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A nonlinear diffusion model for granular segregation

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Abstract

We study a set of nonlinear diffusion equations describing the evolution of densely packed particles under gravity subject to random vibrations. Although the thermodynamics of the model predicts no phase separation at all, the dynamics displays both normal and reverse segregation depending on the mass of the species present in the system.

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Among the complex properties displayed by vibrated (or sheared) granular materials, segregation is one of the more fascinating and less understood. Subject of intense research in the last years, several mechanisms have been proposed to explain the demixing phenomenon observed in simulations and experiments on granular mixtures. Size-segregation for example, may occur simply because small particles sift through the pores among large particles: this geometric mechanism has been called percolation [1–3]. Segregation may also be due to convection, where large particles take the upward stream but are unable to enter the thin downward stream near the walls. This hydrodynamic mechanism has been discussed in Ref. [4]. It has also been suggested that the segregation is a condensation phenomenon [5–8], but this seems to be controversial. Moreover, several studies also deal with only one intruder, either biased [9] or not [10–13].

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In densely packed systems, crystallization is usually kinetically avoided and one can ask whether segregation phenomena may emerge from a nontrivial dependence of particle mobility upon density. For the sake of simplicity one can choose a system whose thermodynamics is trivial. Recently, we have studied a nonlinear diffusion equation [14] describing the dynamics of mono-disperse, noninteracting particles in the presence of gravity. This equation can be thought of as a macroscopic, coarse-grained description of a gravity driven version of the Kob and Andersen lattice gas model [15], which has been shown to present several features of vibrated granular materials such as slow compaction and segregation [16]. The unusual behavior of such a lattice system comes from the nontrivial dependence of the particle's mobility on the density, and most of its dynamical properties are well reproduced by the nonlinear diffusion model [17].

Whether this simple approach is able to describe the onset of segregation in the case of a binary mixture is the question addressed in this contribution. Specifically, is it possible to pass from the normal Brazil-nut effect to its reverse version by changing some of the control parameters of the system? If so, how can one control the degree of mixing and the final relative distribution of the particles? To answer these questions, we adopt the same approach which has proven successful in the monodisperse case. Specifically, we shall present a preliminary study of a binary mixture of equal-sized particles, whose segregation mechanism is based on the differential mobility.

The Hamiltonian for this system can be written as

$$H = g \sum_j m_j h_j \ , \tag{1}$$

where the sum is over all particles in the system, m_j and h_j are the mass and height of particle j, respectively.

The exact Helmholtz free energy functional for this mixture is [14,18]

$$\beta F[\rho_1, \rho_2] = \int_0^H \mathrm{d}z \left[\left(1 - \sum_{i=1}^{2} \rho_i \right) \ln\left(1 - \sum_{i=1}^{2} \rho_i \right) + \sum_{i=1}^{2} \rho_i \ln \rho_i + z \sum_{i=1}^{2} \gamma_i \rho_i \right] \ , \tag{2}$$

where $\rho_i = \rho_i(z,t)$ is the local density of specie i at height z and time t, $\gamma_i = m_i g / k_B T$ is the inverse gravitational length and H is the box height.

We assume that the local densities are governed by a continuity equation $\partial_t \rho_i(z,t) + \partial_z J_i(z,t) = 0$, with the current given by the Fick's Law, $J_i(z,t) = -\Gamma(\rho_i)\partial_z \mu_i(z,t)$ where $\Gamma_i(\rho_i)$ is the Onsager's mobility and μ_i is the local chemical potential, $\mu_i(z,t) = \delta F / \delta \rho_i$. Thus, the evolution is described by two coupled nonlinear diffusion equations:

$$\frac{\partial \rho_i(z,t)}{\partial t} = \frac{\partial}{\partial z} \left\{ \Gamma_i(\rho_i) \left[\frac{1}{\rho_i} \frac{\partial \rho_i}{\partial z} + \frac{1}{1 - \rho_1 - \rho_2} \left(\frac{\partial \rho_1}{\partial z} + \frac{\partial \rho_2}{\partial z} \right) + \gamma_i \right] \right\} \ , \tag{3}$$

where the time is now measured in units of $1/\Gamma_0 k_B T$.

