The Brazil Nut and Reverse Brazil Nut Effects

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Abstract

In this paper, we will consider various theoretical models of and experimental results for the so-called Brazil nut effect (BNE). This phenomenon occurs when large grains rise to the top of materials composed of grains of different sizes subjected to shaking [1]. The opposite phenomenon (large grains sinking) is called the reverse Brazil nut effect (RBNE), and its existence is by no means universally acknowledged [2] and is even absent in some theories of the BNE [1, 3]. One of the models of the BNE is statistical mechanical in nature, and we will explore a phase transition that occurs in this model.

Introduction

The study of the mechanism behind the Brazil nut effect may be somewhat esoteric, but the applications of the effect are well-known: if you have a can of mixed nuts and have eaten all of the visible Brazil nuts, a sure way to get more is to simply shake the can. This will cause the larger nuts, a group in which the Brazil nuts are certainly included, to rise to the top. In addition to this modest domestic application, the Brazil nut effect is of importance to industries in which homogeneity of a mixture is necessary for good product quality [4]. Theoretical and experimental studies of this effect do not employ mixed nuts, of course, using instead beads and other (inedible) materials generally referred to as granular mixtures (in general, the constituent particles in a Brazil nut experiment or theoretical model are called grains). That such a simple effect could have caused as much disagreement as it has is almost unthinkable, but the Brazil nut effect continues to be a problem not amenable to a simple solution. There are many competing theories as to which mechanism is the dominant force behind the effect [5], as well as varying opinions of the relative importance of interstitial air pressure, vibration amplitude and frequency, and friction in causing the effect. There is also some debate about the so-called reverse Brazil nut effect (RBNE), in which larger grains fall to the bottom of a mixture subjected to shaking. Many models predict that this effect should take place under certain circumstances, but there are some that doubt this prediction, citing the lack of experimental evidence [2].

In this paper, we will explore the various mechanisms that have been put forth as explanations for the BNE, and we will see how the results of important experiments reinforce or contradict each of these models. We will pay close attention to the predictions made regarding the transition from the BNE to the RBNE for each model. After this, we will show how a statistical mechanics approach to the problem can be formulated and used to explore the BNE/RBNE transition.

Possible Mechanisms behind the BNE

One of the first papers to try to explain the Brazil nut effect hypothesized that the tendency of smaller grains to fill in voids underneath the larger grains during the "free fall" portion of the shake (when the container is accelerating downwards at a rate greater than g) is the dominant physical

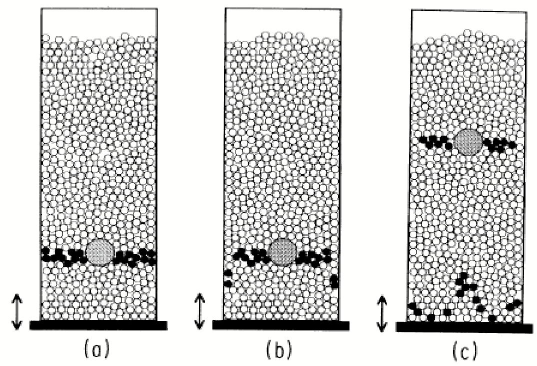

Figure 1: Convection process in a granular mixture. In (b), one can already see the fountain-like movement of the grains up the middle and down the sides; (c) shows the grains on the bottom moving towards the center and up the middle. Taken from [3].

mechanism behind the effect [1]. A Monte Carlo simulation was performed to test this hypothesis, with each "shake" being simulated as a random (but local) rearrangement of grains. Because voids left under large grains could only be filled by small grains, and because the only way a large grain could move back down would be if many smaller grains moved out, the larger grains moved inexorably upward. In this way, the simulated system found a local potential energy minimum, but not the global minimum attained by having the larger grains on the bottom.

