Marginal states of hard disks in a one-dimensional channel

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(Dated: May 7, 2020)

We have studied a class of marginally jammed states in a system of hard disks confined in a narrow channel—a quasi-one-dimensional system—whose exponents are not those predicted by theories valid in the infinite-dimensional limit. The exponent $\gamma$ which describes the distribution of small gaps takes the value 1 rather than the infinite dimensional value $0.41269 \ldots$. Our work shows that there exist jammed states not found within the tiling approach of Ashwin and Bowles. The most dense of these states is an unusual state of matter that is asymptotically crystalline.

There has been remarkable progress in our understanding of the properties of marginally [1, 2] jammed states of hard spheres [3–8]. The most striking predictions are for the values of the exponents that describe the geometry of the marginally jammed system of hard spheres, such as the distribution of small gaps $h$ between the spheres, $g(h) \sim 1/h^\gamma$, as $h \to 0$. The exponent $\gamma = 0.41269 \ldots$, according to the infinite-dimensional replica-symmetry-breaking [9] mean field theory [7]. Numerical results in dimensions $d = 3$ to 10 [4] are consistent with the exponent being independent of dimension and equal to its value for $d \to \infty$.

This is a striking result which remains unexplained. Indeed, possible issues with the infinite-dimensional approach applied to $d = 3$ have been noted in [10]. There is also evidence that the exponents might not actually be independent of dimension, at least for shear-driven (and hence anisotropic) jammed states [11]. Despite this, it is commonly expected that the “upper critical dimension” is 2 [4, 12–15]. That is, the exponents should maintain their infinite-dimension values down to two dimensions; this expectation is supported by numerical evidence for logarithmic corrections to scaling in $d = 2$ [16–18]. In this paper we present evidence that marginally-jammed states in a one-dimensional system of hard disks have very different values for the exponents; for example, we find that $\gamma = 1$ exactly. Our result therefore provides further evidence for an upper critical dimension for marginally-jammed packings.

The one-dimensional system of hard disks in a narrow channel has been extensively studied in other contexts [19–31]. The channel width available to the centers of the disks has in this paper the value $h = 0.95\sigma$ so that the disks, which have diameter $\sigma$, cannot pass each other, but can touch their nearest and next-nearest neighbors, as shown in Fig. 1. The packing fraction $\phi$ is defined as $\phi = N\pi\sigma^2/(4H_dL)$, where $N$ is the number of disks in a channel of length $L$ and width $H_d = h + \sigma$.

The jammed states for channel widths $h < \sqrt{3}\sigma/2$ have already been studied [24, 32]. The complexity of these jammed states is nonzero and all of the states are marginal, in the sense that there are just enough contacts to ensure stability. However, when $h < \sqrt{3}\sigma/2$ there are no small gaps at all between the disks, whereas for the range of $h$ studied in this paper, $\sqrt{3}\sigma/2 < h < \sigma$, there are gaps that can be arbitrarily small: their distribution is described by the exponent $\gamma = 1$. The jammed states with arbitrarily small gaps have nonzero complexity and are also marginal; however, most of the jammed states in our system are not marginal.

Recently Ikeda [33] has studied the case when the diameters of the disks have a broad dispersion in size and obtained $\gamma = 0$. When he used his method on our monodisperse system he found only jammed states that were not marginal (private communication). His method for finding jammed states is similar to that used in higher dimensional systems [34, 35]. Our marginally jammed states seem to be invisible to these methods. It is the case that different preparation methods can result in ensembles of jammed states with very different properties. For example, for channel widths $h < \sqrt{3}\sigma/2$ one particular preparation protocol can generate an ensemble of jammed states which are hyperuniform in a situation where the overwhelming majority of states do not have hyperuniformity [32]. The fact that Ikeda found $\gamma = 0$ for his polydisperse system while we have $\gamma = 1$ in the range $\sqrt{3}\sigma/2 < h < \sigma$ for our monodisperse system suggests that there might be a breakdown of universality for this exponent in one-dimensional systems, in that it might depend on the width of the channel, polydispersity, and the preparation method used for obtaining the jammed states.

