

## Rise of a Brazil nut: A transition line

Sergio Godoy,<sup>1</sup> Dino Risso,<sup>2</sup> Rodrigo Soto,<sup>1</sup> and Patricio Cordero<sup>1</sup>

<sup>1</sup>*Departamento de Física, FCFM, Universidad de Chile, Santiago, Chile*

<sup>2</sup>*Departamento de Física, Universidad del Bío-Bío, Concepción, Chile*

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Using molecular dynamics we study the behavior of a large particle immersed in a bed of smaller ones. The system is bidimensional, consisting of many rough inelastic hard disks of equal size plus a larger one: the intruder. All possible parameters of the system are kept fixed except for two dimensionless parameters determining the frequency and amplitude of the vibrating base. A systematic exploration of this parameter space leads to determining a transition line separating a zone in which the Brazil nut effect is observed and one in which it is not. The results strongly suggest that, in the region of the parameter space in which the study is made, there is a minimum amplitude and a maximum frequency for the Brazil nut effect to take place. These results compare well with isolated results from other authors.

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### I. INTRODUCTION

For several years physicists have systematically been studying the behavior of granular matter [1–5]. Granular matter steadily excited behaves in several respects like a standard fluid but it exhibits some peculiar behavior of its own. Of the many phenomena that granular matter presents under external excitations, one can mention the formation of clusters, avalanches, piling, pattern formation, sound propagation, and segregation.

We are presently interested in the size segregation phenomenon in the case of a vibrated granular system containing one larger particle (the intruder) which, under appropriate conditions, rises to the top. This phenomenon is known as the Brazil nut effect (BNE) and it was so named by Rosato and co-workers [6]. We would like to distinguish this phenomenon from a similar one, also called BNE, in which there is not one intruder but a binary mixture, each species, typically occupying roughly the same volume. In the case of a binary mixture—differing by the size of the grains, or the density, etc.—it is interesting to study the conditions under which the two species segregate and which species migrate to the top (BNE and reverse BNE), but this case is different as it has additional effects involved such as the interactions among the large particles [7].

There are many experimental and simulational studies of segregation and in their conclusions authors attribute it to a variety of mechanisms such as void filling [6,8,9], arch formation [10–12], percolation [13,14], condensation [13–15], buoyancy [7,16–18], inertia [18,19], convection [11,12,18,20–24], and competition between buoyancy and geometric forces [25,26]. In Ref. [27] the authors tabulate seven possible mechanisms in the case when both types of grains have the same mass.

The above mechanisms are valid at least in the case when there is no interstitial fluid, otherwise other mechanisms arise [5]. We concentrate on the case when no such fluid has any significant effect. Which mechanism dominates depends on the region in the huge control parameter space in which the system is located. One may count about 20 possible parameters. Among them are the geometry of the container, the

amplitude and frequency of the vibration of the system, the number of small grains, the size of them and the intruder's size, the densities of the grains and the mechanical properties associated with collisions.

At present there is no generally accepted theory to anticipate which mechanisms are dominant for the segregation phenomena and it would be necessary to make a huge number of experiments and/or molecular dynamic simulations to determine the relevant mechanisms in each case.

There is a wide literature on the analysis of experimental or molecular dynamic results where only one parameter is varied. A few authors vary more than two parameters but give only a few values to each one of them. Many authors vary the density ratio and/or the diameter ratio, which is different than what we do.

In this paper we report a systematic molecular dynamic study—using a quite efficient event-driven simulator program, [28,29]—to find the conditions under which there is or there is no BNE, varying only the parameters which determine the movement of the vertically vibrating base, namely, its amplitude  $A$  and the angular frequency  $\omega$ . The system consists of many small inelastic disks and an intruder in a box with three rigid and rough walls: The vibrating base and the lateral walls, which do not move.

For the system under study, the single intruder is a significant part of the whole system (sidewise it represents 20% of the system) and since we use lateral rough walls the friction with these walls tends to trigger a downward convective current in each side of the box inducing an upward convective current in the middle of the system. We argue that an interplay between the energy influx and the amplitude of the vibrating base are the basic ingredients inducing the convective movement.