Another possible dominant mechanism is convection. An experiment conducted in 1993 with one large grain in a cylindrical tube filled with smaller grains found that intermittent shaking (referred to as "taps") caused convection currents that brought the large grain to the top [3]. The currents ran up through the center of the cylinder and then down the sides in narrow channels. The side channels were too narrow to admit the large grain, so it stayed on the top surface. An illustration of this mechanism is shown in figure 1. The experiment also seemed to indicate that, for a given rms acceleration, the curve of height versus tap number for the larger grain is independent of the size ratio of the grains. Moreover, the experimenters found a scaling function that collapsed all the data for different rms accelerations onto a single curve by redefining the depth of the large grain below the surface. This function is given by [3]:

$$\widetilde{\Delta} = \frac{a_0 \Delta}{a_{rms} - a_0} \tag{1}$$

In the above, Δ is the depth of the large grain below the surface and a_0 is the minimum tap (shaking) acceleration needed to produce convection. The scaling form indicates that the effective depth of a large grain goes to infinity as the acceleration approaches the minimum convection acceleration, meaning that convection is the mechanism driving the grain to the top of the mixture [3]. It is important to note that this mechanism could not lead to a RBNE (at least with a cylindrical container: it was found that the convection currents in a martini glass-shaped container brought large grains near the bottom), and that the effect observed depended heavily on friction between the container and grains.

It would seem that the convection mechanism, being an experimental observation, might be a final explanation for the BNE, but there are some valid criticisms. For one thing , it is not clear that it can describe a situation in which small and large grains appear in a more even mixture. Perhaps more importantly, it can be shown that convection currents are confined to the edges of containers with a small height/width ratio [6], and thus cannot have as great an effect as they do in the 1993 experimental setup. With these criticisms in mind, let us look at yet another mechanism for producing the BNE: condensation. This mechanism, which is the first we've looked at that predicts the RBNE, was first examined via molecular dynamics (MD) simulations [6]. The idea is basically this: a system of grains under the influence of gravity will, below a certain "temperature" T_c (the molecular dynamics equivalent of shaking amplitude and frequency; higher temperature corresponds to more violent shaking), condense into a solid packed state with individual grains confined to certain positions. In a binary mixture, the critical temperatures for the two species of grains are different, and obey the relation [6]:

$$\frac{T_c\,(A)}{T_c\,(B)} = \frac{m_A d_A}{m_B d_B} \tag{2}$$

Here m_A and m_B are the masses of the species and d_A and d_B are the diameters. If the system is quenched at a temperature between these critical temperatures, then the larger grains will condense, while the smaller grains are still fluidized [6]. In the MD simulations under consideration, the condensed state comprised of the larger grains fell to the bottom of the simulation container, and then, depending on the mass and diameter ratios of the two types of grains, either stayed there or was pushed up by a buildup of the smaller grains percolating through holes in between the larger grains. In this way, the simulation resulted in either a BNE or RBNE depending on the mass and size ratios of the grains. The crossover condition between the two effects is [6]:

$$\left(\frac{d_A}{d_B}\right)^{d-1} = C\,\frac{m_A}{m_B} \tag{3}$$

Here d is the spatial dimension and C is a constant of order unity. If the LHS of the above equation is greater than the RHS, then percolation dominates and the BNE occurs. If the LHS is greater than the RHS, condensation dominates and the RBNE occurs. It should be said that there are many valid criticisms of the condensation mechanism. One focuses on the assumption that each species can be considered as interacting only with itself; that is, that the condensation of one species is not affected very much by the presence of the other species [2]. This assumption ignores the drag exerted on the condensed state by the fluidized state, an effect observed in experiments [2]. Another more subtle criticism is that, even with a temperature above both species' critical temperatures, it is possible for the BNE and RBNE to occur due to competition between entropy and energy considerations [7]. This line of thermodynamic thinking will eventually let us analyze the details of the crossover from the BNE to the RBNE, but for now let us just say that it is a way of understanding the results of the MD simulations without resorting to an idea as suspect as non-interacting grain condensates [7].

