id} = -\frac{1}{V_{id}}\left(\frac{\partial V_{id}}{\partial p}\right)_s = \beta_a + (\beta_b - \beta_a)\phi \tag{2}$$

β_a and v_b being the adiabatic compressibility of pure components. In eq. 2 ϕ is the volume fraction of the specie *b*, while the volume fraction of the specie *a* is $(1-\phi)$.

The leading idea is that any (attractive or repulsive) inter-specie interaction can produces the appearance of non-vanishing (negative or positive) mixing volumes resulting in an excess (negative or positive) compressibility, $\Delta\beta_s$. The trouble is that eqs. 1 and 2 imply the definition of an ideal liquid, which is a misleading idea because no zero order model can exist for liquid, in principle. This point is immediately understood when the Gibbs free energy of a binary mixture is written as:

$$G = x_a G_0^a + x_b G_0^b + RT\left(x_a \ln x_a + x_b \ln x_b\right) + \Delta G_f \tag{3}$$

where G_0^i (i=a,b) are the reference states, the third term is the random mixing contribution and the quantity ΔG_f is an excess term accounting for the formation of a binary stoichiometric phase [8]. This last term contains both enthalpic and entropic contributions, which cannot be easily disentangled. Besides the case of very low density regimes, which correspond to the ideal gas phase, the enthalpic term cannot be null in a liquid mixture. As a consequence, the behavior observed in a liquid mixture always will be diverging from linearity. In few words, to compare the experimental behavior against the ideal one represents a misleading approach. The only safe information that one can be extract from such a deviation is just the trivial

knowledge that we are dealing with a liquid. In order to understand if a preferred hetero-coordination is established via intermolecular interaction, we should calculate the deviation respect to a binary mixture in which the two components are fully randomly mixed. Such a reference system can be identified, following Hildebrandt [9.10], as a *regular solution*.

A widely adopted approach to model the excess Gibbs free energy (as well as any other excess thermodynamic quantity) makes use of empirical polynomial expansion [11] as a function of the concentration. In terms of the volume fraction, such an expansions can be written as:

$$G_{ex}(\phi) = \phi \cdot (1-\phi) \sum_{1=0}^{n} G_i \cdot (1-2\phi)^i \tag{4}$$

Aim of this work is to discuss the effective possibility of extracting information about the nature of intermolecular interaction in binary mixture from the analysis of the concentration dependence of some excess thermodynamic quantities, namely excess molar volume and adiabatic compressibility. The experimental data will be compared with the prediction of a primitive model in order to understand the role played by entropic and enthalpic.

A simple model

The most basic model for a liquid mixture is obtained through the adoption of a hard sphere potential [12,13]. In this approach, the inter-species interaction is described in terms of two like collision diameters, d_a and d_b, and by an inter-species collision diameter

$$d_{ab} = \frac{1}{2}(d_a + d_b)(1+\Delta) \tag{5}$$

In eq. 5, Δ is a dimensionless parameter accounting for any deviations of unlike excluded volumes from additivity. In spite of its simple formulation, the model is able to produce a rich variety of thermodynamic behaviors, as the value of Δ is varying. Of course, in order to evaluate a thermodynamic parameter an equation of state must be adopted. The simplest equation of state is the virial expansion, whose partial coefficients are fully analytical up to the third order

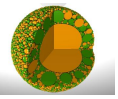
$$\frac{p}{k_B T} = \sum_{i=1}^{\infty} b_i \rho^i \tag{6}$$

where p is the pressure, T the absolute temperature, k_B the Boltzmann constant, b_i the virial coefficients (b_1=1) and $\rho = \rho_a + \rho_b$ is the total number density given by the sum of the two partial densities. For a binary hard-sphere mixture, b_2 and b_3 depend explicitly on the molar fraction of the two species and on the collision diameters, while the number density depends on the packing fraction, η, through the relation

$$\rho = \frac{6}{\pi\left[x d_a^3 + (1-x) d_b^3\right]}\eta \quad ; \quad (x = x_a, \quad 1-x = x_b) \tag{7}$$

CCl_4/$CHCl_3$ mixtures.

Carbon tetrachloride/chloroform mixtures can be representative of the simplest situation. Both molecules are roughly spherical, their sizes are not too much different, and the density of the mixture linearly depends on the volume fraction, within the



experimental accuracy. However, other thermodynamic quantities clearly deviate from linearity. In fig. 1 we plot the dependence of the excess compressibility respect to the behavior described by eq. 2, as a function of $CHCl_3$ volume fraction.

The adiabatic compressibility, β_S, is related to the isothermal compressibility, β_T, through the relation

$$\beta_S = \beta_T \frac{c_v}{c_p} = \rho k_B T \frac{c_v}{c_p} \chi_T \tag{8}$$

Where c_v and c_p are the isochoric and isobaric specific heats, and β_T is the isothermal susceptibility which can be obtained by differentiating eq. 6 with respect to the number density

$$\chi_T^{-1} = \frac{1}{k_B T}\left(\frac{\partial p}{\partial \rho}\right)_T = \sum_{i=2}^{\infty}(i-1)b_{i-1}\rho^{i-2} \tag{9}$$

For an hard sphere mixture [13]

$$c_v = \frac{3}{2} N k_B T \tag{10}$$

and

$$\frac{c_p}{N k_B} = \frac{3}{2} N k_B + \rho k_B T \beta_T \left(\frac{p}{\rho k_B T}\right)^2 \tag{11}$$

where N is the number of particles.

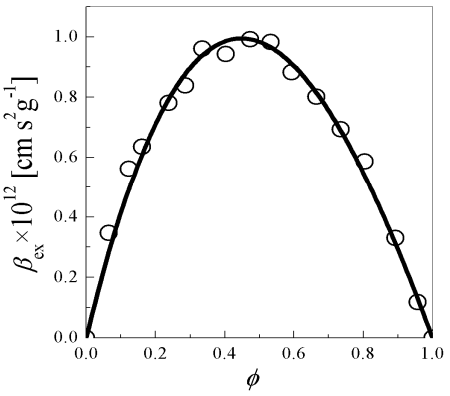


Fig. 1

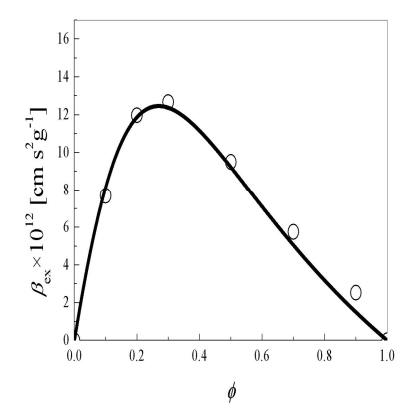


Fig. 2

Eq. 8 can be used to fit the experimental excess compressibility data. The procedure should involve the determination of the values of four parameters, namely d_a, d_b, Δ and η. However, we will assume that the value of η must be low enough to allow random mixing. Under such a condition its value will affect only the amplitude of the excess compressibility with no effect on its shape. We adopted the value η=0.2 and a pre-factor has been inserted in order to fit the amplitude. In addition it must be noted that the shape of the excess compressibility depends only on the ratio d_b/d_a and not on the values of each diameter. The fitting curve reported in fig. 1 has been obtained for d_b/d_a=0.79 and Δ=0 (additive mixture) which are realistic values for $CCl_4/CHCl_3$ mixtures.

CCl_4/penthanol mixtures

Binary mixtures of linear alcohols in carbon tetrachloride exhibit an almost linear dependence on the concentration. Contrary to the previous situation in such a case the ability of intermolecular interaction via hydrogen

bonding implies the occurrence of aggregative phenomena. The local connectivity must be a function of the alcohol volume fraction. At high alcohol content it is expected that it tends to preserve is local connectivity which becomes completely lost at enough high dilution. So it the excess compressibility can carry information about these concentration dependent aggregative phenomena. In fig. 2 the excess compressibility data are reported for carbon tetrachloride/penthanol mixtures. The maximum excess compressibility is observed at $\phi \sim 0.3$. The continuous line in fig. 2 represents the best fit with eq. 8 obtained for $d_b/d_a=0.81$ and $\Delta=-0.1$. A non-zero Δ value implies that some interaction among unlike molecules is taking place. In particular, a value $\Delta<0$ models a less rigid structure than that corresponds to purely additive hard-sphere. The obtained result agrees with literature suggestion that, at intermediate concentration, electrostatic interaction beyond excluded volume interaction results in nontrivially random coordination between the solvent and the alcohol [14,15].

Poly-(ethylene glycol)/H_2O mixture.