The result is the determination of a line—in this two-dimensional (2D) parameter space determining the movement of the base—the transition line, separating a BNE zone from a non-BNE zone. The transition line shows that there is a minimum amplitude and a maximum frequency beyond which no BNE is observed. In this paper we present this simulational result (the transition line) without attempting a deep theoretical elaboration concerning the detail dynamics behind the phenomenon.

TABLE I. Values associated to the geometry and the dissipation coefficients of the system used in all of our simulations.

$N=1200$	Number of small grains
$\sigma_{\text{intruder}}/\sigma=8$	Grains' diameter ratio
$L_x/\sigma=40$	Width of the box
$r_n=r_t=0.98$	Restitution coefficients
$\kappa_s=\kappa_d=0.7$	Friction coefficients

In Sec. II we describe the model and the control parameters. Section III presents the simulational results and a comparison is made with previous studies in which they use the amplitude and frequency as control parameters as we do. A summary and conclusions are presented in Sec. IV.

## II. SYSTEM

The system of small grains and the intruder is in a box with a vertically vibrating base whereas the lateral walls are rough and remain motionless. The interactions within the system are the instantaneous and dissipative collisions between the grains and between the grains and the walls.

We model the grains and the intruder as rough hard disks with translational and rotational degrees of freedom. The collision rule, defined in [30,31], depends on the normal and tangential restitution coefficients  $r_n$  and  $r_t$  and the static and dynamic friction coefficients  $\kappa_s$  and  $\kappa_d$ . This collision rule incorporates the standard law of friction (Coulomb's law) distinguishing static and dynamic friction. In its derivation, instead of taking into consideration the notion of force it is necessary to consider, of course, the instantaneous momentum exchanged. In the appropriate limit this rule also gives the grain-wall collision rule.

In order to make a systematic study of the bidimensional system in a reasonable time we fix most of the control parameters. We restrict our study to a system of 1200+1 particles inside a box of width  $L_x=40\sigma$ , where  $\sigma$  is the diameter of the small grains. The mass density of the intruder equals that of the smaller grains and the ratio between their diameters is 8. All the restitution coefficients are the same, normal and tangential, namely, grain-grain, grain-intruder, grain-wall, intruder-wall, and all friction coefficients are the same as well. This is summarized in Table I.

It should be noted that since the intruder has the same mass density as the small grains, the intruder is denser than the system of small grains even when the latter are close packed, because of the interstitial voids.

We use, for numerical accuracy, a vibrating base which does not move sinusoidally but in a periodic vertical parabolic movement given, in the range  $0 \leq t \leq T$ , by

$$y_{\text{base}} = \begin{cases} \frac{8A}{T^2}(2t-T)t, & 0 \leq t < \frac{T}{2}, \\ \frac{8A}{T^2}(2t-T)(T-t), & \frac{T}{2} \leq t < T, \end{cases}$$

where  $A$  is the amplitude,  $T$  is the period, and  $t$  is time. Due to the parabolic movement, the base's acceleration is piecewise constant,  $a_{\text{base}} = \pm \frac{32A}{T^2} = \pm \frac{8}{\pi^2} A \omega^2$ .

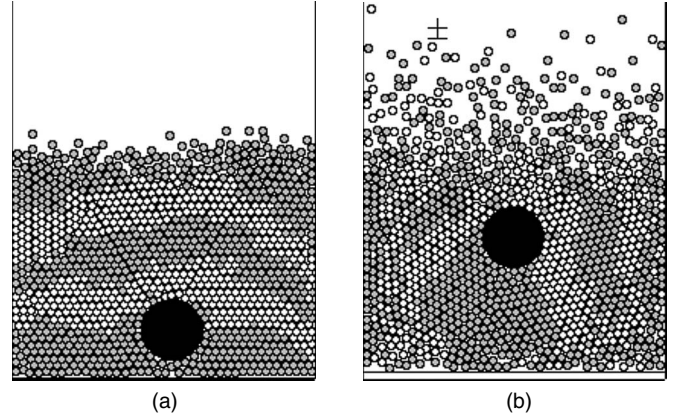


FIG. 1. Two snapshots of the system with different levels of excitation. The width of the box is  $40\sigma$ . The values of  $(\Gamma; \zeta)$  on the left-hand side are  $(3.0; 1.5)$  and on the right-hand side  $(6.0; 4.0)$ . The shades of gray show how initially horizontal layers have evolved.