As a final mechanism, we consider inertia. The idea behind this mechanism is that, during the period in the shaking cycle when the container is being accelerated down at a rate greater than g but is still moving up, the inertia of the larger grains will allow them to break through a thin layer of smaller grains [5], which are moving more slowly due to their participation in stress chains and possibly the effects of air pressure [5]. When they come back down, small grains will have filled in their previous positions [8]. Over the course of each cycle, the large grains will thus move up a certain distance $\delta(h)$, which can be related to their starting energy (that is, their kinetic energy when the acceleration of the container is at $-g$) in the following way [5]:

$$KE_i = \frac{m}{2}v_0^2 = \delta(h)\beta(h) \tag{4}$$

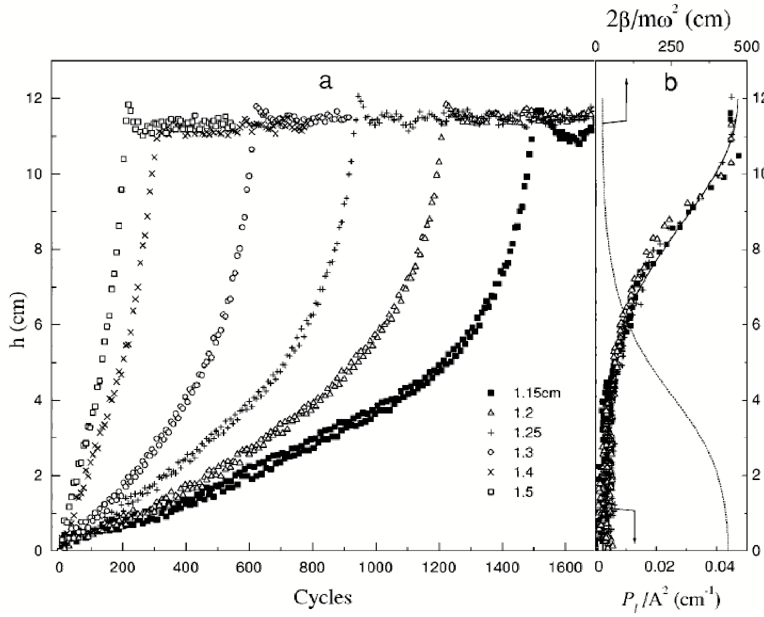

Figure 2: On the left (a) there is a plot of height vs. cycle number for six different runs with different vibration amplitudes. The runs with larger amplitudes are on the left side of the graph. On the right is a plot of $\delta(h)/A^2$ vs. h (note that $\delta(h)$ is just the derivative of h with respect to cycles) for three different runs. As advertised, they collapse onto the same curve. The dotted curve represents $\beta(h)$, which can be obtained from $\delta(h)$ by simply taking the inverse. Taken from [5].

Here $\beta(h)$ is a height-dependent average frictional force which captures the interaction of the large grains and the small grains, and v_0 is, for a container shaken in a sinusoidal manner with frequency ω and amplitude A, given by [5]:

$$v_0^2 = A^2\omega^2 - \frac{g^2}{\omega^2} \tag{5}$$

Note that the change in potential energy of the large grain has been ignored. If the parameters of the shaking are such that the second term in the above equation can be ignored, then the ratio of $\delta\,(h)$ to A^2 should be independent of A. Indeed, this was found experimentally to be true [5]. Figure 2 shows the results of this experiment, in which the full path of a large grain to the top was measured and not just its rise time.

There are evidently many different theories for the mechanism behind the Brazil nut effect, each with its apparent strengths and weaknesses. The convection mechanism is obviously a real phenomenon, but it is not clear under which conditions (container geometries, grain sizes and geometries, etc.) it is true. Indeed, in the experiment which motivated the inertial mechanism explained previously, convection was observed, but was not strong enough or widespread enough to cause the BNE [5]. The condensation/percolation mechanism seems suspect, and may be conceptually flawed and convoluted. The original explanation in terms of void-filling may very well be true, and is even compatible with the inertial mechanism, but, at least in the form presented here, it is a bit light on predictive power. Moreover, it seems somehow not general enough, almost akin to saying that the sun is hotter than a lamp because it emits more photons. The inertial mechanism is appealing and can even explain the RBNE [8], though not for a set of parameter ranges that would appeal to those committed to the condensation or thermodynamic mechanisms (the large grains have to be less dense than the small grains, for one thing). It is likely that all of these mechanisms are important to the BNE, but that, for certain parameter regimes, one or more mechanisms dominate.

Statistical Mechanics Approach

One of the criticisms of the condensation argument was that it was really nothing more than a thermodynamics argument put in different terms [7]. It is possible to formulate the problem in terms of a binary liquid and obtain results in agreement with MD simulations [7], but there is also another way to attack the problem: head on, by computing a partition function for a lattice model and using that partition function to calculate, for instance, the average height of one species [9]. It is this approach that shall occupy us for the remainder of this paper.