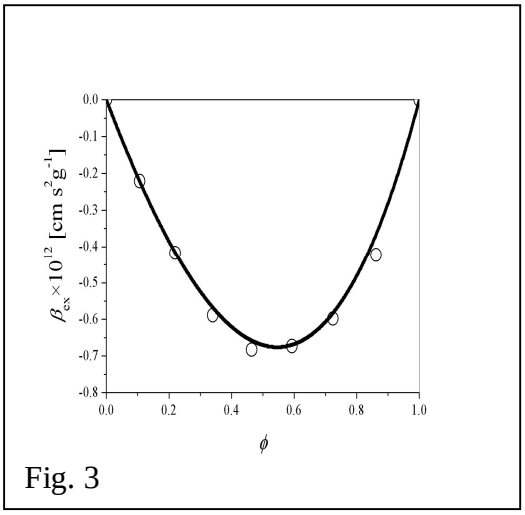


Fig. 3

In fig. 3 the excess compressibility data are reported for an aqueous solution of poly-(ethylene glycol) (molecular weight 600). Also in this system the existence of aggregative phenomena must be taken into account. In addition, this system exhibits a negative excess compressibility, differently from the other systems before examined. The continuous line in fig. 3 represents the best fit with eq. 8 and demonstrates that the proposed model seems to work also under this situation. The best fit has been obtained for $d_b/d_a=1.04$ and $\Delta=-5\cdot10^{-4}$. In this case, a positive Δ value models a more rigid structure which is consistent with the existence of hetero aggregation phenomena via hydrogen bonding. The low value of the Δ parameter agrees with the experimental observation that volumes are almost additive.

Liquid crystal in CCl_4.

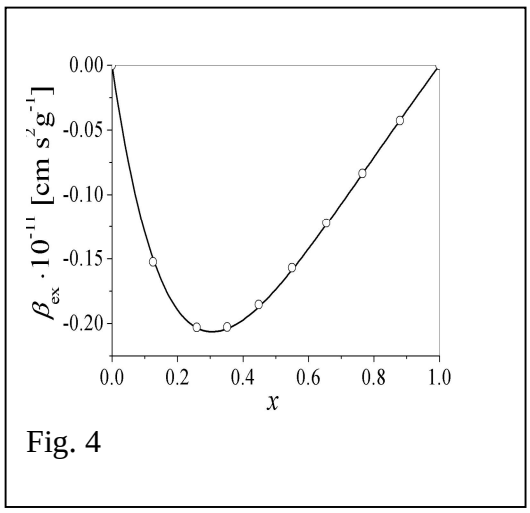


Fig. 4

The adopted approach seems able of reproducing also data from mixtures where one of the two components definitely deviates from a spherical shape. A good example can be represented by a solution of a liquid crystal (ME6N in our case) in carbon tetrachloride. In addition, in this system the volumes of the mixture clearly deviate from linearity. As above mentioned, in this case only the solvent can be described as spherical. In the case of the liquid crystal the value of the parameter d appearing in the model can be assumed only as an average radius. In spite of these difficulties, the model appears able to fit both the excess

compressibility data (see fig. 4) and the number density (calculated from the experimental molar volume, see fig. 5). The best fits have been obtained for d_b/d_a=1.202 and Δ=-0.00712. A positive value of the Δ parameter agrees with the idea that, due to the non-spherical shape of one of the two components, the mixture can exhibit a more dense local structure factor than that would be allowed by a purely additive hard-sphere model. An attempt of fitting the same data with a model for a mixture of hard-sphere/hard-ellipsoid [16] produced results undistinguishable from those reported in Figs. 4 and 5.

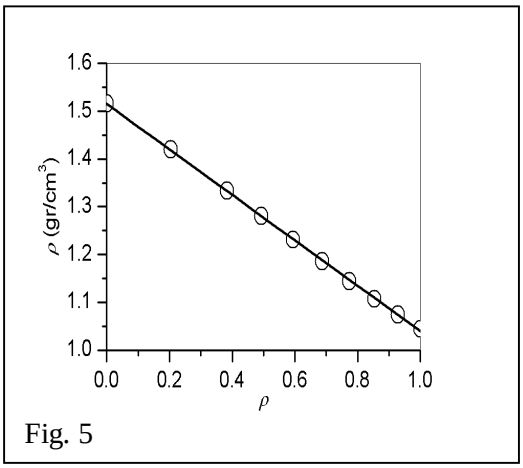


Fig. 5

In this case, the best fitting has been obtained for an aspect ratio of of the ellipsoid of 3.8 while the ration between the smaller size of the ellipsoid and the hard-sphere radius was 0.788. These values are in agreement with the sizes of the involved molecules and no need for accounting a non-additive factor has been detected.

Concluding remarks

The reported results lead to conclude that any observed non-ideality in binary mixtures depends mainly on excluded volume effects and particularly on their non-additive nature. This suggests that geometrical effects play the major role in determining both the sign and the amplitude of excess properties, in agreement with the indication from Prigogine-Flory-Patterson theory [17-19]. In addition, it has been shown that an excess compressibility is observed also in system which fulfill volume additivity. This finding agrees with the Flory statement that the choice of the null volume state as the ideal one is rather arbitrary because it does not imply that all the other thermodynamic quantities should follow the same linear concentration dependence [17].

Reference

[1] J. Lamb, in *Physical Acoustic*, edited by W.P. Mason (Academic, New York, 1965). Vol. IIA**.**

[2] J.P. Boon and S. Yip, *Molecular Hydrodynamic* (Mc Graw-Hill, New York, 1980).

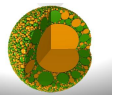
[3] J.-E. Otterstedt, R.W. Missen, *Trans. Faraday Soc.* **57**, *879*, 1962.

[4] G.C. Paraskevopoulos, R.W. Missen, *Trans. Faraday Soc.* **57**, *869*, 1962.

[5] A. Arce, E. Rodil, A. Soto, *J. Solution Chem.*, **35**, *63*, 2006.

[6] H. Pfeiffer, K. Heremans, *Chem. Phys. Chem.*, **6**, *697*, 2005.

[7] B.U. Kadam, A.P. Hiray, A.B. Sawant, M. Hasan, *J. Chem. Eng. Data*, **51**, *60*, 2006.



[8] J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1966).

[9] J.H Hildebrandt, *J. Chem. Phys.*, **15**, *225*, 1948.

[10] J.H. Hidebrandt, *Nature*, **168**, *868*, 1951.

[11] O. Redlich, A.T. Kister, *Ind. Eng. Chem.*, **40**, *345*, 1948.

[12] F. Aliotta, J. Gapinski, M. Pochylski, R.C. Ponterio, F. Saija, G. Salvato, *J. Chem. Phys.*, **126**, *224508*, 2007.

[13] T. Boublik, J. Nezbeda, *Collect, Czech. Chem. Commun.*, **51**, *2302*, 1986.

[14] H. Torii, *Chem. Phys. Lett.*, **193**, *153*, 2004.

[15] M. Musso, H. Torii, P. Ottaviani, A. Asenbaum, M. G. Giorgini, *J. Phys. Chem. A*, **106**, *10152*, 2002.

[16] F. Aliotta, M.G. Giorgini, R.C. Ponterio, F. Saija, *J. Mol. Liq.*, **153**, *67*, 2010.

[17] P. J. Flory, *J. Am. Chem. Soc.*, **87**, *1833*, 1965.

[18] H. Tra Van, D. Patterson, *J. Solution Chem.*, **11**, *793*, 1982.

[19] M. Costas, D. Patterson, *J. Solution. Chem.*, **11**, *807*, 1982.

The influence of cohesion on the behavior of granular systems

G. Lumay, S. Dorbolo and N. Vandewalle

GRASP, University of Liege, Belgium

Introduction

The existence of cohesive forces inside a granular material is known to influence drastically the macroscopic properties of the assembly. The cohesion could be related to capillary bridges, electric charges, or van der Waals interactions. When the weight of one grain is higher than the sum of the cohesive forces acting on the grain, the cohesive forces do not play an important role on the granular assembly. In this configuration, the macroscopic behavior of the granular material is controlled by the friction between the grains, the restitution coefficient and the grain shape. However, when the grains are small (typically less than 50 μm), the macroscopic behavior of the pile is mainly governed by the cohesive forces. These cohesive forces are difficult to quantify and to control experimentally. Therefore, the properties of a model cohesive granular material are investigated. The cohesion is induced by an external magnetic field which can be adjusted. The granular material is made of soft ferromagnetic metallic grains. The influence of the magnetic cohesion between the grains on the static, the quasi-static and the dynamic properties of the assembly is analyzed experimentally. The static properties are investigated through the packing fraction. The quasi-static properties are analyzed with a compaction experiment and the study of the flow in a rotating drum gives some informations about the dynamical behavior of a cohesive granular material. Finally, after the study with the model cohesive granular material, the measurements are performed with two types of granular materials: silicon carbide abrasives and flours. These selected materials allow to show practically the influence of the cohesion on the macroscopic properties of the assembly.

Packing fraction

We present an experimental protocol that allows one to tune the packing fraction of a random pile of ferromagnetic spheres from a value close to the lower limit of random loose packing η_{RLP}=0.56 to the upper limit of random close packing η_{RCP}=0.64 (see Figure 1). This broad range of packing fraction values is obtained under normal gravity in air, by adjusting a magnetic cohesion between the grains during the formation of the pile. Attractive and repulsive magnetic interactions are found to affect strongly the internal structure and the stability of sphere packing. After the formation of the pile, the induced cohesion is decreased continuously along a linear decreasing ramp. The controlled collapse of the pile is found to generate

various and reproducible values of the random packing fraction. [New Journal of Physics **9,** 406 (2007)]

Compaction dynamics

The influence of a magnetic interaction between the grains on the compaction dynamics of a granular pile submitted to a series of taps is investigated. The granular material used to perform this study is a mixture of metallic and glass grains. The packing is immersed in homogeneous external magnetic field. The magnetic field induces an interaction between the metallic grains that constitutes the tunable cohesion.