Among the several possible density-dependent functionals for the mobility of a homogeneous system (i.e., without gravity), of particular interest are those that vanish at a given density ρ_c, typical of a dynamical arrest transition. Following Refs. [14,17] we focus on a power law form, generalized to two particle species:

$$\Gamma(\rho_i) = \Gamma_0\, \rho_i\, \Theta(\rho_c^i - \rho_i) \left(1 - \frac{\rho_1 + \rho_2}{\rho_c^i}\right)^{\phi_i} . \quad (4)$$

Notice that the mobility of one specie is also affected by the particle density of the other specie, and the mobility of particle i vanishes if the total density at a certain height z is equal or above ρ_c^i. When $\rho_c^1 = \rho_c^2 = \rho_c$ and $\phi_1 = \phi_2 = \phi$ we recover the original, mono-disperse case, while if $\rho_c^i = 1$, $\phi_i = 1$ the ith particle is unconstrained. To complete the description, the boundary conditions have to be specified. In the current study, the system is closed at the bottom, $J(0,t) = 0$, and at the topmost layer $z = H$ it is either in contact with a particle reservoir, $\rho(H,t) = \rho_{\rm R}$, or closed, $J(H,t) = 0$ (fixed number of particles).

We define the jamming transition as the locus in the parameter space $(\gamma_1, \gamma_2, \rho_{\rm R}^1, \rho_{\rm R}^2)$, at which a layer of critical density first appears at the bottom of the system, $\rho_1(0,\infty) + \rho_2(0,\infty) = \min(\rho_c^1, \rho_c^2)$. For example, in the particular case of equal reservoir and critical densities, $\rho_{\rm R}^1 = \rho_{\rm R}^2 = \rho_{\rm R}$ and $\rho_c^1 = \rho_c^2 = \rho_c$, the jamming transition occurs at

$$e^{\gamma_{2c} H} = \frac{(1 - 2\rho_{\rm R})\rho_c}{\rho_{\rm R}(1 - \rho_c)} - e^{\gamma_1 H} . \quad (5)$$

This line separates a regime where the dynamics is (exponentially) fast and the stationary profile is the equilibrium one (obtained through the minimization of the Helmholtz free energy), and another regime, at lower vibrations, where the dynamics is slow and the equilibrium and the stationary profiles no longer coincide. Once the system enters the latter regime, it gets out of equilibrium and the asymptotic stationary density profile is approached very slowly. Notice that as in the mono-disperse case, here the critical line between the two regimes does not depend on the exponents ϕ_i, but only on the critical densities.

In the case where the masses are equal, the equilibrium profiles, apart from a possible trivial dependence on the number of each type of particles, are the same. On the other hand, the stationary state obtained from the numerical solution of Eqs. (3), at low vibrations, presents a segregated configuration: larger (or more constrained) particles go to the top while the less constrained (smaller) prefer the bottom part of the system. This effect is purely dynamical. Interestingly, the profiles seem to present three different regions, instead of the two appearing in the mono-disperse case [14]: a small slope (probably going to a flat plateau for $t \to \infty$) part at low z, a rapidly decaying region for large z and, at intermediate heights, a more complex, with one decreasing and one peaked profile, as can be seen in Fig. 1, for both cases.