Before writing down and then computing a partition function for the Brazil nut problem, we need to show that such an approach is even justified. Consider a system of grains of the type we've been looking at. For a given energy, there are many possible configurations of grains. The basic notion of the statistical mechanics approach is that all of these states are equally likely when the system is subjected to shaking (taps), and that the macrostate associated with this energy has an entropy given in the usual way by $S = \ln \Omega$, where Ω is the number of microstates (configurations) in the macrostate. A "configurational temperature" can thus be defined as $\beta = 1/T = \frac{\partial S}{\partial E}$. It can be shown that a proper probability distribution for the microstates in the system with average energy E is given by the Boltzmann distribution [10]:

$$P_i = \frac{e^{-\beta E_i}}{Z} \tag{6}$$

Here Z is the usual sum over states. The situation is actually more complicated in the case of a binary mixture of the type present in the Brazil nut problem. Here we must define two temperatures, and the probability is given by [10]:

$$P_{i,j} = \frac{e^{-\beta_1 E_{1i} - \beta_2 E_{2j}}}{Z} \tag{7}$$

Though it may seem farfetched that a system with almost no movement could explore its entire possible phase space (or even a significant portion of it), this form of the probability function correctly predicts the macroscopic properties of a granular mixture under taps, giving the same results as a time-average of the system. We can use this idea to explore the BNE in a model system.

Phase Transition in the Brazil Nut Problem

We start with a lattice model of a binary granular mixture. The model works as follows: we only consider mechanically stable microstates–that is, microstates in which grains are supported by other grains underneath them [9]–and we don't allow lattice sites adjacent to sites occupied by large grains to be filled. Besides those requirements, the rest is straightforward. The energy of each microstate is simply the gravitational potential energy, and any macroscopic observables of interest can be computed as ensemble averages. Written out in all its glory, the full Hamiltonian is [9]:

$$\mathcal{H} = \mathcal{H}_{hc} + \sum_{z,i} m_1 g z \, \delta_{n_{zi},1} + \sum_{z,i} m_2 g z \, \delta_{n_{zi},2} \tag{8}$$

The labels z and i denote the layer and position in each layer of each site, respectively. The n_{zi} are the occupancy variables of each site (z, i), equal to either 0 (no grain present), 1 (small grain present), or 2 (large grain present) [9]. The exclusion rule is captured in $\mathcal{H}_{hc}$, which has an explicit and tractable expression [9]. The partition function is then the trace of $e^{-\mathcal{H}_{hc}-\beta_1 E_1-\beta_2 E_2}$ over all mechanically stable states.

The partition function of this model, and thus all the quantities of interest to the Brazil nut problem, can be approximated using mean field theory. The method used is related to Bethe's solution of the Ising model, though it is quite a bit more complicated [9]. We shall not go through all the detail here, but simply state the results of the calculation. Specifically, we will look at how the parameter $\Delta h/h$ varies with the parameter δ. These two parameters are defined by:

$$\frac{\Delta h}{h} = \frac{h_1 - h_2}{h_1 + h_2} \tag{9}$$

$$\delta = \frac{2m_1 - m_2}{2m_1 + m_2} \tag{10}$$

Here h_1 and h_2 are the thermal averages of the mean heights of the two grain species, and $\Delta h/h$ is clearly a measure of whether we are dealing with the BNE or the RBNE. The main results are shown in figure 3. There are many important things to note. The first is that the model is able to reproduce both the BNE and RBNE depending on the mass ratio of the two grain types. The competition is clearly between entropy and gravity, much like in the condensation problem [7]. This model has no dependence on microscopic (that is, on the scale of the grains) details (save for hard-core repulsion), and so seems to indicate that the BNE and RBNE are driven by global "thermodynamic" mechanisms [9]. The second thing to note is that there is a phase transition occurring in this system, though not the transition one would naïvely expect. As the number of small grains per unit surface N_1 is increased, the rate at which $\Delta h/h$ changes with δ gets bigger and bigger, until, at a critical value N_{1c}, the transition becomes infinitely steep. In other words, we go from a situation in which there is a smooth crossover from the BNE to the RBNE as δ is varied to a situation in which any deviation of δ from some value δ_c results in either a large BNE or RBNE [9]. The situation is roughly analogous to the Ising model, where for $T > T_c$ we have paramagnetic (smooth crossover from $M < 0$ to $M > 0$ as H is varied) behavior, while for $T < Tc$ we have a sharp transition from all the spins pointing up to all the spins pointing down as H is varied [9]. With this in mind, we can identify $\Delta h/h$ as our order parameter (analogous to M), δ