The compaction characteristic time τ and the asymptotic packing fraction η_∞ have been measured as a function of the Bond number Bo which is the ratio between the cohesive magnetic force and the grain weight. These measurements have been performed for different fractions of metallic beads in the pile. When the pile is only made of metallic grains (see Figure 2), the characteristic compaction time increases as the square root of the Bond number. While the asymptotic packing fraction decreases as the inverse of the Bond number. For mixtures, when the fraction of magnetized grains in the pile is increased, the characteristic time increases while the asymptotic packing fraction decreases. A simple mesoscopic model based on the formation of granular chains along the magnetic field direction is proposed to explain the observed macroscopic properties of the packings. [Phys. Rev. E **80**, 041302(2009)

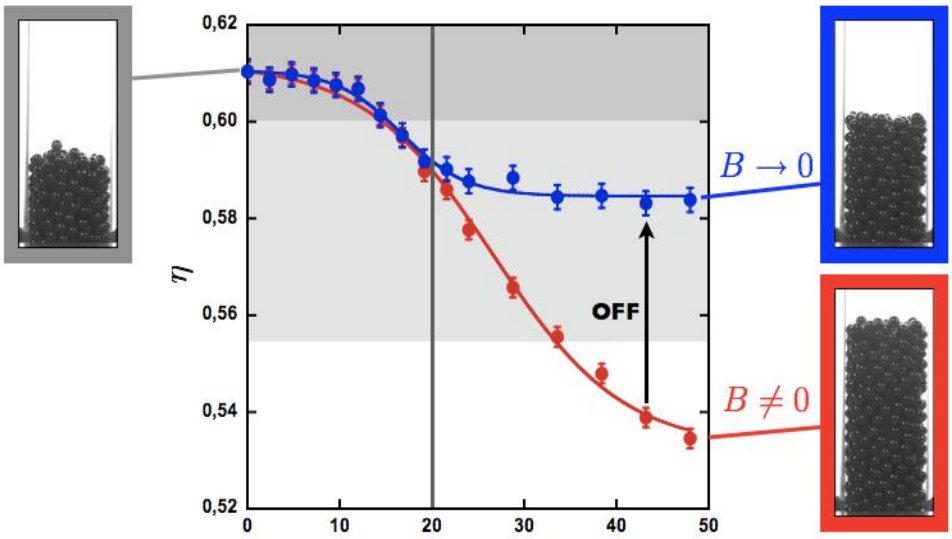


Figure 1. (in red) Packing fraction η as a function of the applied magnetic field B (expressed in Gauss). (in blue) Packing fraction $\eta_{B\to 0}$ after switching off the magnetic field. Hyperbolic tangent curves, fitting the data, are guides for the eye. The dark grey region denotes the usual RCP values, while the light grey region represents settling (RLP) experiments. The vertical line at B = 20 Gauss corresponds to the situation for which the magnetic force between two contacting grains along the magnetic field is equal to the weight of a grain. Snapshots of the upper grains, just above the coils illustrate the changes of the packing arrangements.

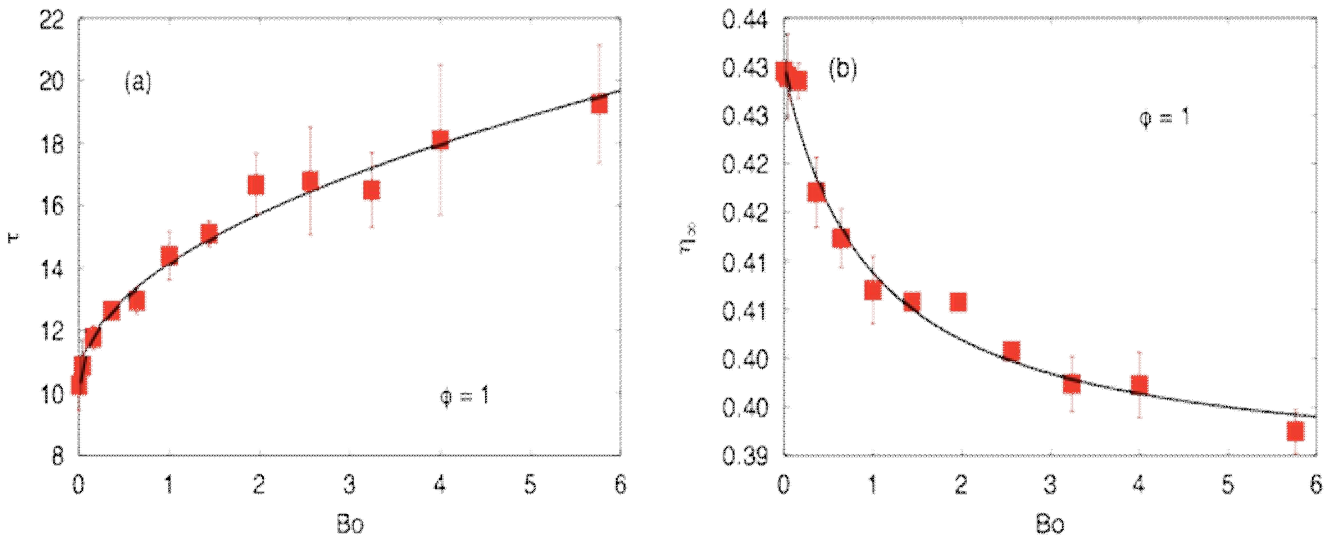


Figure 2. (a) Evolution of the compactions characteristic time τ as a function of the Bond number Bo, i.e. the ratio between the magnetic force acting on two contacting grains and the weight of one grain. The continuous line is a fit with a square root law $\tau = \tau_0 + a\ Bo^{0.5}$. The only fitting parameters is a = 3.8 +/- 0.2. The value of the characteristic time when Bo = 0 is $\tau_0 = 10.3$. (b) Decrease of the asymptotic packing fraction η_∞ with the Bond number Bo.

Flow in a rotating drum

The influence of a magnetic interaction between the grains on the flow of a granular material in a rotating drum is investigated. The magnetic cohesion is induced by applying a homogeneous external magnetic field B oriented either parallel or perpendicular to the gravity g. The drum rotating speed has been selected to obtain a continuous flow when the magnetic field is switched off. We show that, for both magnetic field orientations, the cohesion is able to induce a transition between the continuous flow regime to the discrete avalanche regime (see Figures 3 and 4). The avalanche dynamics is periodic when $B \perp g$ and irregular when $B \| g$. Moreover, the maximal angle of stability θ_m increases strongly with the cohesion strength and could be higher than 90° when $B \perp g$. A toy model based on the stability of a magnetic block on a magnetic inclined plane is proposed to explain this behavior. [Phys. Rev. E **82**, 040301 (2010)]

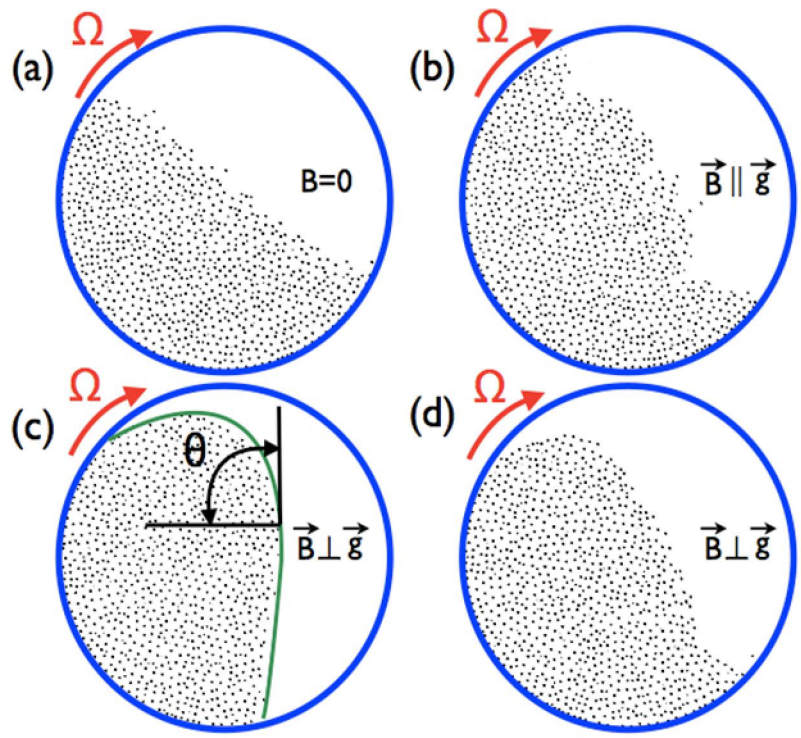


Figure 3. Snapshots of the granular flow inside the drum rotating at an angular speed Ω for different orientations of the magnetic field **B**. (a) The magnetic field is off. (b) **B** // **g** and the value of the Bond number, i.e. the ratio between the magnetic force acting on two contacting grains and the weight of one grain, is Bo=10. (c) and (d) **B** ⊥ **g** and Bo=10. The snapshot (c) and (d) have been taken respectively just before and after an avalanche. The measurement of the angle θ is schematized on snapshot (c).