Ashwin and Bowles [36] claimed to have constructed the complete jamming landscape for disks all of the same size when $\sqrt{3}\sigma/2 < h < \sigma$. They argued that all the jammed states in the system could be constructed from 32 varieties of tile together with rules limiting which tiles could be joined to other tiles. Figure 1 shows two configurations that can be described by their tiling procedure: a unit cell of the state of maximum density (the “buckled crystal”) and an asymmetric pentagon. In the tiling picture, the gaps between disks take on a finite number of nonzero discrete values. However, we have discovered that the Ashwin-Bowles picture is incomplete: there are jammed states that would require an infinite number of tiles. We first became aware of this by studying the jammed states produced Lubachevsky-Stillinger [37] quenches; these states regularly contained jammed disks at distances from the walls that were not among those considered by Ashwin and Bowles. As a consequence of this we shall not be using the tiling approach. Our work is mainly analytical; we resort to numerical methods only to verify the stability of the jammed states.

The coordinates of a disk will be labelled $(x, y)$, where $y$...
is measured from the mid-point of the channel. A disk which is just touching a wall has \( y = \pm y_1 \), where \( y_1 = h/2 \); it will be referred to as a 1-disk (see Fig. 1). A 4-disk may have positions \( \pm y_4 \), where \( y_4 = \sqrt{3}\sigma/2 - h/2 \approx 0.391025 \); it is at the apex of an equilateral triangle whose other vertices are 1-disks. One further disk position, \( y_2 \), frequently arises in quenches; it is defined by the pentagonal arrangement of disks shown in Fig. 1(b).

The jammed states that we focus on in this paper (see Fig. 3) consist of tilted equilateral triangles of disks, stabilized by additional 1-disks. The triangles have varying orientations that are specified by the following algorithm. We refer to Fig. 2:

1. Disk (a) touches the wall, \( y_a = \pm y_1 \). An equilateral triangle of disks (bcd) has its first disk, (b), touching the opposite wall, \( y_b = \mp y_1 \), and its second disk, (c), touching disk (a). Given the values of \( (x_a, y_a) \) and \( (x_b, y_b) \), the positions of disks (c) and (d) can be obtained exactly, e.g. by solving the four equations specifying the contacts (ac), (bc), (bd), and (cd).

2. Two more disks, (e) and (f), are placed at \( \pm y_1 \), touching their next-nearest neighbors, (c) and (d), respectively.

3. Steps 1 and 2 are repeated with disks (e) and (f) replacing (a) and (b), respectively.

At step (2) one could, instead of placing one pair of disks, choose to put in two pairs, as shown in Fig. 3(b): the stability of the jammed state is unaffected. States with a nonzero complexity can be obtained by placing the additional pairs of disks at random in the configuration generated by the deterministic algorithm 1–3.

The algorithm 1–3 generates configurations like those shown in Fig. 3(a) and (b). The \( y \) coordinates of the colored disks approach a limiting value, \( y_{\text{Teal}} \), which in our diagrams is represented by the color teal (intermediate between green and blue). The limiting state is crystalline; it is depicted in Fig. 4.

The jammed states in Fig. 3(a) and (b) do not satisfy periodic boundary conditions. Periodic states can be constructed as shown in Fig. 3 (c), (e) and (f): two regions containing tilted equilateral triangles of disks are sandwiched between disks at positions 1 and 4, which form a region of buckled crystal. These sandwich states are characterized by an inversion of the tilted equilateral triangles near their midpoint.

We next discuss the stability of the sandwich states. They are manifestly \textit{locally jammed}, as this only requires each disk to have three contacts, not all on the same semicircle. We have checked these states for stability against a collective displacement of any number of disks by using an extension of the linear programming algorithm discussed in Ref. [38]. The algorithm not only checks for linear stability but also finds a stable state that the system can reach when it is not stable, as illustrated in Fig. 3(d) for the case \( N = 24 \). (Sandwich states with just one unit cell of buckled crystal within them have values of \( N \) which are multiples of 8.) Details of the algorithm can be found in the Supplemental Material. We find that the sandwich states containing one unit cell of buckled crystal are stable for \( N = 8 \) and \( N = 16 \) and for all \( N \geq 96 \). However, for \( N = 24, 32, \ldots, 88 \), the sandwich states can be made stable by the addition of a second unit cell of buckled crystal; an example is shown in Fig. 3(e) for the case \( N = 24 + 6 = 30 \).

The sandwich states can be regarded as marginally stable for large \( N \). A truly marginal state is one in which the number of contacts of the disks is equal to the number of their degrees of freedom \( N_f \). The latter is \( 2N - 1 \) (not counting the uniform translation of the entire system along the \( x \)-axis); the number of contacts in periodic sandwich states with one unit cell of buckled crystal as shown in Fig. 3(c) is \( N_c = 2N + 2 \), so \( N_c - N_f = 3 \); i.e., there are just three more constraints than required for strict marginality. Thus, for large \( N \geq 96 \), the sandwich states approach the condition of marginal stability, in the sense that the ratio \( (N_c - N_f)/N \) can be made arbitrarily small.