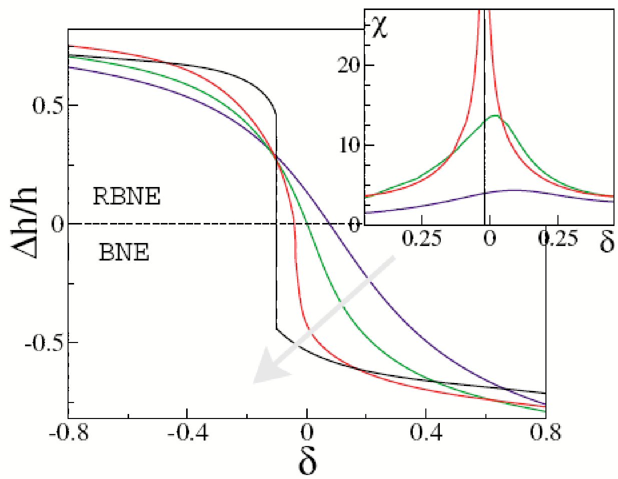

Figure 3: The main part of the figure shows $\Delta h/h$ as a function of δ for various values of N_1. The inset shows the susceptibility as a function of δ for various values of N_1. Note the divergence as $N \to N_{1c}$. Taken from [9].

as our ordering field (analogous to H), and N_1 as our inverse temperature [9]. The analogy is not exact since the value of δ which causes $\Delta h/h$ to be zero depends on N_1, but it is close. Indeed, the equivalent of the magnetic susceptibility, which is given by [9]

$$\chi(\delta, N_1) = N_{tot}\left(\left\langle \Delta h^2 \right\rangle - \langle \Delta h \rangle^2\right) \tag{11}$$

has a power law divergence $\chi \propto (N_1^{-1} - N_{1c}^{-1})^{-\gamma}$ near the critical point (see figure 3), with γ found to be close to 1 [9]. This is the same behavior found in the Ising model. Similarly, $\Delta h/h$ varies as $(N_{1c}^{-1} - N_1^{-1})^{\beta}$ near the critical point, with β numerically found to be close to the Ising value of 1/2 [9].

What exactly is happening physically as N_{1c} is approached? The explanation that has been put forth concerns something called the depletion force [9], which is an effective force between large grains due to the presence or absence of small grains. When this force is greater than some critical value, the larger grains undergo a sort of condensation and a phase separation occurs, dragging the heavier phase to the bottom [9]. Since this force becomes greater as N_1 is increased, and since it is this parameter that drives the phase transition, this explanation is entirely plausible.

Conclusions

The underlying physical mechanism behind the BNE is still not well understood. There are a number of competing theories as to what the dominant mechanism is, including reorganization of grains, convection, condensation/percolation, and entropy/gravity. The last of these is intriguing because it comes from a statistical mechanics argument and can be used to determine the nature of the crossover from the BNE to the RBNE without having to worry about the microscopic details of the interaction. It can be shown that a statistical mechanical model of a binary granular mixture undergoes a phase transition from a "paramagnetic" phase in which varying the mass ratio of the grains smoothly alters the average difference in height of the large and small grains to a "ferromagnetic" phase in which this difference in height jumps sharply as a function of mass ratio. The critical exponents of this transition in mean field theory are identical to those found for the Ising model. Experimental studies of the BNE are still somewhat inconclusive regarding the existence of the RBNE in the parameter regimes predicted by theory, although the effect has been observed [8]. Since one of the main features that separates some theoretical mechanisms from others is their prediction regarding the RBNE, testing this effect in a laboratory setting is of the utmost importance to unravelling the Brazil nut problem.

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