In the present study the control parameters are the amplitude and frequency of the vibrating base,  $A$  and  $\omega$ , or rather, the parameters  $\Gamma$  and  $\zeta$  which represent the dimensionless base acceleration and velocity, respectively,

$$\Gamma = \frac{8}{\pi^2} \frac{A\omega^2}{g}, \quad \zeta = \sqrt{\frac{2}{\sigma g}} A\omega, \quad (1)$$

where  $g$  is the acceleration of gravity. In our study we explore the region  $2.0 \leq \Gamma \leq 12$  using  $\Delta\Gamma=0.5$ . The control parameter  $\zeta$  is varied around the BNE transition with  $\Delta\zeta=0.25$ . The minimum and maximum values of  $\zeta$  are 1.0 and 10.0, respectively. (The explored region is shown in Fig. 5.) With present day computers all of these molecular dynamics (MD) simulations represent about 1 year of CPU time.

The mean kinetic energy gets larger when  $\zeta$  is increased at fixed  $\Gamma$ . When  $\Gamma$  is increased at fixed  $\zeta$  the mean kinetic energy slightly increases until  $\Gamma \approx 10$ , beyond which the mean kinetic energy roughly remains constant. This is consistent with Ref. [32] where it is shown that in the limit of large  $\Gamma$  the injected power increases with  $\zeta$ .

We restrict our study to cases in which the system does not get too excited, remaining relatively dense, as seen in Fig. 1. In fact in the neighborhood of the intruder the density of the intruder can be as high as 90% of the close-packing density.

## III. RESULTS

The initial condition places the intruder in contact with the base (namely, its center is at height  $4\sigma$  from the base), the base is at its lowest position, and the small particles are set in a loose triangular order.

Figure 2 illustrates the observed behavior of the height of the intruder for  $\Gamma=6.0$  and three values of  $\zeta$ , comparing it with the height  $H_S$  of the center of mass of the small grains. The intruder does not rise above  $H_S$  for small  $\zeta$ , while it moves and remains up for intermediate values of  $\zeta$  and it moves above and below  $H_S$  for larger values of  $\zeta$  (phenom-

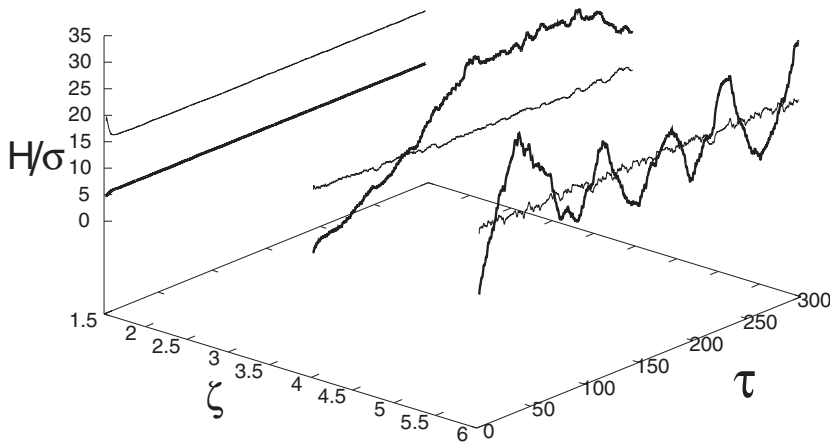


FIG. 2. The evolution of the height of the intruder,  $H$  (bold line), and the height of the center of mass of the small grains,  $H_S$  (light line), as a function of the number of cycles of the base  $\tau$ . The curves correspond to  $\Gamma=6.0$  and three values of  $\zeta$ : 1.5, 4.0, and 6.0. The height  $H_S$  is roughly  $15\sigma$  in all cases. The intruder does not rise above  $H_S$  for small  $\zeta$ , while it moves and remains up for intermediate values of  $\zeta$  and it moves above and below  $H_S$  for larger values of  $\zeta$ .

enon sometimes called “whale effect”). This last behavior is caused by an intense convective current: The intruder moves up along the central part of the box, reaches the surface of the granular fluid, moves toward one of the walls where it is pushed down by the convective roll, next moves horizontally to the center of the box, starts moving up again, and so on.