Cohesion in well known powders

The studies performed with the model cohesive granular material have shown that the cohesive forces decrease the packing fraction, slow down the compaction dynamic and increase both angle of repose and flowing angle. Moreover, the cohesion induces some fluctuation of the flow. These conclusions have been checked with a set of well known powders: silicon carbide abrasives and flours. [Powder Technology **224**, 19 (2012)]

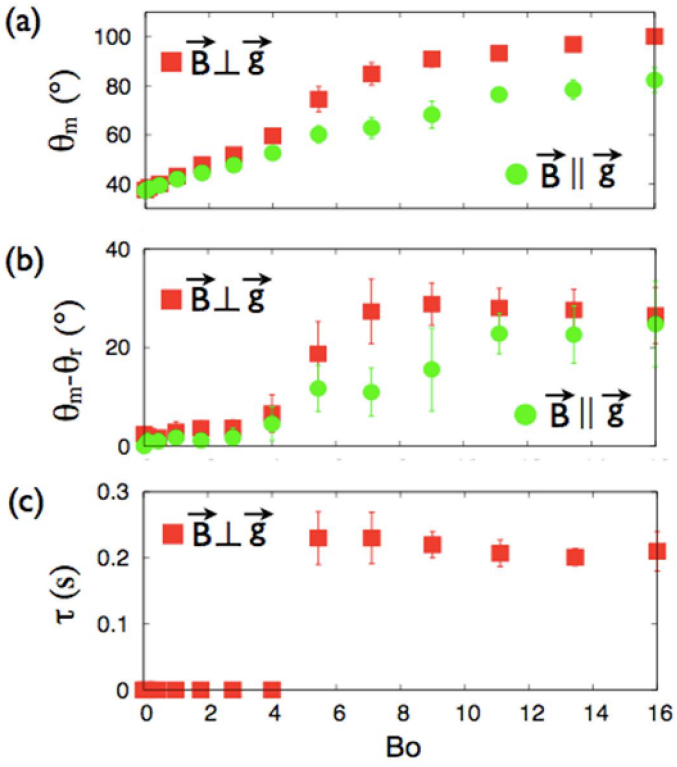
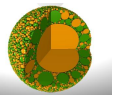


Figure 4. (a) Evolution of the maximum angle of stability θ_m as a function of the Bond number Bo for the two orientations of the magnetic field. (squares) $\mathbf{B} \perp \mathbf{g}$. (circles) **B** // **g**. The maximum angles θ_m and the repose angles θ_r have been calculated from five sets of data. (b) Evolution of the avalanche angular amplitude θ_m-θ_r as a function of Bo. (c) Average avalanche time τ as a function of Bo. The values of τ are not displayed for the case **B** // **g** due to the large fluctuations found in the measurements.

Conclusion

The effect of cohesive forces inside a granular assembly on the macroscopic properties of the pile has been analyzed experimentally with a model system. This model cohesive granular material is made of soft ferromagnetic grains inside a tunable magnetic field. The magnetic field allows to adjust the cohesion between the grains. The influence of the magnetic cohesion on (i) the packing fraction, on (ii) the compaction dynamics and on (iii) the flow has been analyzed. The cohesion is able to stabilize a pile with a low packing fraction and slow down the compaction dynamics. The flow is also drastically affected by the magnetic interactions. Due to the anisotropy of the magnetic interaction, the orientation of the field according to the gravity is an important parameter. Finally, The results obtained with this model cohesive granular material have been extrapolated to real powders.



Performing of the momentum dynamics in 1D models of granular systems

O. Gerasymov and A. Spivak

Department of General and Theoretical Physics
Odessa State Environmental University, Ukraine

During a few recent decades, the scientific community shows a heightened interest to the investigation of complex open systems where the energy dissipation results in the initiation of essentially nonlinear dynamic processes. Among such systems, one undoubtedly rates is so-called granulated materials (GMs). GMs consist of a large number of particles (granules) with complex surface morphology and wide size dispersion. The interaction between granules takes place only due to inelastic collisions. Therefore GMs represent the example of an open system that particularly does not obey the energy conservation law.

The complexity of processes which occur in GMs stimulates their studying with the help of simple models, where particles interact inelastically, whereas the energy dissipation is compensated due to supply from boundaries. Direct physical experiments with GMs ([1]) testify the possibility of asymptotic stationary states to exist in them. This open, the principle, possibility of the application of statistical mechanics methods to their investigation.

The one-dimensional models of granular systems can facilitate a better understanding of physical processes in such structures and could be interpreted as the first step in the investigation of more complicated three-dimensional systems.

The physical problem of transport of the impulse impacted from the boundaries into inhomogeneous nonlinear 1D system of beads have been intensively studied by many authors, see for instance [1–9]. We consider the general problem of the impulse propagation in gravitationally preloaded granular chain. We show that the equation of motion for the propagating momentum, formulated in form of difference-differential equation adopt analytical solution expressed by means of Bessel functions of an integer order.

1. Deterministic Stationary States in a Vertical 1D System of Inelastic Particles

Let us consider a system of N structureless particles of equal mass located vertically in vacuum (in the absence of friction) in the field of gravity forces $\vec{g}$. The energy losses due to binary collisions between particles can be compensated at the expense of the reflection of the lower particle from the horizontal “hot” solid substrate which represents, thus, an energy source for the system. In the case where such a reflection is absolutely elastic, the system is practically closed. In contrast, in the case where the hot substrate is able to supply an arbitrary (but definite) energy to the system, the latter is open.

The proposed model is constructed in such a way that, at arbitrary velocities of

collision of an incident particle with the substrate, the velocity at the time moment of reflection also has the same constant value (let it be ω_0). Generally speaking, ω is the quantity distributed with certain weight $\Phi(\omega)$. In our model, the initial velocity after a collision with the substrate obeys the distribution in the form of the Dirac delta-function $\Phi(\omega)=\delta(\omega-\omega_0)$.

Due to the binary character of collisions, the velocities of the particles before a collision (ω_1, ω_2) and after it (ω_1', ω_2') satisfy the following relations:

$$\omega_1' = \omega_1 - \frac{1+\varepsilon}{2}\omega_{12}, \qquad \omega_2' = \omega_2 + \frac{1+\varepsilon}{2}\omega_{12}, \tag{1}$$

where $\omega_{12}=\omega_1-\omega_2$; ε denotes the inelastic loss coefficient (at $\varepsilon=1$, collisions are absolutely elastic and the summary kinetic energy conserves; at $\varepsilon<1$, dissipative energy losses take place).

In the postulated stationary state, the periods of motion of the particles between collisions are equal to certain constant T_N.

Taking into account the uniformly accelerated character of motion of particles between collisions, we obtained the following expression for the oscillation period T_N [1]:

$$T_N = \frac{2\omega_0}{g}\cdot\left[N+\frac{1-\varepsilon}{3(1+\varepsilon)}(N-1)(2N-1)\right]^{-1}. \tag{2}$$

Thus, as follows from (2), the period of the oscillatory motion of the N-th particle in the stationary state in the constructed model system depends on all parameters of the model ω_0, g, and ε and reaches its maximal or minimal values in the limits of absolutely elastic ($\varepsilon=1$) and inelastic ($\varepsilon=0$) collisions, respectively.

The stationary motion in such a model system leads to the vertical stratification (i.e. layering) of the system into a sequence of intervals, within every of which the corresponding particles participate in a simple periodic motion (see Fig.1). In this case, collisions within every pair of particles occurs in framework of relevant fixed length intervals.

