Reversible polydisperse parking lot model

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We use an improved reversible parking lot model to study the compaction of vibrated polydisperse media. The particle sizes are distributed according to a truncated power law. We introduce a self-consistent desorption mechanism with a hierarchical initialization of the system. In this way, we approach densities close to unity. The final density depends on the polydispersity of the system as well as on the initialization and will reach a maximum value for a certain exponent in the power law.

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I. INTRODUCTION

The vibratory compaction of granular materials has long been of importance in technological applications such as high performance concrete or ceramics which have to withstand extreme stress. Extensive experimental studies have been conducted on monodisperse systems. Knight *et al.* [1] investigated density relaxation of a column containing monodisperse spherical beads subject to a long sequence of taps while Nowak *et al.* [2] studied density fluctuations in vibrated granular materials.

Theoretical work dealing with vibrated powders was conducted by Barker and Mehta [3,4]. Studies addressing the compaction under shear and/or tapping were done by Pouliquen *et al.* [5], Nicolas *et al.* [6], and Luding *et al.* [7].

Several models were introduced to describe the dynamics of a granular system under compaction, including a lattice model [8] and the Tetris model [9] as a special case of a frustrated lattice gas. The study of polydisperse systems dates back to the ancient Greeks where Apollonius of Perga studied the problem known as "Apollonian packing" [10,11]. This problem deals with the question of how to tile the space with circles by iteratively placing between every three circles a circle tangentially touching all three. The Apollonian packing is a special case of the so called "space filling bearings" in which a plane is tiled with circles touching one another such that the whole area is covered with circles [12-15]. These space filling bearings fill space with a particle size distribution given by a truncated power law. Different studies of polydisperse packings were conducted by Aste [16], Dodds and Weitz [17], and Brilliantov et al. [18,19].

The aim of our work is to study the time evolution of density in polydisperse systems under vibratory compaction. The size distribution of the particles obeys a truncated power law (different than the one used by Brilliantov). We modified the one-dimensional reversible parking lot model [20-22] where identical particles adsorb on an interval with an adsorption rate k^+ and desorb with a rate k^- , such that the system is hierarchically initialized and the equilibrium state with the highest density is reached through self-consistent desorption.

II. THE MODEL

We first explain the classical parking lot model [21] and its reversible variant [20]. Afterwards we introduce our generalization to polydisperse systems and the self-consistent desorption probability.

A. The parking lot model

In the classical parking lot model (PLM), identical particles of size *r* try to adsorb with an adsorption rate k^+ on randomly chosen places along an interval of length *l*. The adsorption fails if the chosen place is partially occupied by a previously adsorbed particle. Because of the irreversible adsorption mechanism the system will reach a so called jammed state with a final density of $\rho_{jam} \approx 0.7475$.

Krapivsky and Ben-Naim extended this model to the reversible parking lot model [20]. Here particles will additionally desorb with a desorption rate k^- (Fig. 1) and the density of the system's equilibrium state can be different from ρ_{jam} . This equilibrium state is determined by the ratio between the adsorption and the desorption rates, $k = k^+/k^-$. For the final density ρ_{ss} the following leading behavior in the two limiting cases was found:

$$\rho_{ss}(k) \cong \begin{cases} k & \text{for } k \leqslant 1 \\ 1 - \ln(k)^{-1} & \text{for } k \gg 1. \end{cases}$$
(1)

In the limit of $k \rightarrow \infty$ ($k^+ = 1, k^- \rightarrow 0$), also called the desorption controlled limit, the interval is completely filled with particles and $\rho_{ss} = 1$ when time goes to infinity.

B. Generalization to a polydisperse model

Granular materials that reach highest densities consist of particles with different sizes. Such media are called polydisperse. We will simulate such media using a polydisperse PLM.

The behavior of a polydisperse PLM is governed by the size distribution of the particles, the amount of particles



FIG. 1. The reversible parking lot model with an interval of length *l* and particles of equal size *r*. Particles adsorb with a rate k^+ and desorb with a rate k^- .



FIG. 2. The self-consistent reversible polydisperse parking lot model with an interval of length l, particles of different sizes r, and the reservoir. Particles adsorb with a rate k^+ and desorb with a conditional probability p(r) which also depends on the distribution of holes in the interval.

available in the system, the initialization process, and the dependence of the desorption rate on the particle size. Figure 2 shows the setup for the polydisperse parking lot model.

Unlike the case of monodisperse systems we introduce a reservoir because it turns out to be necessary to restrict the number of particles of each size in order to impose a given size distribution. For a system with *K* particles of which K_1 are adsorbed on the interval, this reservoir will contain the remaining $K_2 = K - K_1$ particles.