In the cases when the intruder remains below  $H_S$  the evolution of the height of the intruder is seen in Fig. 3: The intruder slowly moves up in discrete steps until it apparently settles at a certain small height for as long as the simulations last: 1500 cycles of the vibrating base.

Figure 4 shows the inverse of the time it takes for the intruder to reach the height  $H_S$  for  $\Gamma=5.5$  as a function of  $\zeta$ . It suggests that there is a clear transition between regimes with very large rising times (eventually infinite) and regimes where the intruder moves above  $H_S$  in a finite time. Longer simulations would give values for the inverse of the rising time indistinguishable from zero for  $\zeta < 3.2$ , hence they cannot alter the result. In all cases in the present study—in which the intruder did move to the top—convection was present. When the intruder did not reach the top there was sometimes a short transient period with convection, but we never saw sustained convection when the intruder stayed below the center of mass of the system.

To characterize the locus, in the  $\Gamma$ - $\zeta$  space, of the transition mentioned above we ran three simulations associated to each point in the grid. To decide whether there was BNE or not we check—as was similarly done in Ref. [16]—if the intruder reaches a height above  $H_S$ , during an entire cycle of the base, for at least two of the three simulations. This procedure provides a series of transition points to which we have adjusted the parabola,

$$\zeta_t(\Gamma) = (0.062 \pm 0.001)(\Gamma - 1)^2 + (1.84 \pm 0.06), \quad (2)$$

which is shown in Fig. 5. It was checked that a linear term in Eq. (2) has a coefficient consistent with zero. The observed BNE takes place above this transition line,  $\zeta > \zeta_t(\Gamma)$  and it is always seen to be associated with convection.

The transition line would be somewhat lower if we had allowed the system to evolve for more than the 1500 cycles that we arbitrarily set. However, as Fig. 4 suggests, it cannot be too far from the one we have found even though for smaller values of  $\Gamma$  graphs like Fig. 4 are not so neat.

In what follows we compare our results with those obtained in studies where this comparison is meaningful: There is one intruder, its density is the same as that of the small particles, the lateral walls are rough and the frequency or the amplitude of the base are used as control parameters. Refer-

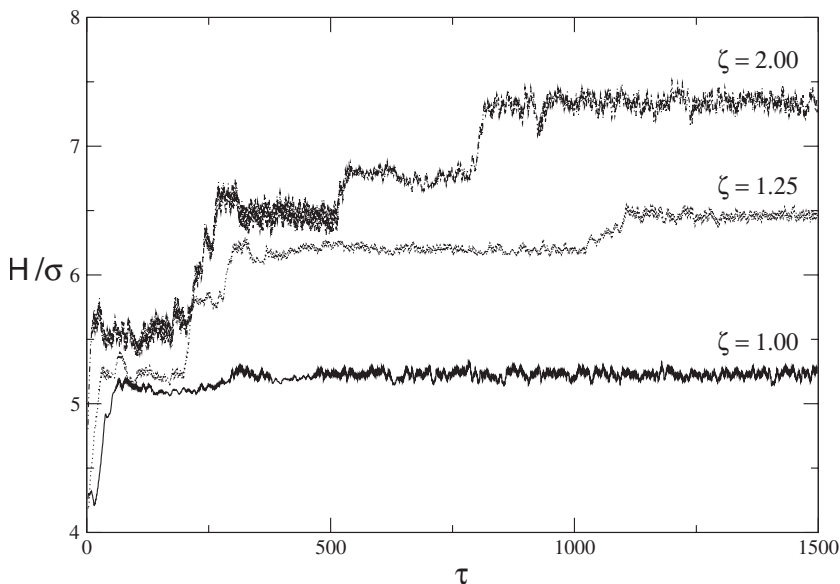


FIG. 3. Evolution of the height of the intruder during 1500 cycles of the base for  $\Gamma=3.5$  and the values for  $\zeta$ : 1.0, 1.5, and 2.0. The intruder moves up in steps but it does not reach  $H_S \approx 15\sigma$ .