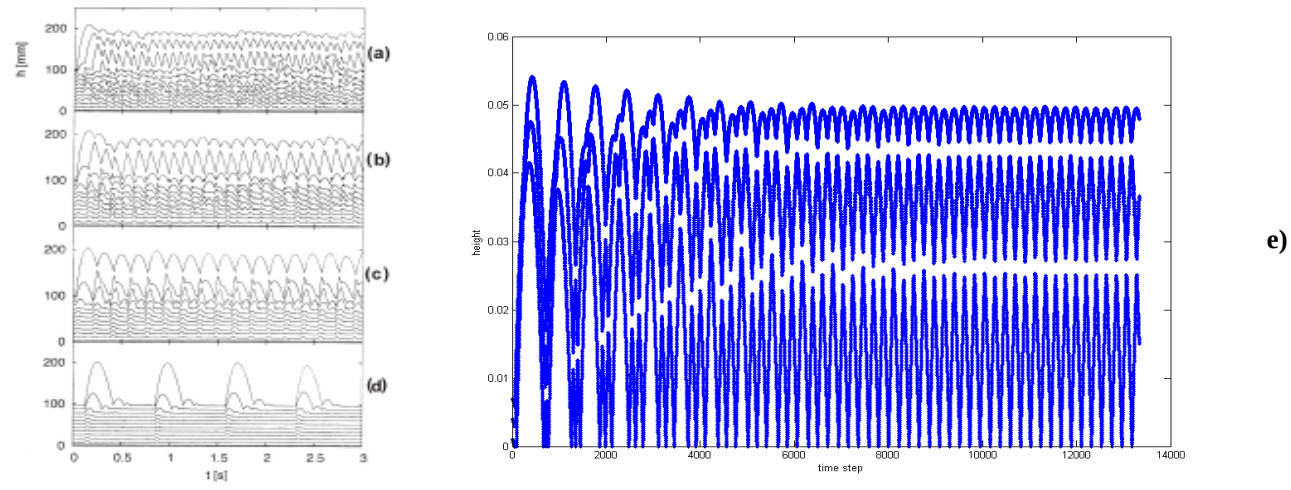
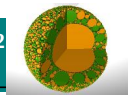


Fig. 1. Trajectories (in real spice) of grains in column of beads subjected to gravity under the vertical tapping (a, b, c, d – correspondent to the following frequencies of tapping: a) – 13.8 Hz; b) – 8.93 Hz; c) – 5.61 Hz; d) – 1 . 37Hz) [1]; e) numerical calculation of stationary states in a vertical 1D system of 3 inelastic particles in a gravitational field.



The size of the system, where the described stationary motion occurs, can be found with the help of the formula

$$L = \frac{gT^2}{8}\cdot\left(1+4\sum_{i=1}^{N-1}\frac{A}{(1+A)^2}\left(1+2(N-i)\right)\right), \qquad (3)$$

where $A = \dfrac{(1+2\varepsilon)-(1-\varepsilon)(N-i)}{(2+\varepsilon)+(1-\varepsilon)(N-i)}$ denotes the ratio of the time, during of which the i-th particle moves upward, to the time, during of which it moves in the opposite direction. Every distinctive term in (3) determine the size of the corresponding interval, where the i-th particle performs their periodic motion. The condition, where at least one of these terms becomes negative, corresponding to the criterion of decay of the constructed stationary state:

$$\varepsilon \geq \varepsilon_c = (N-2)/(N+1) \qquad (4)$$

It follows from relation (4) for the critical value of the inelastic loss coefficient ε_c that, for systems that include only one or two particles, the stationary states are formed for arbitrary small values of ε. If the number of particles in a system exceeds two, then the stationary states exist under condition of the particular condition for the coefficient of inelastic energy losses.

Thus, the asymptotic states cannot exist in the large enough systems with a strongly inelastic collisions. Therefore within the considered model stationary state practically does not exist at sufficiently large N, i.e. in the case of large size systems.

The obtained results testify to the fact that, in large-scale systems or systems with strong dissipation, the supply of energy to the system from outside is insufficient for the creation of the existence conditions for stationary states (the dissipative and external energy flows cannot stably compensate one another).

2. Horizontal 1D System of Inelastic Particles

Now let us consider the problem of stability of a stationary state by the example of a one-dimensional system consisting of two inelastic particles. The hot boundary of the system is specified in such a way that the particle nearest to the wall always reflects from it with the same constant velocity v_0. The reflection of the second particle from the opposite side is performed absolutely elastically, i.e. without any energy losses.

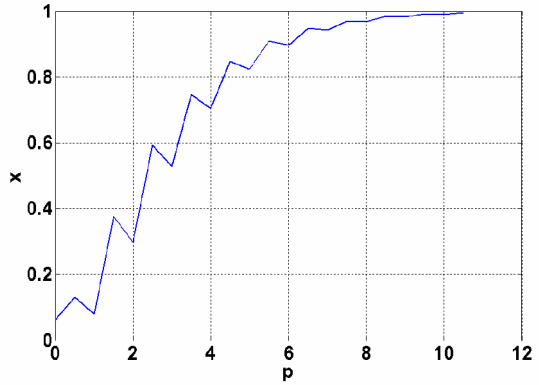
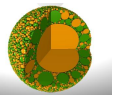


Fig. 2. Numerical simulations of the position of particles plotted against the number of collisions. (L=1, v_0 =1, ε =0.5, v_1 =0.0250, w_2 =0 .675, x_0 =0 .0632).

Finally the described system tends to a stationary state after a series of collisions. One can obtain the following recurrent relation for the velocity:

$$v_{k+p} = \varepsilon^p (v_k - v_\infty) + v_\infty, \qquad (5)$$

where v_∞ is the velocity of a particle which corresponds to the motion in the stationary mode. From numerical simulation one can see that $\lim_{p\to\infty} x_p = L$ (Fig.2).



Therefore it is convenient to describe the kinetic processes which occurs in GMs with the help of the relevant order parameter [10].

Let determine the order parameter $\varphi(p)$ of the considered system as follows: $\varphi(p)=(v_{k+p}-v_k)/(v_\infty-v_k)$. Using (5), we obtain the equation for $\varphi(p)$:

$$\varphi(p)=1-\varepsilon^p. \qquad (6)$$

It is follows from (6) that, with increasing of the coefficient of inelastic energy losses ε, the relaxation time τ_0 increases. When $\varepsilon\to 1$, $\tau_0\to\infty$. Therefore system does not tend to quasistationary state even asymptotically. This results was also is confirmed experimentally [11].

3. Modeling of momentum transition in inhomogeneous granular chain

Consider the system which is organized as a vertical column of identical grains. The current displacement φ_n of the n-th grain which belong to the system satisfies the following linearized equation of motion [12]:

$$\frac{d^2\varphi_n}{d\tau^2}=\kappa_n\varphi_{n+1}-(\kappa_n+\kappa_{n-1})\varphi_n+\kappa_{n-1}\varphi_{n-1}, \qquad (7)$$

where $\tau=t\sqrt{g\delta}(\gamma/g)^{1/2\delta}$ - rescaled time, $\gamma=E\sqrt{d}/\left[3m(1-\nu^2)\right]$ - is a force constant, m - is a mass of an individual grain, d - is the diameter of an unloaded particle, E - is a Young elastic modulus, ν - is the Poisson ratio [13]. Here $\kappa_n=n^{1-1/\delta}$ can be treated as a new force constant which becomes dependent on the position (on the number of the beads) in the column (the character which happens due to presence of gravity). The exponent δ could reach different values. Hertzian contacts between beads give $\delta=3/2$. Note, that in what follows we will ignore the role of dissipation in the present study. The equations of type Eq.(7) belong to class of difference-deferential equations which is a case of functional-differential equations [14].

When $\delta=1$, in this case $\tau=t\sqrt{\gamma}$ and $\kappa_n=1$, therefore we can write Eq.(7) in the follows form

$$\frac{d^2\varphi_n}{d\tau^2}=\varphi_{n+1}-2\varphi_n+\varphi_{n-1}, \qquad (8)$$

Note the expression on the right side of Eq.(8) is the finite-difference approximation to the second order partial derivative. As it was shown in [12,14] this equation has a rigorous solution:

$$\varphi_n(\tau)=C\cdot J_{2n}(2\tau), \qquad (9)$$

where J_{2n} is a Bessel function of an integer order (see Fig.3). The solution in form of linear combination of functions like (9) formally can satisfy to an appropriate initial conditions.

Therefore, the rigorous solution of the linearized equations of motion which governed the moments propagation in inhomogeneous granular chain shows oscillation behavior as a function either of rescaled time τ or against number of position n. The solution of type (9) valued in every internal points of the system.

In order to satisfy Eq.(8) to appropriate boundary conditions we construct the linear combination of the functions, given by Eq.(9). For instance, the linear form

$$\varphi_n(\tau)=x_0\cdot\left[J_{2n-2}(2\tau)+J_{2n}(2\tau)\right], \qquad (10)$$

as it is shown on Fig.3a almost accurately reproduce the data of numerical simulations made for Eq.(8) under the $\delta = 1$ and under the following boundary conditions

$$\varphi_1(0) = x_0, \quad \dot{\varphi}_1(0) = 0 \tag{11}$$

(which is the case of excitation by means of deterministic shifting of the out-most grain in the chain).

The dynamic excitation which correspond to the following boundary conditions:

$$\varphi_1(0) = 0, \quad \dot{\varphi}_1(0) = v_0. \tag{12}$$

The solution of Eq.(8) which satisfy the boundary conditions (12) can be written down by means of following linear transformation

$$\varphi_n(\tau) = v_0 \cdot \int_0^{\tau} [J_{2n-2}(2\tau) + J_{2n}(2\tau)] d\tau \,. \tag{13}$$

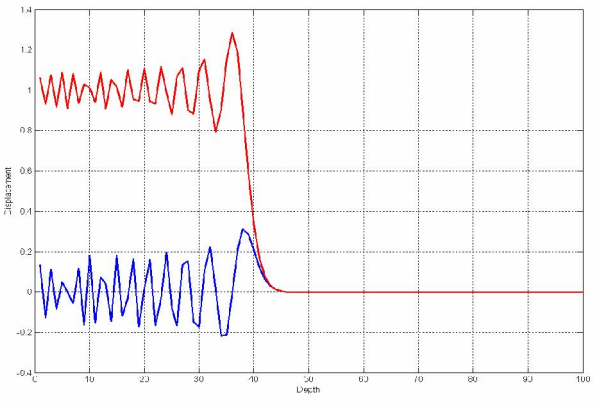


Fig.2. Displacement (φ_n) plotted against the depth (n): theoretical curve which follow from Eq.(9): for static excitation (blue) and for the dynamic excitation (red).