We restrict the size of the particles to the interval $\overline{R} = [r_{min}, r_{max}]$ which we will refer to as the "range of particle sizes." For all simulations discussed here, r_{max} is set to unity and the size distribution of all particles is given by a truncated power law

$$P(r) = ar^{-b}, \quad r \in \overline{R}, \tag{2}$$

where *a* is a normalization factor chosen such that $\int_{r_{min}}^{r_{max}} P(r) dr = l$. We allow the exponent *b* to take values in the range of 1.306 < b < 1.802, the same range as that found for two-dimensional space filling bearings [13]. We also apply periodic boundary conditions to the system. Its density ρ is given by

$$\rho = \sum_{i=1}^{K_1} r_i / l, \tag{3}$$

where K_1 is the total number of adsorbed particles and r_i is the length of the *i*th adsorbed particle.

As in the classical PLM, the particles attempt to be adsorbed with the adsorption rate k^+ . This rate is defined as the number of particles attempting to be adsorbed per time unit. A particle of given size *r*, randomly chosen among the adsorbed particles, will desorb with a conditional desorption probability p(r).

Desorbed particles are put back into the reservoir. The conditional probability can be calculated through

$$p(r) = \sum_{i=1}^{K_1} {'(h_i - r)/l.}$$
(4)

Here K_1 is the total number of holes which is the same as the number of adsorbed particles when using periodic boundary conditions. The variable h_i is the length of a single hole, which can be zero in the case of two touching particles. The primed sum only considers terms with $h_i > r$. Thus p(r) will be zero if the particle size r is larger than any available hole.

We call p(r) the "self-consistent desorption probability" because of its dependence on the hole distribution. It changes in time as the configuration in the interval changes.

This approach is justified because in an experiment, a particle can only leave its place if there is a large enough hole where it can move to. The holes of the system are stored in a list H which is updated after each adsorption and desorption.

In the monodisperse parking lot model a constant desorption rate removes particles regardless of their local environment. Therefore, the system ultimately reaches an equilibrium state independent of the initial condition. This is not the case in a polydisperse system where the self-consistent desorption is implemented. If we would use a constant desorption rate in the polydisperse system, the result would be a final density lower than the ρ_{jam} obtained in the monodisperse model.

1. Dynamics

Now we will explain the dynamics of the system. The word "random" will denote a homogeneously distributed random number generator unless stated otherwise.

First the particles available to the system are generated. For this a total number of *K* particles is put into an initially empty reservoir (list). The size r_k of each particle is sampled randomly from the power law distribution given in Eq. (2). The total number *K* of particles is given by $\sum_{k=0}^{K} r_k = l$. Thus the generation of particles is stopped as soon as the sum of the lengths of all particles is equal to or larger than *l*. We call the size distribution of particles in the reservoir at this time (t=0) the " t_0 distribution."

Next an initial distribution of particles on the interval is generated. We will call this the "initialization of the interval." This is necessary because for an almost empty interval, p(r) is close to unity for all particles and any adsorbed particle would most likely desorb again. A further justification for this initialization is given in Sec. III A.

In order to reach highest densities a hierarchical initialization is used. This idea was inspired during a visit to Losert's [23] laboratory at the University of Maryland. The reservoir is sorted by size such that $r_1 > r_2 > \cdots > r_K$. Then each particle, starting with the biggest particle r_1 , is given *I* trials to adsorb. During the initialization, the desorption probability is set to zero. This resembles the filling of a recipient in an experiment, where the large particles are loaded first and the system is not vibrated.

For each adsorption trial, a random point in the interval is chosen. If the chosen place is not even partially occupied the particle will adsorb. If the particle did not adsorb after its *I*th trial it is left in the reservoir and one continues with the next smaller one. The initialization is finished when each particle had up to *I* trials for adsorption. The density resulting from this initialization is called ρ_{init} .

The parameter *I* has a meaning only during the initialization process. It plays no role during the adsorption/desorption mechanism. Here, with a rate k^+ , a particle is randomly picked from the reservoir and adsorbed if possible on a random position. If the adsorption is not possible, the particle will be put back into the reservoir. For desorption a

particle on the interval is randomly picked at each time step. With the probability p(r), given by Eq. (4), it is put back into the reservoir. Each time the distribution of particles in the interval changes, the list of holes *H* is updated accordingly.