The normal/reversed segregation transition can be obtained by opportune tuning of the control parameters. For example, by changing the relative masses, one can pass from one phase to the other. This is exemplified in Fig. 2 where the difference between the centers of mass of both species are plotted as a function of γ_1 (while γ_2 is kept constant). One sees that for small ratio of the mass of particles 1 relative to 2, we

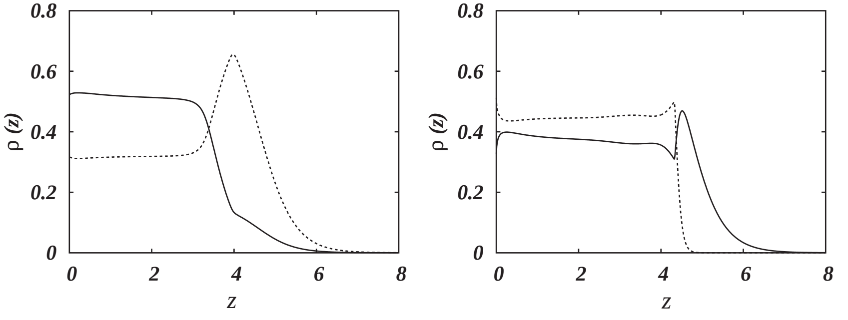

Fig. 1. Long time profiles for the case where $\rho_c^1 = \rho_c^2 = \rho_c$ but $\phi_1 \neq \phi_2$. The parameters are $H = 10$, $\rho_c = 0.84$, $\phi_1 = 4$ and $\phi_2 = 3$. The values of (γ_1, γ_2) are (2.302, 2.302) (left) and (13.812, 2.302) (right). On the left we can see the normal Brazil-nut effect: larger particles (species 1, dashed line) segregate on the top of the system; while on the right, the positions are exchanged leading to the reverse Brazil-nut effect. It is easy to show that for the case on the left, the sum of both profiles is the result obtained in Ref. [14] for the mono-disperse case.

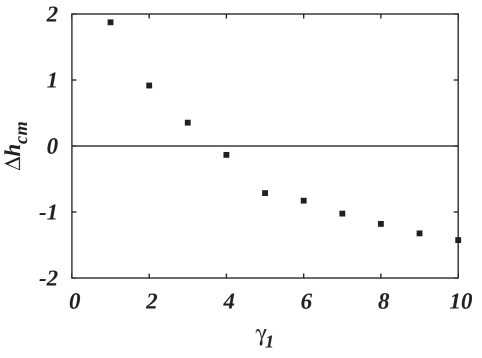

Fig. 2. Difference of the height of the center of mass for both species of particles, $\Delta h = h_{\rm cm}^1 - h_{\rm cm}^2$, versus γ_1, while $\gamma_2 = 2.302$ is kept constant (the other parameters are the same as in Fig. 1).

obtain the normal segregation pattern, with more constrained particles at the top ($\Delta h = h_{\rm cm}^1 - h_{\rm cm}^2 > 0$), while by increasing γ_1, (or, what is the same, the mass of particle 1), the centers of mass exchange positions and the less constrained particles go to the top ($\Delta h < 0$). This transition, in particular the precise mechanism involved and its experimental realization, have been the center of a recent debate in the literature [5–8]. Work is in progress to obtain a closer comparison of our model with the available experimental data and previous models.

In brief, we presented macroscopic transport equations describing the phenomena of normal and reverse segregation in a thermally vibrated system of particles under the action of gravity. The mechanism of segregation studied by us, purely dynamical, depends on the differential mobility of particles. It is similar to the percolation mechanism, where small particles, being more mobile, can move downwards more easily than larger ones. Both normal and reverse segregation are present depending on the masses of both particles. Several issues are still open. For example, recent experimental results [8] show that the presence of the reverse Brazil-nut effect is suppressed if the filling height is too large, and work is in progress to check how our model depends on it. Moreover, our system receives energy in a way analogous to a thermal reservoir, while in vibrated systems energy is usually injected from below and dissipates as the flow of energy goes up. Thus, it seems that the vertical dissipation (temperature gradient) is not a necessary ingredient for the segregation. To conclude, much theoretical and experimental efforts are still necessary to elucidate the general conditions under which segregation occurs in granular systems.

Acknowledgements

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