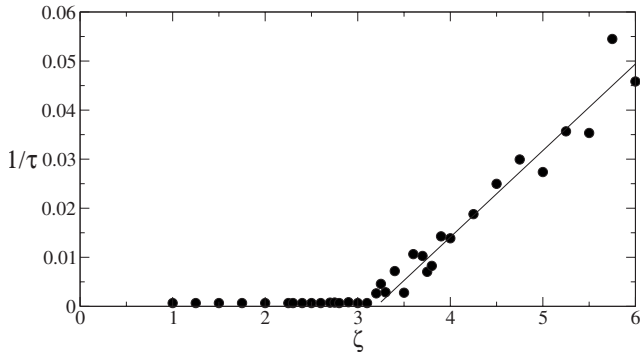


FIG. 4. Inverse of the number of cycles  $\tau$  it takes for the intruder to reach the height  $H_S$  for  $\Gamma=5.5$  as a function of  $\zeta$ . The straight line is a guide to indicate that there is a transition at about  $\zeta \approx 3.2$ . The points for  $\zeta < 3.2$  are not zero, but the inverse of the maximum number of cycles of our simulations,  $1/1500$ .

ences [11,12,20] vary the amplitude of the base while [21] varies the frequency. References [11,20] are experimental while [12,21] are time driven simulations; Ref. [20] is fully three dimensional while Ref. [11] refers to experiments in a Helle-Shaw cell. We did not find any references simultaneously varying the two parameters.

Although it is not necessary, in order to do this comparison, we change our control parameters from  $(\Gamma, \zeta)$  to  $(\tilde{\omega}, \tilde{A})$ , obtained from Eq. (1) where

$$\tilde{A} \equiv \frac{A}{\sigma}, \quad \tilde{\omega} \equiv \sqrt{\frac{\sigma}{g}} \omega. \quad (3)$$

Note that what was a parabola in the  $\Gamma$ - $\zeta$  plane now—in this frequency-amplitude plane—has a tongue shape as seen in Fig. 6. The new curve has been extended, for low frequencies, well beyond the region where the parabola was determined. The light gray zone in the interior of the tongue contains the BNE points that we have simulated. We reiterate

that the BNE points that we have observed are all related to convection in the granular fluid.

The transition line shows that there is a minimum amplitude ( $\tilde{A}_{\min}=0.57$ ) and a maximum frequency ( $\tilde{\omega}_{\max}=3.10$ ) beyond which no BNE is observed. One reason why there is a maximum frequency is because at larger frequencies the energy flux has a shorter penetration length [32,33]. At a certain frequency the upper layers of the system do not get enough energy influx to allow the intruder to pass through. Under such circumstances there is a gaslike fluid layer underneath.

For a given amplitude, the frequency must be above a certain threshold to ensure a sufficient energy influx to allow the intruder to move up. This is why the extrapolation of the transition line shown in Fig. 3 is qualitatively reasonable.

One of the reasons why there is a minimum amplitude to have BNE is because the up and down movement of the system produces friction with the lateral walls and this friction is larger when there is a larger pressure, namely, when the system is being pushed up. The result, on average, is a downwards force on the particles and the main obstacle for convection is possible jamming. For a given frequency there is a minimum amplitude to produce the friction necessary to have convection.

The results from the four papers cited above are consistent with our findings as it can be seen in Fig. 6. This comparison should have a limited significance because none of the other authors use the values summarized in Table I. To our surprise, however, the comparison tends to agree with our results making us believe that the transition line is not strongly dependent on the specific values of the other parameters. In this comparison, the important point is that all the four articles show the same tendency: For a given frequency there is an amplitude below which the intruder does not rise; for a given amplitude, there is a frequency below which the intruder does not rise either. The transition these authors observe is roughly where our MD results indicate. In the pre-