The marginally stable configurations have gaps that become vanishingly small for \( N \to \infty \). They are the gaps between disks of types (d) and (e) in Fig. 2; see also Fig. 3(a). From the geometry of the state, the sizes \( h_i \) and \( h_{i+1} \) of consecutive gaps can be related algebraically. For large values of \( i \), the relation simplifies to

\[
h_{i+1} = h_i/b,
\]

(1)
where the constant $b \simeq 1.219$ for $h = 0.95\sigma$. This implies that for an infinite sequence the distribution of gaps would be of the form

$$g(h) = \frac{1}{h \ln b},$$

as $h \to 0$; thus, the exponent for gap sizes is $\gamma = 1$. A distribution varying as $1/h$ at small $h$ is not normalizable, but this is not a problem in practice because, for any finite value of $N$, there is a smallest gap whose size is of order $\exp(-cN)$, where $c > 0$. The result $\gamma = 1$ should be contrasted with $\gamma = 0.41269\ldots$ for jammed states of spheres in the limit $d \to \infty$; the latter value of $\gamma$ is also consistent with simulation results for all $d \geq 3$ [4].

Extra 1–1 disk insertions do not change the form of $g(h)$. Neither do they change the value of $N_c - N_f$; it remains at 3. Because any of the 1–1 pairs can be replaced by two 1–1 pairs,
in the limit of large $N$, these values, as is the inequality \(\gamma \to \infty\),

Notice that the inequality 
\[
\phi \geq \frac{N}{4} - 3, \\
\]
where $N$ is the number of disks before the insertions are made. When $N$ is large, the resulting states have packing fractions in the range $0.8064 < \phi < 0.8068$; the jammed states at the upper and lower limits of the density range are shown in Figs 4 and 5, respectively. Within this range of densities, the sandwich states are marginal and have a nonzero complexity.

States of the type discussed above consist of short lengths of buckled crystal alternating with noncrystalline regions of fixed length. Our construction can clearly be generalized to create aperiodic structures in which the lengths of the buckled-crystal and noncrystalline regions vary. We note that the distribution of small gaps, $g(h)$, will in general be related to the distribution of lengths of the noncrystalline regions, because the size of the smallest gap in one of these regions depends (exponentially) on its length. It may also be noted that each additional region of buckled crystal increases the excess number of contacts, $N_c - N_f$, and so takes the system further from marginality.

Another much studied quantity for marginal jammed states is the exponent associated with the distribution of small contact forces $f$, $P(f) \sim f^{\theta}$. We used the algorithms in Ref. [39] to determine the forces in the contacts when a unit force is applied along the $x$ axis. The smallest force, which occurs near the center of the sandwich state (see Fig. 6 for the case $N = 352$), seems to approach a nonzero value ($\approx 0.005$) as $N \to \infty$. The existence of a gap in $P(f)$ suggests that $\theta = \infty$. Notice that the inequality [40] $\gamma \geq 1/(2 + \theta)$ is satisfied by these values, as is the inequality $\gamma \geq (1 - \theta)/2$.

The sandwich state of Fig. 3(f) is a curious state of matter. In the limit of large $N$ it approaches the crystalline state of Fig. 4. However, it never quite reaches that state: the equilateral triangles of disks all have slightly different orientations and the small gaps persist. If one were to compute the structure factor [41] of the state it would have for $N \to \infty$ the delta function peaks of the crystal in Fig. 4. It could thus be regarded as an asymptotic crystal. But if one regards it as a crystal, its unit cell is the length of the system. We suspect that similar states might already have been found in other systems with restricted geometries; for example, the packing of spheres within a long cylinder, as considered in Ref. [42], where certain jammed states, constructed so as to satisfy periodic boundary conditions, were found to have a unit cell that was as large as the system.

We should like to thank P. Charbonneau, and E. Corwin for discussions. We would especially like to thank Harukuni Ikeda for running his code for finding jammed states on our system.

**SUPPLEMENTAL MATERIAL: LENGTH-COMPRESSION ALGORITHM**

The supplemental material describes how we used a linear programming method to determine the stability of jammed states of hard disks in a channel. Although the results are specific to our system, the methods are general and have been derived and discussed in detail by A. Donev and coworkers [38]. Our discussion of the methods is therefore brief, and the reader is referred to Ref. [38] for a careful description.

