The reversible polydisperse Parking Lot Model

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Abstract

We use a new version of the 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.

I. INTRODUCTION

The vibratory compaction of granular materials has long been of importance in technological applications like 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.

Several models were introduced to describe the dynamics of a granular system under compaction, including a lattice model [3] and the Tetris model [4] as a special case of a frustrated lattice gas. The study of polydisperse systems reaches back to the ancient Greeks where Apollonius of Perga studied the problem know as 'Apollonian packing' [5, 6]. This problem deals with the question 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' (SFB) in which a plane is tiled with circles touching one another such that the whole area is covered with circles [7, 8, 9, 10]. These space filling bearings fill space with a particle size distribution given by a truncated power law. Different studies of polydisperse packings where conducted by Aste [11], Dodds and Weitz [12] and Brilliantov et al. [13, 14].
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 \cite{15, 16, 17} 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 \cite{16} and its reversible variant \cite{15}. 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 \cite{15}. Here particles will additionally desorb with a desorption rate $k^-$ (Figure 1) and the density of the system’s equilibrium state can be different from $\rho_{jam}$. This equilibrium state is determined by the ratio between the adsorption and the desorption rates $k = k^+ / k^-$. For the final density $\rho_{ss}$ the following leading behavior in the two limiting cases was found:

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

For the final density $\rho_{ss}$ the following leading behavior in the two limiting cases was found:

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 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.

![Diagram of the polydisperse Parking Lot Model](image)

FIG. 2: The self consistent reversible polydisperse Parking Lot Model with an interval length $l$, particles of different size $r$ 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.

Unlike to 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 $\mathcal{R} = [r_{min}, r_{max}]$ 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:

$$P(r) = a \cdot r^{-b}, \quad r \in \mathcal{R} \quad (2)$$

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 found for two dimensional space filling bearings [8].

We also apply periodic boundary conditions to the system. Its density $\rho$ is given by.

$$\rho = \frac{K_1}{l} \sum_{i=1}^{K_1} r_i / l \quad (3)$$

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 $p(r)$. This conditional probability can be calculated through:

$$p(r) = \frac{\sum_{i=1}^{K_1} (h_i - r)}{l} \quad (4)$$
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 $\rho_{jam}$ obtained in the monodisperse model.

1. Dynamics

Now we will explain the dynamics of the system. The word 'random' will denote an equally 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 a power law distribution 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 $l$. 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 section III A.

In order to reach highest densities a hierarchical initialization is used. This idea was inspired during a visit to W. Losert’s 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 $\rho_{\text{init}}$.

Now the adsorption/desorption mechanism is activated. 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 does not get a second trial but 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.

In this model we have 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 time after the initialization (the dynamics). Here a single time step in the system 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.

### III. MONTE CARLO RESULTS

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

The alignment of the particles on the interval $l$ at a certain time is visualized in a spatio-temporal diagram by plotting at each time step the system by 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 spatio-temporal diagram as displayed in Figure 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 (desorption is always turned off in this case).

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 Figure 4 we display the size distribution of the adsorbed particles at the end 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. All simulations show the same overall behavior for different values of \( \overline{R} \) and \( b \). In addition we show the distribution for a 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.
FIG. 5: Desorption probability of the self consistent system as a function of the particle size in a semi-logarithmic 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: \( l = 5000, r_{\text{min}} = 0.001, r_{\text{max}} = 1, k^+ = 1, I = 1000, b = 1.33, \) average \( K = 89618 \). Data are averaged over 10 runs.

B. Desorption Probability

The desorption probability \( p(r) \) right after the initialization of the interval and at the end of the simulation is shown in Figure 5. The probability depends on the hole distribution and therefore changes in time. The solid line in Figure 5 shows the probability at the end of the initialization process \( (t \approx 10^7) \). The dotted line shows \( p(r) \) at the end of our simulation \( (t \approx 10^9) \). The probability \( p(r) \) decreases the denser the system gets.

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

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: \( \rho_\infty = 1, \Delta\rho_\infty = 0.967, B = 2.829, \tau = 19339 \). Data are averaged over 10 runs. The system parameters are the same as in Figure 5.

The development of the density is shown in Figure 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 process takes place. From this point on, adsorption- and desorption take place simultaneously; the density rises slower.

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 \( \rho_\infty, \Delta \rho_\infty, B \) and \( \tau \) depend on the experimental setup. Here \( \rho_\infty \) is the final density while \( \Delta \rho_\infty \) is the difference between this value and the density at \( t = 0 \). The parameters \( B \) and \( \tau \) 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]. The dotted line in Figure 6 is the fit using Eq. (5). We 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 closer in the following section.

D. Discussion

Using the self consistent desorption, the final density mostly depends on the initialization. Large particles that could not adsorb during the initialization are, in general, excluded from the interval for the rest of the simulation. The initialization is characterized by \( \rho_\text{init} \). Three parameters determine this density. The number of trials \( I \), the exponent in the power law \( b \) and the range of particle sizes \( \bar{r} \).

\[ I (\text{number of trials during initialization}) \]

FIG. 7: Dependence of \( \rho_\text{init} \) on the number of trials \( I \). Displayed are three curves with different \( r_{\text{min}} \) while \( r_{\max} = 1 \) is kept constant for all three runs. The maximal possible density is determined by \( r_{\text{min}} \) and reached for very large \( I \). System parameters: \( l = 5000, r_{\max} = 1, k^+ = 1, b = 1.33 \) and \( K \approx 89000 \). Data are averaged over 9 independent runs.