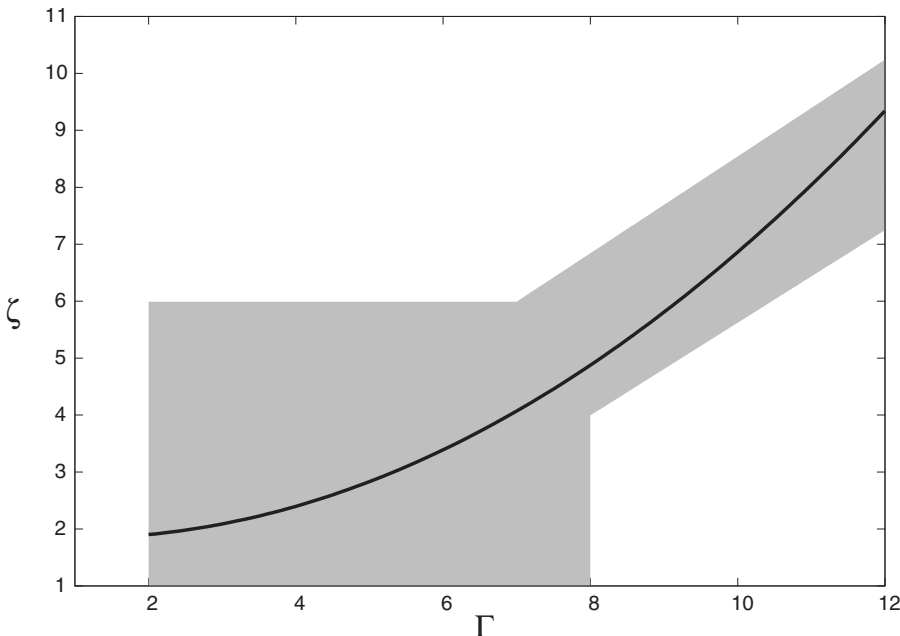


FIG. 5. The gray zone represents the explored points in the  $\Gamma$ - $\zeta$  parameter space. The solid curve defined by Eq. (2) separates the region where the intruder goes up (above the curve) from the region underneath where it does not.

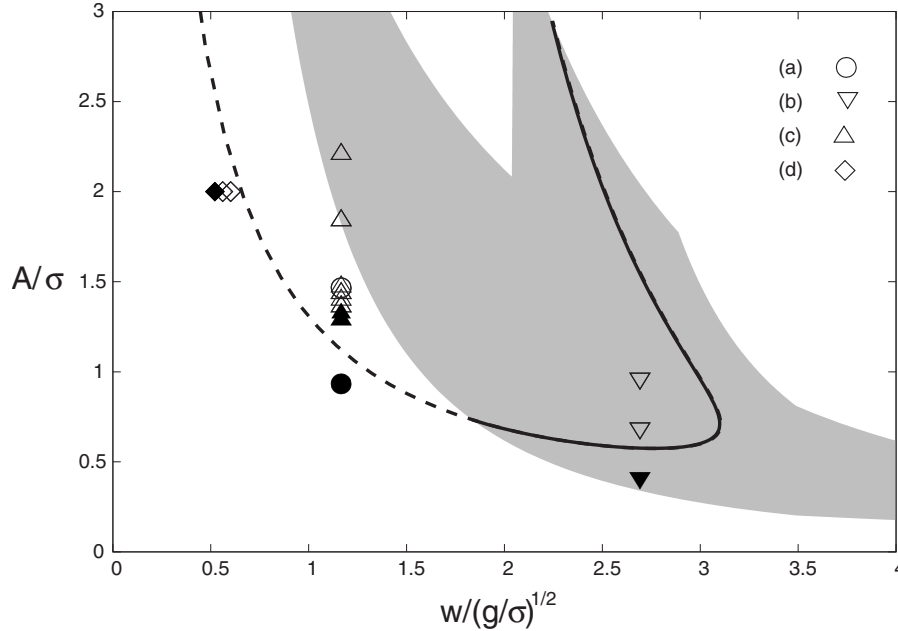


FIG. 6. The transition line (bold line) drawn in the  $\tilde{A}$  and  $\tilde{\omega}$  plane and its extrapolation outside the explored region (gray zone) using Eq. (2) (dashed line). The open symbols correspond to cases in which other authors reported the intruder going up in a time less or equal to our total simulation time, solid symbols represent the intruder rising in a time longer than our total simulation time or the intruder not rising above the height of the center of mass. (a) Values explored by Ref. [11],  $\tilde{\omega}=1.166$  and  $\tilde{A}=0.933$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.466$ . (b) Values explored by Ref. [20],  $\tilde{\omega}=2.692$  and  $\tilde{A}=0.413$ ,  $\tilde{\omega}=2.692$  and  $\tilde{A}=0.689$ ,  $\tilde{\omega}=2.692$  and  $\tilde{A}=0.965$ . (c) Values explored by Ref. [12],  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.287$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.323$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.360$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.397$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.434$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.471$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=1.838$ ,  $\tilde{\omega}=1.166$  and  $\tilde{A}=2.206$ . (d) Values explored by Ref. [21],  $\tilde{\omega}=0.521$  and  $\tilde{A}=2.0$ ,  $\tilde{\omega}=0.561$  and  $\tilde{A}=2.0$ ,  $\tilde{\omega}=0.602$ , and  $\tilde{A}=2.0$ .