2. Definitions of time

In this model we introduce two different definitions of time. The first definition covers the initialization of the system. Here one time step consists of a single adsorption trial. The second definition considers the dynamic part of the model. Here a single time step consists of an adsorption and a desorption trial. Adsorption is attempted with the rate k^+ while desorption is checked every time step. These two definitions are of significant difference. Nevertheless we will put them on the same scale in our density plots in order to investigate dependencies on different parameters. When talking about time we mostly refer to the definition of time during the initialization.

III. MONTE CARLO RESULTS

In this section we give an overview of the performed simulations. We always use an adsorption rate $k^+ = 1$. Thus, one adsorption trial is performed during each time step in the dynamic regime.

Let us first investigate the behavior of the system during the initialization. The alignment of the particles on the interval l at a certain time during the initialization is visualized in a spatiotemporal diagram by plotting at each time step the system with a height of one pixel and a width proportional to l. The density is gray scale encoded using white pixels for zero density and black pixels for density one. The darkness of the pixel depends linearly on the density. Arranging these pictures in chronological order results in the spatiotemporal diagram as displayed in Fig. 3 which shows the time evolution of the system during the initialization process.

Because of the hierarchical initialization the big particles, shown as regions of high density, are adsorbed first. As time progresses the interval is consecutively filled with smaller and smaller particles which settle in the remaining gaps until the system reaches a high density before dynamics start.

A. Size distribution

The hierarchical initialization avoids the exclusion of large particles and thus leads to an adsorption of almost all particles. In the ideal case of a completely filled interval, the t_0 distribution and the distribution of adsorbed particles for a system in its final state would be identical.

In Fig. 4 we display the size distribution of the adsorbed particles at the end of the dynamic part of the simulation. The solid line shows the distribution for a self-consistent desorption rate as given by Eq. (4) at the end of the simulation which coincides very well with the t_0 distribution which is omitted for clarity. The slope in this plot corresponds to the exponent of the power law, which is 1.33 in this case. All simulations show the same overall behavior for different values of \overline{R} and b. In addition, we show the distribution for a



FIG. 3. Spatiotemporal diagram of the initialization process. System parameters: l=300, $r_{min}=0.001$, $r_{max}=1$, $k^+=1$, I=1000, b=1.33, and K=5420. Density at the end of the initialization: $\rho \approx 0.985$.

system with constant desorption rate using no initialization. For large particles the distribution deviates very strongly from the t_0 distribution which justifies our hierarchical initialization.

B. Desorption probability

The desorption probability p(r) right after the initialization of the interval and at the end of the dynamic part of the simulation is shown in Fig. 5. The probability depends on the hole distribution and therefore changes in time. The solid line in Fig. 5 shows the probability at the end of the initialization process ($t \approx 10^7$). At this time, the transition from the initialization to the adsorption/desorption process takes



FIG. 4. Particle size distribution for the self-consistent system (solid line, I=1000) and a system with a constant desorption rate using no initialization (dotted line). The slope in the plot corresponds to the exponent of the power law, which is -1.33. In both cases we display the distribution at the end of the simulation.



FIG. 5. Desorption probability of the self-consistent system as a function of the particle size in a semilogarithmic plot. For a denser system the probability is smaller. The solid line is the probability at the end of the initialization process $(t \approx 10^7)$. The dotted line shows p(r) at the end of the simulation $(t \approx 10^9)$. System parameters: l = 5000, $r_{min} = 0.001$, $r_{max} = 1$, $k^+ = 1$, I = 1000, b = 1.33, and average K = 89 618. Data are averaged over ten runs.

place. The dotted line shows p(r) at the end of our simulation $(t \approx 10^9)$. The probability p(r) decreases as the system gets denser.

The probability p(r) will become zero for large particles at some time and they will not be able to desorb anymore. This leads to a stable configuration with highest densities including all the large particles in the interval.

C. Density evolution

The development of the density is shown in Fig. 6. Here the density evolution for different numbers of trials I are shown. The inset enlarges the time interval where the transition from the initialization to the adsorption/desorption pro-



FIG. 6. Density as a function of time in the self-consistent system for different values of *I*. The dotted line is the fitted curve according to Eq. (5). Fit parameters: $\rho_{\infty}=1$, $\Delta\rho_{\infty}=0.967$, B=2.829, and $\tau=19$ 339. Data are averaged over ten runs. The system parameters are the same as in Fig. 5.

cess takes place and we use a different definition of the time from this point on. Now adsorption and desorption take place simultaneously; the density rises logarithmically with time.