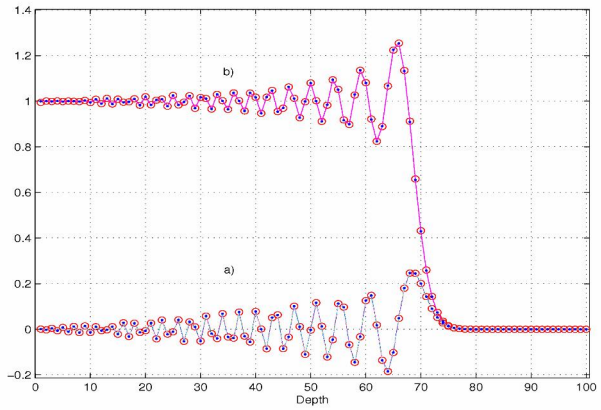


Fig.3. Displacement (φ_n) plotted against the depth (n): numerical simulation of Eq.(8) - lines, theoretical curve which follow from Eq.(10) and Eq.(13) - circles, a) for static excitation, b) for the dynamic excitation, respectively.

On Fig.3b the comparison between the data of numerical simulations made for Eq.(8) and theoretical results which follow from Eq.(10) end Eq.(13) are presented.

Analyzing the data shown on a Fig.3 one can conclude that momentum dynamics in weakly inhomogeneous granular chain could not be described in a single wave approximation.

Consider now the case of multiple signal reflections from the boundaries of the finite system when occurs the superposition of the reflected and incident waves. We found that the relations (10) and (13), can be satisfied by the following functions:

$$\varphi_n(\tau) = x_0 \cdot \sum_{k=1}^{K} sign(v)[J_{v-1}(2\tau) + J_{v+1}(2\tau)], \tag{14}$$

$$\varphi_n(\tau) = v_0 \cdot \sum_{k=1}^{K} sign(v) \int_0^{\tau} [J_{v-1}(2\tau) + J_{v+1}(2\tau)] d\tau \,, \tag{15}$$

where $v = sign(\sin\frac{\pi k}{2})\cdot(2n-1) + sign(\cos\frac{\pi k}{2})\cdot(k - mod(k,2))(2N-1)$, K - multiplicity of the signal along chain. On Fig.4 the proposed approximations are shown.

When $\delta = 3/2$ (Hertzian-chain) the solution of Eq.(7) which corresponds to dynamic excitation, can be approximated by the following expression

$$\varphi_n(\tau) = \mathrm{v}_0 \cdot \left(\frac{\eta}{2}\sqrt{\kappa_n}\right) \cdot \int_0^{\tau} \left[J_{2n-2}\left(\eta\sqrt{\kappa_n}\tau\right) + J_{2n}\left(\eta\sqrt{\kappa_n}\tau\right)\right] d\tau\,, \quad \text{where } \eta = 1 + \frac{1}{\delta}. \qquad (16)$$

On Fig.5 the result of numerical calculations performed by means of analytical formulas are represented.

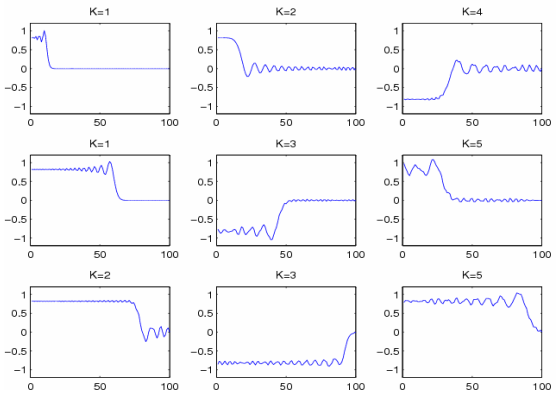


Fig.4. Displacement (φ_n) plotted against the depth (n): numerical simulation of Eq.(8) for case of multiple signal reflections from the boundaries in the system ($N = 100$), with initial condition: $\varphi_1(0) = 0,\ \varphi_1'(0) = v_0$.

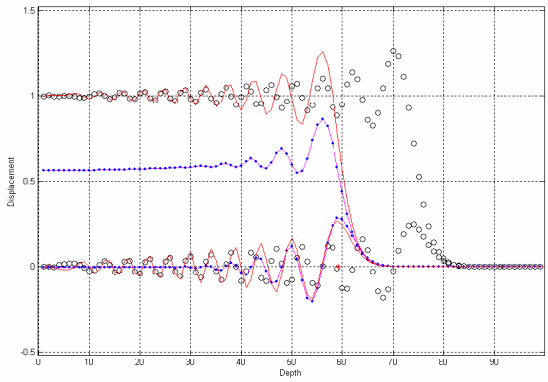


Fig.5. Numerical simulations (denoted by points) of Eq.(7) for the displacement φ_n against depth (n); analytical solution (solid line) of Eq.(16).

We demonstrate the possibility of existence the deterministic stationary states in 1D model of Hertzian chains which approached asymptotically. It has been shown the multiwave character of the solution of differential-difference equation of motion which governed the momentum transmission in inhomogeneous Hertzian chain under the condition of weak inhomogeneously.

Reference

[1] O.I.Gerasymov, N.Vandewalle, G.Lumay, S.Dorbolo, A.Ya.Spivak, N.Khudyntsev, O.Klymenkov, Ukr. Fiz. Zh. 53 (2008) p.1128.
[2] E.Fermi, J.Pasta, S.Ulam, Los Alamos Sc.Lab.Rep. LA-1940 (1955) p.978.
[3] V.T.Zakharov, A.V.Shabat, Zh.Eksp.Teor.Fiz.(JETP) 619 (1971) p.118.
[4] P.L.Bhatnagar, *Nonlinear waves in one dimensional dispersive systems*, Clarendon, Oxford, 1979.
[5] V.Nesterenko, *Dynamics of Heterogeneous materials*, Springer, New York, 2001.
[6] C.Coste, E.Falcon, S.Fauve, Phys. Rev. E 56 (1997) p.6104.

[7] S.Sen, J.Hong, J.Bang, E.Avalos, R.Doney, Phys. Rep. 462 (2008) p.21.
[8] E.Avalos, T.Krishna Mohan, S.Sen, Phys. Rev. E 67 (2003) p.060301(R).
[9] E.Falcon, C.Laroche, S.Fauve, C.Coste, Euro. Phys. J. B 5 (1998) p.111.
[10] O.I. Gerasimov, P.P.-J.M. Schram, and K. Kitahara, Ukr. Fiz. Zh. 48 (2003) p.885.
[11] F. Cantelaube and D. Bideau, Europhys. Lett. 30 (1995) p. 133.
[12] O.I.Gerasymov, N.Vandewalle, Dopov. Nac. akad. nauk Ukr. N8 (2012) p.67.
[13] L.D.Landau, *Theory of elasticity*, 3rd ed. Butterworth-Heinemann, 1986.
[14] E.Pinney, *Ordinary Difference-differential equations*, University of California Press, Berkley and Los Angeles, 1955.

Packing of wires in cavities and growing surfaces

Hans Herrmann

ETH Zürich, Switzerland

We investigate the morphologies and maximum packing density of thin wires packed into spherical cavities. Using simulations and experiments with nylon lines, we find that ordered as well as disordered structures emerge, depending on the amount of internal torsion. We find that the highest packing densities are achieved in a low torsion packing for large systems, but in a high torsion packing for small systems. An analysis of both situations is given in terms of energetics and comparison is made to analytical models of DNA packing in viral capsids. In two dimensions we also find that wires can crumple into different morphologies and present the associated morphological phase diagram. Our results are based on experiments with different metallic wires and confirmed by numerical simulations using a discrete element model. We show that during crumpling, the number of loops increases according to a power-law with different exponents in each morphology. Furthermore, we observe a power-law divergence of the structure's bulk stiffness similar to what is observed in forced crumpling of a membrane. We also investigate the morphology of thin discs and rings growing in circumferential direction. Recent analytical results suggest that this growth produces symmetric excess cones (e-cones). We study the stability of such solutions considering self-contact and bending stress. We show that, contrary to what was assumed in previous analytical solutions, beyond a critical growth factor, no symmetric e-cone solution is energetically minimal any more. Instead, we obtain skewed e-cone solutions having lower energy, characterized by a skewness angle and repetitive spiral winding with increasing growth.

These results are generalized to discs with varying thickness and rings with holes of different radii. Simple experiments with cardboard confirm the simulations.