vious two paragraphs we have described what we believe are the dominant mechanisms. It is clear from comparing Figs. 5 and 6 that the description of the transition line is much simpler using the parameters  $\Gamma$ - $\zeta$  than using  $\omega$ - $A$ .

#### IV. SUMMARY AND CONCLUSIONS

In this paper we have studied under which conditions an intruder immersed in a bed of smaller grains goes up (Brazil nut effect, BNE) when the system is subjected to vibrations. We have determined a transition line—in the 2D parameter-space characterizing the movement of the base—which separates a BNE zone from a non-BNE zone.

To this end we have made use of MD simulations of a bidimensional system of grains (inelastic disks) in a box with a vibrating base. The mass density of the intruder is equal to that of the smaller grains. The collisions are instantaneous and inelastic. The vibration of the base is characterized by the dimensionless acceleration and velocity,  $\Gamma$  and  $\zeta$ , defined in Eq. (1).

The present study fixes the values of all possible control parameters except for  $\Gamma$  and  $\zeta$ . In our study the intruder is large: Its diameter,  $\sigma_{\text{intruder}}$ , is one-fifth the horizontal size of the box and it is typically one-quarter of the effective height of the system. In other words, the intruder is an important fraction of the system as a whole. Under these conditions the friction of the grains with the lateral walls—which may trigger convective currents in the system—plays an important

role. If we study the same system, except that now the lateral walls represent periodic boundary conditions, the intruder does not rise in the zone of the parameter space that we explore. The friction among particles is also important even though we do not report this effect, but summarily we can say that if we use zero friction coefficient between grains (keeping the roughness of the lateral walls) the intruder does not rise either.

Simulations were run for at most 1500 cycles of the base. For a given value of  $\Gamma$  and values of  $\zeta$  sufficiently large it is seen that the intruder crosses the height of the center of mass of the small grains,  $H_S$ , eventually reaching the top of the system. The time taken by the intruder to reach  $H_S$  increases when  $\zeta$  decreases. Figure 4 suggests that this time diverges at a transition point. For smaller values of  $\zeta$  the intruder slowly moves up in steps not reaching  $H_S$  in the 1500 cycles that each simulation lasts, as seen in Fig. 3.

It was found out that in the  $\Gamma$ - $\zeta$  plane there is a transition line  $\zeta_t(\Gamma)$ , such that for  $\zeta > \zeta_t(\Gamma)$  the BNE takes place. The observed BNE was always seen associated with convection. In fact, we are quite certain that the class of BNE that we are reporting is directly connected to the convective currents induced by the friction of the small grains with the lateral walls. But we must point out that there are many possible mechanisms which may be competing.

The characteristics of the transition line  $\zeta_t(\Gamma)$  that we have determined tell us that there is a maximum frequency and a minimum amplitude of the vibrating base beyond

which no BNE should be observed. Our results compare well with the results of other authors, as seen in Fig. 6, in spite that in their studies they use values different from those in Table I. We cannot discard that there could be other transition lines, dominated by different effects, in a different region of our parameter space.

From observing Fig. 5 it is seen that the phenomenon is more sensitive to the variation of  $\zeta$  than of  $\Gamma$ . In fact we have observed that the energy flux into the system is only slightly dependent on  $\Gamma$  but significantly dependent on  $\zeta$ . When the energy flux is larger the system is more fluidized even though the densities are still not too far from close packing.

Since in the present case, convection is induced by friction with the lateral walls, and this convection is enhanced by larger values of the amplitude of the base, then for a given  $\zeta$  smaller values of  $\Gamma$  (which imply larger amplitudes) enhance convection. In other words convection can take place with a smaller energy influx (value of  $\zeta$ ) when  $\Gamma$  is smaller. This is why the transition line  $\zeta_c(\Gamma)$  is an increasing function.

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