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QUANTUM MECHANICAL APPROACH TO RANDOMLY-PACKED BEDS OF SPHERES IN THE CONTAINER*

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A b s t r a c t. In the paper a proposal for a new idea of description of granular materials is sketched. The quantum mechanical like theory is applied to the problem of the randomly packed spheres in the container.

K e y w o r d s: sphere packing, granular materials

INTRODUCTION

Randomly or regularly packed beds of spheres have been the subject of many papers and books. They constitute a relatively simple model not only for grains [1,2,5,7] or other materials in containers but also, e.g., in informatics, in the theory of error-correcting codes, some mathematical problems in number theory and algebra [3,4]. The problem is rather complicated. Till now even the highest density packing configuration of spheres in a rectangular container is unknown [3]. However, there are known solutions for a series of lattices which are partial solutions of the problem.

Our paper is a preliminary report on possible solution of the sphere packing problem and makes use of a quantum mechanics - like approach instead of standard geometrical considerations, or classical mechanics formalism. It seems to be reasonable to replace very complicated, for irregular packings, geometrical description, which requires solving rather complicated systems of non-linear equations of many variables or analysis of forces acting within spheres, by more homogenous boundary conditions for the quantum mechanical wave function.

Obviously the task is to solve the many-body problem which is still difficult enough. However, considerations along this line are interesting not only for the practical reasons mentioned above, but also as a more interdisciplinary problem of interacting particles with ''hard cores'' needed in physics, chemistry and technology.

THE MODEL

The Hamiltonian of the problem H consists of the kinetic energy term T, the potential well V_c describing the container, the potential of the gravitational field V_g and the short range interaction V_{int} within the spheres simulating their macroscopic properties:

$$H=T+V_c+V_g+V_{int}, \tag{1}$$

where

$$T=\frac{-\mathrm{h}^2}{2M}\sum_k \nabla^2(k), \tag{2}$$

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and

$$V_g = \sum_k M\,g\,(\vec{r}(k)\,\vec{e}_z), \tag{3}$$

with $\vec{e}_x, \vec{e}_y, \vec{e}_z$ denoting versors of the Cartesian frame (z-axis points out in vertical direction), h the Planck constant, M the mass of the sphere and g the gravitational acceleration constant. In the formulae $\vec{r}(k)$ are the radius vectors, dynamical variables for the k-th sphere.

As a possible model of container one can choose the container in the form of the "square" potential well with boundaries $\Gamma = <-l_x/2, l_x/2> \times <-l_y/2, l_y/2> \times <0, \infty)$:

$$V_c = \sum_k V_c(\vec{r}(k)), \tag{4}$$

where

$$V_c(\vec{r}(k)) = \begin{cases} 0, & \text{if } -l_x/2 \le \vec{r}(k)\vec{e}_x \le l_x/2, \\ & -l_y/2 \le \vec{r}(k)\vec{e}_y \le l_y/2, \vec{r}(k)\vec{e}_z \ge 0, \\ \infty, & \text{otherwise.} \end{cases} \tag{5}$$

A possible, interesting two-body interaction, which can simulate the behaviour of macroscopic spheres of the radius R, is of the following form:

$$V_{\text{int}} = \sum_{k<l} V_{\text{int}}(|\vec{r}(k) - \vec{r}(l)|), \tag{6}$$

where

$$V_{\text{int}}(|\vec{r}(k) - \vec{r}(l)|) = \begin{cases} V_\infty, & \text{if } |\vec{r}(k) - \vec{r}(l)| < 2R, \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

This type of interaction can also simulate, by allowing overlap among spheres, some mechanical properties of theses objects. In the case of $V_\infty = \infty$ one can exclude the situation when two spheres overlap and come back to the geometrical region. However, in this preliminary report we decided to use another type of the two-body interaction of a similar nature, but simpler in calculation and allowing for a geometrical interpretation. This is the contact δ-interaction:

$$V_{\text{int}} = \sum_{k<l} V_\infty \delta(|r(k) - \vec{r}(l)|), \tag{8}$$

where $\delta(\vec{r})$ is the standard *delta*-Dirac distribution.