As already seen in Figure 6 a larger number of trials \( I \) increases considerably the final density \( \rho_\text{init} \) of the system. In Figure 7 the
dependence of $\rho_{\text{init}}$ 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 $r_{\text{min}}$. Because the system is hierarchically initialized the final density depends on $I$. This dependence can be fitted by:

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

Here $\rho_{\text{max}}(r_{\text{min}})$ is the maximum density the system can reach for the chosen value of $r_{\text{min}}$ in the limit $I \to \infty$ and $\Delta \rho$ is the difference between $\rho_{\text{max}}(r_{\text{min}})$ and the initialization density for $I = 1$. The exponent $f$ is a fit parameter ($f = 0.4406$ for $r_{\text{min}} = 0.001$) giving the logarithmic relaxation towards the highest density. In Figure 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:

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

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

The number of trials $I$ also influences the size distribution of the particles. In Figure 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 absorb first because of the hierarchical initialization and a deviation is only noticeable for small particles. Comparing Figure 9 with Figure 4 reveals that the deviation from the $t_0$ distribution (large $I$) after the initialization almost vanishes when the adsorption/desorption mechanism is activated.

Finally we study which effect $I$ has on the self consistent desorption probability $p(r)$.

![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: $l = 5000$, $r_{max} = 1$, $k^+ = 1$, $b = 1.33$, and $K \approx 89000$.](image1)

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: $l = 5000$, $r_{max} = 1$, $k^+ = 1$, $b = 1.33$, and $K \approx 89000$.

In Figure 10 the desorption probability right after the initialization is displayed for three different $I$. The larger $I$ 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 $R$

![Dependence of $\rho_{init}$ on $r_{min}$ fitted by Eq. (8) ($\rho_{max}(I) = 0.987$, $\Delta \rho = 0.241$, $e = 0.600$ for $I = 1000$ and $\rho_{max}(I) = 0.562$, $\Delta \rho = 0.093$, $e = 0.519$ for $I = 1$). The smallest particle size $r_{min}$ is varied while $r_{max}$ is kept constant. System parameters: $l = 5000$, $r_{max} = 1$, $k^+ = 1$, $b = 1.33$, $K \approx 5200 - 90000$. Data are averaged over 9 runs.](image2)

FIG. 11: Dependence of $\rho_{init}$ on $r_{min}$ fitted by Eq. (8) ($\rho_{max}(I) = 0.987$, $\Delta \rho = 0.241$, $e = 0.600$ for $I = 1000$ and $\rho_{max}(I) = 0.562$, $\Delta \rho = 0.093$, $e = 0.519$ for $I = 1$). The smallest particle size $r_{min}$ is varied while $r_{max}$ is kept constant. System parameters: $l = 5000$, $r_{max} = 1$, $k^+ = 1$, $b = 1.33$, $K \approx 5200 - 90000$. Data are averaged over 9 runs.

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

The hierarchical initialization, starting with the biggest particle, allows the system to densify better because the holes get smaller and smaller. Would the initialization start 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 $\mathcal{R}$ determines the smallest hole that can be filled and thus determines the highest reachable density.

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

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

Here $\rho_{max}(I)$ is the maximal possible density for the applied number of trials $I$ which occurs for $r_{min} \to 0$. 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 $I$, $\rho_{init}$ rises proportionally to $b$. Increasing $I$ reveals, that, for a certain value of $b$, $\rho_{init}$ reaches a maximum. 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 $K$ 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 previous section, the hierarchical initialization generates small holes. Thus, increasing $b$ increases $\rho_{init}$ because more smaller particles, able to fit into these holes, become available. On the
other hand, during each initialization, holes, smaller than \( r_{\text{min}} \), 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 the initialization density \( \rho_{\text{init}} \) will have a maximum.

IV. CONCLUSION

We generalized the reversible Parking Lot Model introduced by Krapivsky and Ben-Naim \[15\] from a monodisperse model to a polydisperse one. This 'self consistent reversible polydisperse Parking Lot Model' results in a final and stable state of very high density.

The crucial part, in order to reach high densities, is the self consistent desorption probability. The use of a constant desorption rate results in an exclusion of larger particles. The system will reach a final state of unrealistic low density. Thus, the small particles must not be allowed to block a larger interval and large particles already adsorbed in the interval need to stay. This is realized through a hierarchical initialization where each particle gets \( I \) trials for adsorption.

To keep the density on a high level we propose a self consistent desorption probability. A particle can only desorb if at least one hole, as large as this particle, exists. The density rises as a power law with the number of trials \( I \) for each particle during the initialization and is fitted well by Eq. (7). The smaller the range \( \overline{R} \), the lower the final density.

The most interesting result is: There exists a value for the exponent \( b \) of the power law of the \( t_0 \) distribution for which the final density reaches a maximum as seen in Figure 12.

In short: A large number of trials \( I \) and a wide range of particles sizes \( \overline{R} \) results in a high final density. The maximal possible density is determined by the exponent \( b \).

In this paper we extended the work of Brilliantov et al. \[13, 14\] by adding the self consistent desorption to the polydisperse RSA in one dimension. We could also apply the expression for the evolution of density, measured experimentally by Knight \[1\] and Nowak \[2\], to our density evolution. As the initialization is the crucial point in our model it would be interesting to see the density evolution of an experiment using our hierarchical initialization.

Future work should focus on the behavior of this model in two or three dimensions and under the influence of gravity. The main difficulty will be the development of a fast algorithm able to determine the hole distribution.
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