Towards the studying of structure of the granular matter

O. Gerasymov, M. Somov

Department of General and Theoretical Physics,
Odessa State Environmental University, Ukraine, Odessa

Granular materials is one of the representatives of soft matter. They are large conglomerations of discrete particles. The size of particles typically varies from few micrometers to few meters. In general the interaction between particles are nonlinear and dissipative. Even being at rest the g.m. are nonequilibrium systems which naturally being in metastable state. The main energy scale in g.m. is their energy in the external field (for instance gravity) which in together with boundary condition influence on the geometry of volume. The ordinary temperature plays no role and thus g.m. are nonequilibrium.

Being complex (dissipative) system, g.m. demonstrate properties which are similar to regular states of matter and at the same time can behave differently from them under special condition.

For instance, experimental investigation of 2D g.m. show the existence of crystal structure with hexagonal ordering which coexist of clusters with different symmetries and transitions between them. A lot of these effects appears in many other systems such as magnetic fluids and g.m., dusty plasma, water drops cluster, etc.

Another type of observable structures of g.m. is s.c. jammed state, in which could be observe the freezing. The first order phase transition between ordered and disordered types of structures are also observed in g.m.. The observed clusterization of local structure are developed in meso- and even in macroscale.

Here we focused in problem of parameterization (quantitative and qualitative) of local structure in meso- and macroscale by means of geometrical and structure invariants methods.

The role of entropy effects in local configurations will be also discussed.

Structure of 2D granular materials

An experimental investigations of 2D granular materials and some other objects of soft matter in meso- and macroscale show that observable structures are similar to some regular (crystallic) states of matter. Transition between states with different symmetries are realized along the variety of scenarios. The character of these scenarios depends on the initial conditions, dimensionality of the system, dissipation, external fields.

On Figure 1 it is shown the picture of real 2D granular systems of discs on surface [1]. Black dots represent positions of the centers of mass of discs. Here we

observe formation of hexagonal clusters in this system. The same structures have been observed in completely different system – dusty plasma [2].

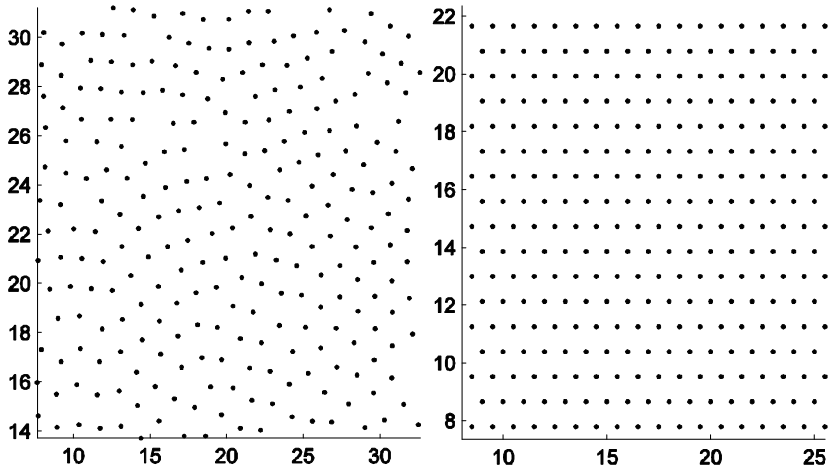


Figure1 - Picture of granular materials in real space (on a left– disordered state; on a right– ordered state with hexagonal symmetry).

The further structure analysis will be developed by means of Voronoi diagram method. To determine Voronoi cell we must enclose the space around the center of each particle which contains all points that much closer for it than another one. On Fig.2 Voronoi diagrams for observed types of structures in 2D systems are depicted.

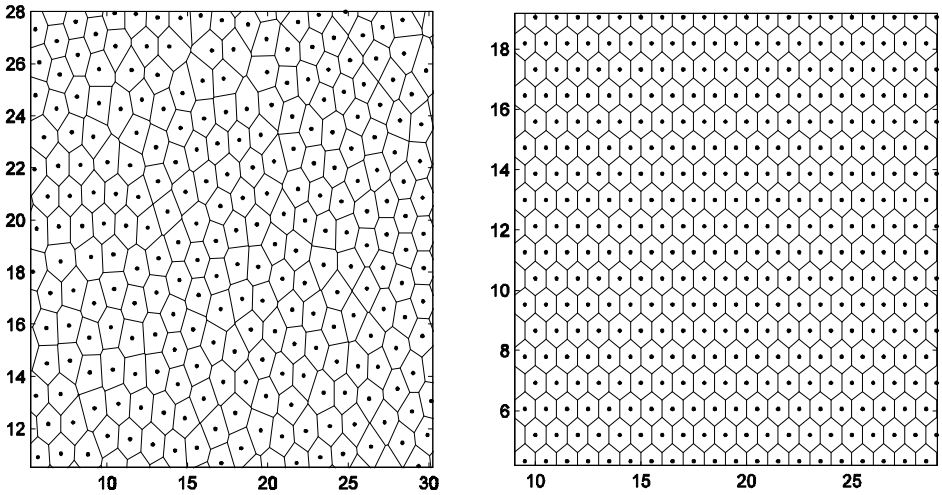


Figure 2 - Voronoi diagrams for 2D g.m. shown in real space on Fig.1.

Obtained results testifies that local structure of different systems in mesoscale has a lot of similarities such as crystallization with preferable hexagonal symmetries.

Anisotropy of the structure of granular materials

The quantitative description of local structure of granular materials has been made in [3] by means of considering of the discrete set of points with certain coordinates of particles which surround center of coordinates.

Along this way geometrical structure $\{G_\alpha\}$ could be identify by means of comparing it with "ideal" set $\{\Gamma_\alpha\}$. Information about "ideal" state could be obtained from alternative sources about structure.

In terms of this approach every states of considered systems can be interpreted as a deviation from ideal set $\{\Gamma_\alpha\}$.

In order to describe transformations of the local structure one can introduce the order parameters and build phase diagram for them. Turning back to set of vectors $\{\vec{r}_\alpha\}$, which determine particle configurations, we limitate them by certain scale r_0. For instance, r_0 could be radii of coordination spheres or lattice constant.

Let introduce the orientation order parameter which defined as follows

$$g_n = \frac{1}{N_n} \cdot \sum_1^{N_n} \exp(iN_n\varphi_n) \qquad (1)$$

where N_n - is a number of particles in n-th shell, φ_n - is relative angle between radii-vectors of given particle in n-th shell and the central one.

Translational order parameter can be introduced as

$$u_2^2 = \frac{1}{N}\sum_i \left[\left\langle |\vec{r}_i|^2 \right\rangle - \left\langle |\vec{r}_i| \right\rangle^2\right], \qquad (2)$$

where N - is a number of particles in the given shell;

$\left\langle |\vec{r}_i|^2 \right\rangle$ - is a mean value of square distance between central and neighboring particles in shell;

$\left\langle |\vec{r}_i| \right\rangle^2$ - is the square of mean distance between central particle and particle in shell under consideration;

The order parameters (1), (2) was performed for the structures showed on Fig. 1.

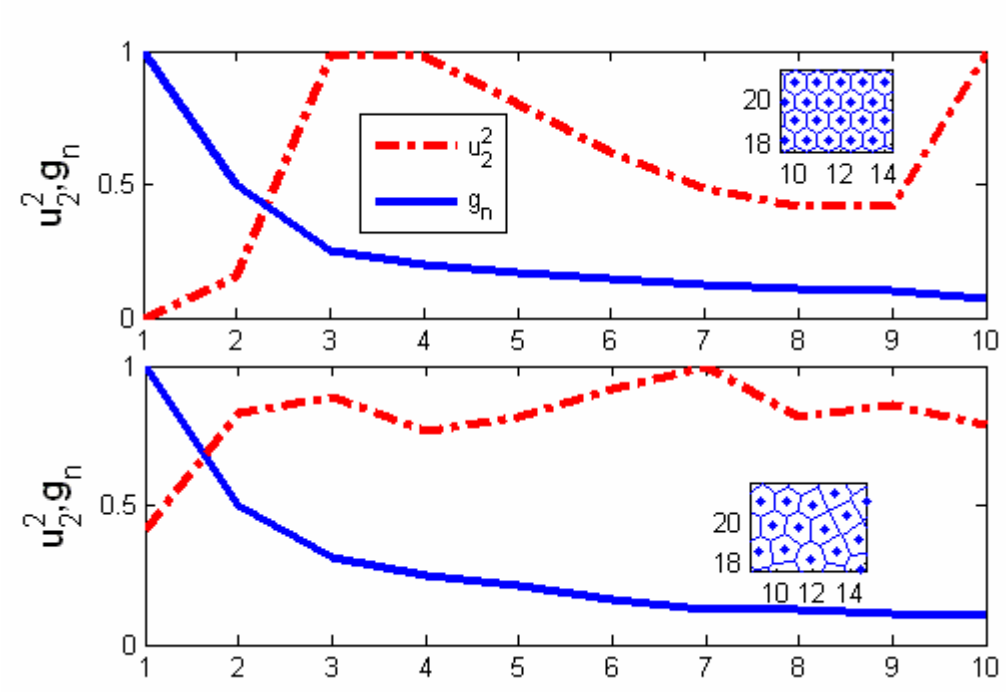
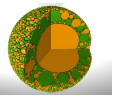


Figure 3 - Phase diagrams constructed in terms of translational and orientation order parameters for structure presented on Fig.1.