In addition, we consider here only the static case and neglect the kinetic energy of the spheres. In this case we do not need to solve the eigenequation for the Hamiltonian. Instead, we chose the form of the single-particle (single-sphere) wave function which is able to simulate a macroscopic sphere of radius R at the position $\vec{R}_k$:

$$\phi_{\vec{R}_k}(\vec{r}_k) = \frac{1}{\Omega_0}\theta(R - |\vec{r}_k - \vec{R}_k|), \tag{9}$$

where

$$\theta(x) = \begin{cases} 1, & \text{if } x \ge 0, \\ 0, & \text{otherwise,} \end{cases} \tag{10}$$

and $\Omega_0 = 4/3\pi R^3$ represents the volume of the sphere.

Note that in principle all arguments of the functions should be dimensionless. To achieve this property one needs to choose a unit length, e.g., l_o=1m and use it as needed. However, by tradition this is not usually done and we will follow this simplification.

N spheres can be described, in the first approach, by the product of the single-particle functions (9):

$$|\vec{R}_1, \ldots, \vec{R}_N> = \prod_{i=1}^{N} \phi_{\vec{R}_i}(\vec{r}_i). \tag{11}$$

Because our spheres are in the rectangular container the space of states consists of the square integrable functions $L^2(\Gamma)$, where the "cube" $\Gamma = <-l/2, l/2> \times <-l/2, l/2> \times <0, \infty>$. Here, l is the length of x and y edges of the "cube". This physical condition restricts the range of the sphere positions and the vectors $\vec{R}_k$ in (9) must belong to Γ. The above implies the scalar product of the wave functions is given by:

$$<\psi_1/\psi_2> = \int_\Gamma d^3\vec{r}\,\psi_1(\vec{r})^*\psi_2(\vec{r}). \tag{12}$$

The eigenstates $|\psi_\nu>$ of the Hamiltonian (1) with the container and interaction given by Eqs (4-7) should describe the configurations of N hard spheres put into the box. They should allow us to find the positions of the spheres by calculating the following matrix elements (average position of k-th sphere):

$$<\vec{r}(k)>=<\phi_{\vec{R}_k}|\vec{r}(k)|\phi_{\vec{R}_k}>. \quad (13)$$

Having positions of the spheres one can calculate the contact numbers for the given configuration and the packing coefficient. Similarly, the eigenenergies $E(\nu)$ of H give the energies of the configurations determined by the sets of quantum numbers ν. This way one can obtain all characteristics needed in our problem. In our case we neglect the kinetic term in the Hamiltonian (1). In addition, we try to obtain only the macroscopic part of the energy. To this purpose one needs to calculate only the appropriate average values instead of solving the full eigenvalues problem.

Following this line we consider the energy of N spheres in the box. The total energy can be thus calculated as:

$$E_N(\vec{R}_1,...\vec{R}_N)=<\vec{R}_1,...\vec{R}_N|V|\vec{R}_1,...\vec{R}_N>. \quad (14)$$

Using the wave function (11) and writing explicitly the operator V (respectively to the formulae above) we obtain:
a) for the box-part potential:

$$<\vec{R}_1,...,\vec{R}_N|V_c|\vec{R}_1,...\vec{R}_N>=\int_{\Gamma^N} d^3\vec{r}_1...d^3\vec{r}_N$$

$$\left(\prod_{k=1}^{N}\phi^*_{\vec{R}_k}(\vec{r}_k)\right)\sum_{n=1}^{N}V_c(\vec{r}_n)\left(\prod_{k'=1}^{N}\phi_{\vec{R}'_k}(\vec{r}'_k)\right), \quad (15)$$

where the last expression is equal to 0 because the potential V_c=0 inside the box;
b) for the gravitational-part potential:

$$<\vec{R}_1,...\vec{R}_N|V_g|\vec{R}_1,...,\vec{R}_N>=$$

$$\sum_{n=1}^{N}\int_\Gamma d\vec{r}_n\phi^*_{\vec{R}_n}(\vec{r}_n)mg(\vec{e}_z\circ\vec{r}_n)\phi_{\vec{R}_n}(\vec{r}_n)=$$

$$mg\sum_{n=1}^{N}(\vec{e}_z\circ\vec{R}_n) \quad (16)$$

is a classical potential energy of the spheres in the gravitational field;
c) for the two-body contact interaction between the spheres:

$$<\vec{R}_1,...\vec{R}_N|V_{\text{int}}|\vec{R}_1,...\vec{R}_N>=$$

$$\sum_{k<n}\int_\Gamma d^3\vec{r}\phi^*_{\vec{R}_k}(\vec{r})\phi^*_{\vec{R}_n}(\vec{r})V_\infty\phi_{\vec{R}_k}(\vec{r})\phi_{\vec{R}_n}(\vec{r})=$$

$$V_\infty\sum_{k<n}\int_\Gamma d^3\vec{r}\phi^2_{\vec{R}_k}(\vec{r})\phi^2_{\vec{R}_n}(\vec{r}). \quad (17)$$

From the properties of the single-sphere function (9), after a few transformations we get:

$$<\vec{R}_1,...\vec{R}_N|V_{\text{int}}|\vec{R}_1,...\vec{R}_N>=$$

$$\frac{V_\infty}{\Omega_o}\sum_{k<n}\int_\Gamma d^3\vec{r}\phi_{\vec{R}_k}(\vec{r})\phi_{\vec{R}_n}(\vec{r}) \quad (18)$$

and at last:

$$<\vec{R}_1,...\vec{R}_N|V_{\text{int}}|\vec{R}_1,...\vec{R}_N>=$$

$$\frac{V_\infty}{\Omega_o^2}\sum_{k<n}vol\left(K(R,\vec{R}_k)\cap K(R,\vec{R}_n)\right), \quad (19)$$

where $K(R,\vec{R}_k)$ denotes the sphere of the radius R and the center determined by the radius vector $\vec{R}_k$. The operator vol (A) denotes the volume of the set A. It means that the interaction energy is proportional to the volume of the overlap of the interacting spheres.

The total energy of N spheres can be thus written as:

$$E_N(\vec{R}_1,...,\vec{R}_N)=mg\sum_{k=1}^{N^{-1}}Z_k+$$

$$\frac{V_\infty}{\Omega_o^2}\sum_{k<n}vol\left(K(R,\vec{R}_k)\cap K(R,\vec{R}_n)\right). \quad (20)$$

It is useful to write the equation (20) in the recurrence form. It allows us to calculate the energy in much more effective way. On the other hand, it enables us to build a pile of spheres adding them one by one. After a short algebra we get:

$$E_N(\vec{R}_1,...,\vec{R}_N) = mg \sum_{k=1}^{N-1} Z_k + \frac{V_\infty}{\Omega_o^2} \sum_{n=2}^{N-1} \sum_{k=1}^{n-1}$$

$$vol\left(K(R,\vec{R}_k) \cap K(R,\vec{R}_n)\right) + mg Z_N + \frac{V_\infty}{\Omega_o^2}$$

$$\sum_{k=1}^{N-1} vol\left(K(R,\vec{R}_k) \cap K(R,\vec{R}_N)\right) =$$

$$E_{N-1}(\vec{R}_1,...,\vec{R}_{N-1}) + mgZ_N + \frac{V_\infty}{\Omega_o^2} \sum_{k=1}^{N-1}$$

$$vol\left(K(R,\vec{R}_k) \cap K(R,\vec{R}_n)\right). \qquad (21)$$

One may calculate a simple integral to obtain the required volume of the common part of the overlapping spheres. The calculation in 3 dimensional space gives:

$$vol\left(K(R,\vec{R}_k) \cap K(R,\vec{R}_n)\right) =$$

$$\Theta\left(2R - \left|\vec{R}_k - \vec{R}_n\right|\right)\left[\frac{4}{3}\pi R^3 - \pi\left|\vec{R}_k - \vec{R}_n\right| R^2 + \right.$$

$$\left. \frac{\pi}{12}\left|\vec{R}_k - \vec{R}_n\right|^3\right]. \qquad (22)$$