Knight [1] and Nowak [2] measured experimentally that the time evolution of density in monodisperse systems can be asymptotically fitted by the expression

$$\rho(t) = \rho_{\infty} - \frac{\Delta \rho_{\infty}}{1 + B \ln(1 + t/\tau)},$$
(5)

where the parameters ρ_{∞} , $\Delta \rho_{\infty}$, *B*, and τ depend on the experimental setup. Here ρ_{∞} is the final density while $\Delta \rho_{\infty}$ is the difference between this value and the density at t=0. The parameters *B* and τ fit the logarithmic behavior of the curve. The same asymptotic behavior was obtained by Krapivsky and Ben-Naim for the reversible parking lot model using a variable desorption constant [2]. For a comparison we plotted the fit of Eq. (5), using a dotted line, in Fig. 6. As we are using a dynamics different from the one in the experiment, the curves do not fit.

One can see that the density after the initialization is very close to the final density. Thus the dominating part in our simulations is the initialization process which we will investigate more closely in the following section. As the final density depends on the initialization, this means that our model is nonergodic.

D. Discussion

The final density mostly depends on the initialization as large particles that could not adsorb during the initialization are, in general, excluded from the interval for the rest of the simulation. Therefore we will concentrate our discussion on the initialization process. The initialization is characterized by ρ_{init} which itself depends on three parameters. The number of trials *I*, the exponent in the power law *b* and the range of particle sizes \overline{R} .

1. Dependence on I

As already seen in Fig. 6 a larger number of trials *I* increases considerably the initial density ρ_{init} of the system. In Fig. 7 the dependence of ρ_{init} on *I* is displayed. Starting from a low density of about 0.55 the density of the system increases until it reaches its maximum density for this value of r_{min} . Because the system is hierarchically initialized the final density depends on *I*. This dependence can be fitted by

$$\rho_{init}(I) = \rho_{max}(r_{min}) - \Delta \rho I^{-f}.$$
(6)

Here $\rho_{max}(r_{min})$ is the maximum density the system can reach for the chosen value of r_{min} in the limit $I \rightarrow \infty$ and $\Delta \rho$ is the difference between $\rho_{max}(r_{min})$ and the initialization density for I=1. The exponent f is a fit parameter (f= 0.4406 for r_{min} = 0.001) giving the logarithmic relaxation towards the highest density. In Fig. 8 the curve fitted with Eq. (6) is the dotted line.

A better fit can be accomplished when in Eq. (6) the last term is multiplied by the last term given in Eq. (5). The resulting expression has the form:



FIG. 7. Dependence of ρ_{init} on the number of trials *I*. Three curves are displayed with different r_{min} while $r_{max} = 1$ is kept constant for all three runs. The maximal possible density is determined by r_{min} and reached for very large *I*. System parameters: l = 5000, $r_{max} = 1$, $k^+ = 1$, b = 1.33 and $K \approx 89\,000$. Data are averaged over nine independent runs.

$$\rho_{init}(I) = \rho_{max} - \frac{\Delta \rho}{1 + B \ln(1 + I/\tau)} I^{-f_n}.$$
 (7)

In Fig. 8 this results in the full line coinciding with the simulation data. The value of f_n is $f_n = 0.3163$ for $r_{min} = 0.001$.

The number of trials I also influences the size distribution of the particles. In Fig. 9 the size distribution for two different values of I is displayed. The distribution of adsorbed particles at the end of the simulation coincides better with the t_0 distribution for larger I.

The deviation from the original distribution depends on the value of I because a larger I gives each particle more trials for adsorption. For large I, big particles adsorb first because of the hierarchical initialization and a deviation is only noticeable for small particles. Comparing Fig. 9 with Fig. 4 reveals that the deviation from the t_0 distribution (large I) after the initialization almost vanishes when the



FIG. 8. Simulation data of Fig. 7 fitted by Eq. (6)(dotted line, $\rho_{max}=1$, $\Delta\rho=0.4406$, f=0.4109) and Eq. (7) (solid line, $\rho_{max}=1$, $\Delta\rho=0.4406$, B=0.6366, $\tau=21.3$, $f_n=0.3163$). The system parameters are the same as in Fig. 7.



FIG. 9. Comparison of the size distribution at the end of the initialization for a different number of trials *I* (dotted line) with the t_0 distribution (solid line). System parameters: l=5000, $r_{min} = 0.001$, $r_{max}=1$, $k^+=1$, b=1.33, and $K \approx 89\,000$.

adsorption/desorption mechanism is activated. Finally, we study what effect I has on the self-consistent desorption probability p(r).

In Fig. 10 the desorption probability right after the initialization is displayed for three different I. The larger the I the smaller the overall desorption probability. More trials I during the initialization result in smaller holes and a denser system. Hence the overall probability will be lower for a larger I. In all three runs it is zero for the largest particles.