Obtained results show that granular systems naturally are anisotropic. The consequent theoretical description of this systems is complicated in particular, because their anisotropic character.

Vertical density profile in granular materials

An external perturbation of granular systems induces the decreasing of occupied volume. However, an adequate theoretical description of these phenomena is one of the key problem in physics of granular materials. The description of the systems under consideration is complicated by the fact that the standard approaches of statistical physics cannot be used through their non-thermodynamical character and due to absence of equilibrium potential of interparticle interaction.

In order to describe vertical density profile of g.m. we will use the concept of quasistatistical approach. On this way for “inherent” states the free energy functional of the system can be written in form

$$F(\rho) = E(\rho) - \beta^{-1} S(\rho), \tag{2}$$

Where the free energy of the system $E(\rho)$ in gravity field is given by

$$E(\rho) = mg \int\limits_{(V)} z\rho(\vec{r})d\vec{r}, \tag{3}$$

here z - vertical coordinate, β^{-1}- energy scale, ρ - density of the system.

For the $S(\rho)$ we will use well known relation for entropy of lattice gas [4]

$$S(\rho) = -\int\limits_{(V)} d\vec{r}\left\{\frac{\rho}{\rho_0}\ln\frac{\rho}{\rho_0} + \left(1-\frac{\rho}{\rho_0}\right)\ln\left(1-\frac{\rho}{\rho_0}\right)\right\}, \tag{4}$$

where ρ_0 - maximal density of the system.

Calculation of variation derivative $\frac{\delta F(\rho)}{\delta\rho}$ bring us to the density profile in form similar to Fermi-like function

$$\rho(\vec{r}) = \frac{\rho_0}{1+ce^{\Gamma z}}, \Gamma = mg\rho_0\beta \quad . \tag{5}$$

c- constant, which can be determined by comparing with experimental data

The same form of (5) was used in [5] for effective parameterization of experimental vertical density profile in g.m..

We now consider our system in the vicinity of maximum compactivity. Thus, the weak deviation from this state can be interpreted as “melting” of state with given symmetry. In solid state theory for quantitative description of melting often used s.c. Lindemann criteria. It can be written in following form [6]:

$$\gamma_m = \sqrt{\left\langle \left(r - \langle r\rangle\right)^2\right\rangle} \Big/ L \quad , \tag{6}$$

where r – distance between neighboring particles in given state, L – lattice constant, $\langle r \rangle$ - mean distance between neighboring particles in state with given symmetry.

In terms of proposed model the Lindeman-like criteria can be written down as follows

$$\sqrt{z^2 - \langle z \rangle^2} \Big/ L = \frac{\rho_0 c}{\Gamma^2} \cdot A,$$

$$A = \left\{ \rho \frac{\ln^2 \frac{1}{c}\left(\frac{\rho_0}{\rho} - 1\right)}{c\rho_0} - \frac{1}{c}\ln^2 \frac{1}{c} \cdot \left(\frac{\rho_0}{\rho} - 1\right) - \right. \tag{7}$$

$$\left. - 2\left[\ln c \ln \frac{\rho_0}{\rho} + Li_2\left(\frac{\rho_0}{\rho}\right)\right] - \rho_0 c \left[\rho \frac{\ln c}{\rho_0} - \ln \frac{\rho_0}{\rho} + \frac{\frac{\rho_0}{\rho} - 1}{\frac{\rho_0}{\rho}} \ln\left(\frac{\rho_0}{\rho} - 1\right)\right]^2 \right\},$$

here Li_2 - is dilogarithm.

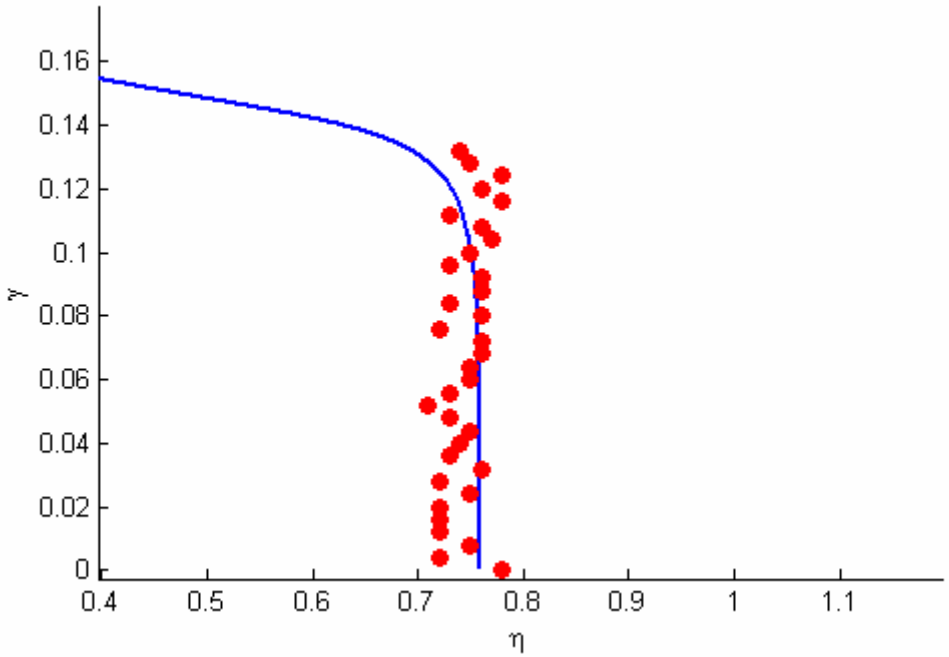
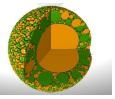


Figure 4 - Parameter γ plotted versus packing fraction η. Solid curve – represent theoretical data, dots- experimental measurements [5].

Obtained theoretical results qualitatively (and in the vicinity of maximally compacted states - even quantitatively) well enough satisfied to the data of experiments.

Entropy analysis of the structure of granular materials

An alternative approach in description of properties of manyparticle systems could be the direct modeling of radial distribution function. A simple expression of



RDF in terms of generalized function can be written down in the following form [7]:

$$g(\vec{r}) = \sum_{\{r_i\}} A_i \delta(r - r_i) \tag{8}$$

where r – is a distance between grains;

r_i - is a distance between particles in the state with given symmetry;

A – is a coefficient which can be determined with help of relevant normalization condition for RDF;

Such a function is able to reproduce the main maximum of RDF, which is correspond to most probable configuration of particles in the 1st coordination sphere. Consider behavior of entropy density, which is an adequate measure of every process which occurs in the system. For entropy excess density we can write down the familiar relation:

$$\frac{S - S_0}{V} = -\frac{k_Б \rho^2}{2} \int g(r) \ln g(r) d\vec{r} \tag{9}$$

Substituting $g(\vec{r})$ given by (8), after the trivial manipulation, one can obtain

$$\frac{S - S_0}{V} = -\frac{k_Б \rho^2}{2} \cdot \sum_{\{i\} \in \Omega}^{N} \ln A_i \tag{10}$$

where Ω - occupied volume, N – is a number of particles in Ω.

As one can see with the increasing of the number of particles the entropy excess also increased as well, and furthermore, the system during the ordering has a tendency to relax to more stable state.

Conclusion

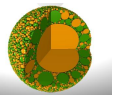
The structural ordering in meso- and macroscale which has been observed in granular materials and some other objects of soft matter (for instance in dusty plasma) has been studied by means of geometrical methods (Voronoi diagrams) and with the help of structural order parameters analysis.

It has been shown that structurization in mesoscale in the physically different systems has a lot of similar characters. Such as: the formation of short- and long-range ordering and tendency to transition to state with a definitive (preferably hexagonal) symmetry.

Studying the phase diagrams which are constructed in terms of translational and orientation order parameters show the naturally anisotropic character of the structure of granular materials.

It is shown that the transition to the ordered state with a given symmetry (or their melting) can be characterized by means of a Lindeman-like parameter. Along this the Fermi-like density profile either in 1D or in 3D granular system has been obtained.

The model of entropy of the lattice gas can be used to perform a vertical density profile of granular materials in the presence of gravity. Obtained theoretical results qualitatively (and in the vicinity of maximally compacted states - even quantitatively) well satisfied the data of experiments.



The possibility of the description of the structural transformation in terms of entropy analysis with help of structural measures expressed by means of generalized functions has been discussed.

References

1. Gerasymov O.I., Zagorodny A.G., Somov M.M., Ukr. J. Phys, Vol.58, N1 (2013) p.32. https://doi.org/10.15407/ujpe58.01.0032
2. F. Boyer, E. Falcon, Phys. Rev. Lett.103, 144501 (2009)
3. Gerasymov O.I., Ukr. Journ. Phys.-2010.-Vol.55, N 5.-P.586-592.
4. A. Isihara, Statistical physics (Moscow, 1973)
5. Holly Kokstein, Paul V. Quinn Sr., Physica A. 374, 1 (2007)
6. Kittel C., Introduction to solid state physics (Moscow, 1978)
7. Gerasymov O.I., Scattering of external radiation's in statistical systems. Solved models (Odessa, 1999)