TEST OF THE MODEL AND RESULTS

As a basic test of the method we constructed computer code simulating the gravitational fall of the spheres into the container. Using the basic formula (21) the program drops sphere after sphere according to a given distribution (here uniform) in *xy* plain. The *N*-th sphere is placed in a given position if the energy $E_N(\vec{R}_1,...,\vec{R}_N)$ gets the local minimum in respect to $\vec{R}_N$ for fixed positions of N-1 spheres. In the first two figures we show the typical configurations obtained by this procedure. Figure 1 shows a configuration for the two dimensional case, the second one is plotted for the spheres in 3 dimensions. However, it is rather difficult to imagine the distribution of the spheres from the Fig. 2. In the Fig. 3 we plotted only the centres of the spheres. One can easily observe the higher density of the centres in the inner part of the container than within the region close to its walls.

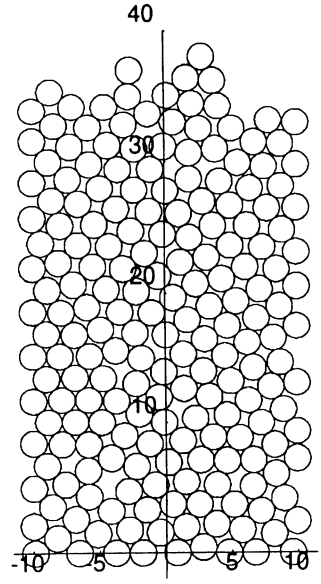

Fig. 1. A typical configuration of 200 circles.

Within this short report we have shown an alternative method for a construction of the theory for granular systems. It seems to be more effective than the methods based on more classical approaches. Its flexibility is caused by splitting, as in quantum mechanics, the notions of the observable and the function of state which practically does not exist in classical mechanics. It leads to more smooth formulae which become, in this way, more tractable. Simple modification of the calculations allows description of the spheres at different sizes. One can also to deform the wave function (9) to obtain the grains of required shapes. Different modifications of the interaction among considered objects should allow us to introduce required physical properties of the constructed granular medium.

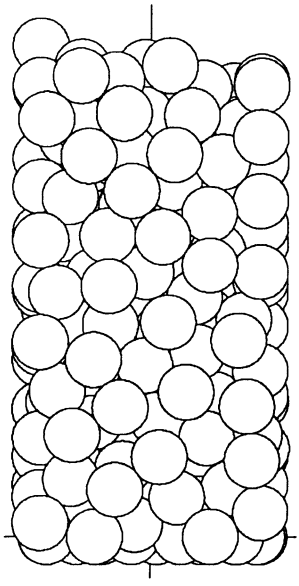

Fig. 2. A typical configuration of 200 spheres.

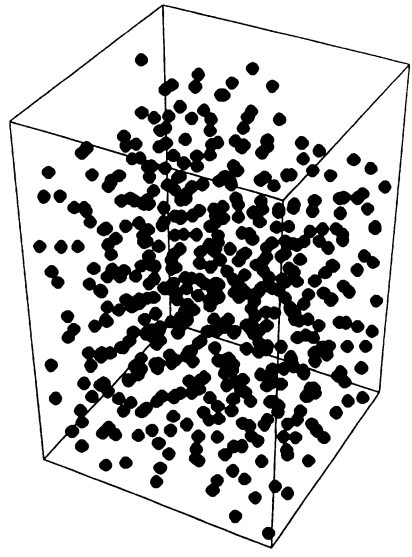

Fig. 3. The distribution of the centers of 200 spheres.

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