2. Dependence on \overline{R}

The maximum density also depends on the range of particle sizes \overline{R} . In Fig. 11 r_{max} was kept constant (unity) while r_{min} was varied. The dependence of ρ_{init} on r_{min} is displayed for two different values of *I*. A larger range of particle sizes \overline{R} results in a higher ρ_{init} . This general behavior is independent of the number of trials *I*.



FIG. 10. Desorption probability for different number of trials *I* in a double logarithmic plot, right after the initialization. It is zero for the largest particles in all three cases. System parameters: l = 5000, $r_{min} = 0.001$, $r_{max} = 1$, $k^+ = 1$, b = 1.33, and $K \approx 89\,000$.



FIG. 11. Dependence of ρ_{init} on r_{min} fitted by Eq. (8) $[\rho_{max}(I)=0.987, \Delta\rho=0.241, e=0.600 \text{ for } I=1000 \text{ and } \rho_{max}(I)=0.562, \Delta\rho=0.093, e=0.519 \text{ for } I=1]$. The smallest particle size r_{min} is varied while r_{max} is kept constant. System parameters: $l = 5000, r_{max}=1, k^+=1, b=1.33$, and $K \approx 5200-90000$. Data are averaged over nine runs.

The hierarchical initialization, starting with the biggest particle, allows the system to densify better because the holes get smaller and smaller. If the initialization started with the smallest particles first, the system would end up in a final state with an extremely low density. The smallest size r_{min} in the range of particle sizes \overline{R} determines the smallest hole that can be filled and thus determines the highest reachable density.

The dependence on the minimal particle size in Fig. 11 can be fitted very well by the equation

$$\rho_{init}(r_{min}) = \rho_{max}(I) - \Delta \rho r_{min}^e.$$
(8)

Here $\rho_{max}(I)$ is the maximal possible density for the applied number of trials I which occurs for $r_{min} \rightarrow 0$. The variable $\Delta \rho$ is the difference between this maximal density and the density the monodisperse system reaches for the same applied number of trials I. Thus we can determine these values through averaging over several independent simulations. The fit parameter e has a value of e=0.6 for I=1 and e=0.519 for I=1000.

3. Dependence on b

The most interesting behavior of the system is revealed when investigating the dependence on *b*. Figure 12 shows this dependence for two different values of *I*. For a small value of *I*, ρ_{init} rises proportionally to *b*. Increasing *I* shows that for a certain value of *b*, ρ_{init} reaches a maximum. For I=100, *b* is approximately 1.62 as shown in the figure. For I=1000 this value shifts to 1.42. Thus the exponent *b* is important to reach high densities. The fine tuning in that regime can then be accomplished by adapting the parameter *I*.

The value of b corresponds to the slope in the log-log plot of the size distribution. For a larger b the probability to find a small particle will increase. The summed up length of the K



FIG. 12. Dependence of ρ_{init} on the exponent *b*. System parameters: l=5000, $r_{min}=0.001$, $r_{max}=1$, $k^+=1$, $K \approx 85\ 000-422\ 000$. Data are averaged over nine runs.

particles in the system must be equal to the length l of the interval for all values of b. Therefore, a system with a larger b has more particles but their average size is smaller.

As mentioned in the preceding section, the hierarchical initialization generates small holes. Thus, increasing *b* increases ρ_{init} because more smaller particles able to fit into these holes become available. On the other hand, during each initialization, holes smaller than r_{min} are generated. They will never be filled and increasing the number of particles *K* in the system enhances the generation of these holes. These two effects act against each other and so there exists a value of *b* for which the initialization density ρ_{init} will have a maximum.

IV. CONCLUSION

We extended the reversible parking lot model [20] and work done by Brilliantov *et al.* [18,19] by adding the selfconsistent desorption to polydisperse random sequential adsorption. The use of a constant desorption rate [20] in our model would result in an exclusion of larger particles. Avoiding segregation and reaching high densities is accomplished with a hierarchical initialization of the system. This makes the model nonergodic as this final density strongly depends on the initialization.

The most interesting result is the existence of a specific value for the exponent b of the power law of the size distribution for which the initialization density reaches a maximum as seen in Fig. 12. Fitting the experimentally measured expression for the evolution of density [1,2] to our density evolution is not satisfactory since our model uses a dynamics different from the one in the experiment.

As the initialization is crucial in our model, it would be interesting to compare our data with experimental ones, using a hierarchical initialization. Of special interest would be the dependence of the finals density on the exponent *b*. Future work should also focus on the extension of this model in two or three dimensions. From small systems we know that here initialization is even more important. In addition, we would expect new and interesting effects due to gravity.

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