If a jammed configuration of hard disks is unstable, that is, if it allows a collective motion of an arbitrary number of disks, then it can be compressed until the system is truly jammed. In our work we consider periodic configurations of $N$ disks in a channel and minimize their length, subject to the constraints of no overlap of disks with each other or the channel walls.
FIG. 7. A configuration of four disks, used in the example of a rigidity matrix given in Eq. (3). In addition to the actual contacts shown by red dots, the rigidity matrix includes potential contacts, such as those between disks (a) and (b), and between disks (c) and (d) and the walls.

The length of the configuration, \( L = x_{N+1} - x_1 \), is a linear function of the 2N-dimensional vector of disk coordinates, \( \mathbf{R} \). Thus, it is natural to consider a linear programming problem in which the function \( L[\mathbf{R}] \) is minimized, subject to the following linearized constraints

\[
\mathbf{A}^T \Delta \mathbf{R} \geq -\mathbf{h}, \\
\Delta x_{N+1} \leq 0, \\
\Delta x_1 = 0, \\
\Delta r_{N+1} = \Delta r_1, \\
\Delta r_{N+2} = \Delta r_2,
\]

where \( \Delta \mathbf{r}_n = (\Delta x_n, \Delta y_n)^T \), \( \Delta \mathbf{R} = (\Delta r_1, \Delta r_2, \ldots, \Delta r_N)^T \) is a set of potential unjamming displacements, and \( \mathbf{A} \) is the rigidity matrix containing all potential contacts (i.e., pairwise contacts with all nearest and next-nearest neighbours). The components of the vector \( \mathbf{h} \) are the sizes of the gaps at each of the potential contacts; the gap sizes are nonnegative. The matrix \( \mathbf{A} \) has two rows for each disk and \( N_C \) columns that represent the \( N_C \) possible contacts. For the example shown in Fig. 7, \( \mathbf{A} \) is given by

\[
\mathbf{A} = \begin{pmatrix}
  a & w & a, b & a, c & b, w & b, c & b, d & c, w & c, d & d, w \\
  a & w & a, b & a, c & b, w & b, c & b, d & c, w & c, d & d, w \\
  b & 0 & -u_{a,b} & 0 & u_{b,w} & u_{b,c} & u_{b,d} & 0 & 0 & 0 \ \\
  c & 0 & 0 & u_{a,c} & 0 & -u_{b,c} & 0 & u_{c,w} & u_{c,d} & 0 \ \\
  d & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

where \( u_{m,n} \) denotes the unit vector directed from the center of disk \( n \) to the center of disk \( m \),

\[
u_{m,n} = \frac{\mathbf{r}_m - \mathbf{r}_n}{\|\mathbf{r}_m - \mathbf{r}_n\|},
\]

and \( u_{m,w} = \pm \mathbf{y} \) is a unit vector directed into the channel from the wall that is nearer to disk \( m \). To implement the periodic boundary condition, two extra disks \( N + 1 \) and \( N + 2 \), which are equivalent to disks 1 and 2, are added to the end of the channel; this avoids having the matrix \( \mathbf{A} \) depend on \( L \), which would make the problem nonlinear. The bottom right section of \( \mathbf{A} \) containing these disks is then

\[
\begin{pmatrix}
  \cdots & N - 1, w & N - 1, N & N - 1, N + 1 & N, w & N, N + 1 & N, N + 2 \\
  \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
  N - 1 & u_{N-1,w} & u_{N-1,N} & u_{N-1,N+1} & 0 & 0 & 0 \\
  N & 0 & -u_{N-1,N} & 0 & u_{N,w} & u_{N,N+1} & u_{N,N+2} \\
  N + 1 & 0 & 0 & -u_{N-1,N+1} & 0 & -u_{N,N+1} & 0 \\
  N + 2 & 0 & 0 & 0 & 0 & -u_{N,N+2} & 0
\end{pmatrix},
\]

and the displacements of disks \( N + 1 \) and \( N + 2 \) are defined by the last two linear constraints, \( \Delta \mathbf{r}_{N+1} = \Delta \mathbf{r}_1 \) and \( \Delta \mathbf{r}_{N+2} = \Delta \mathbf{r}_2 \).

The solution of the linear programming problem described above provides a set of displacements that reduces the length of the system. It is easily shown [38] that any set of displacements that satisfy the linearized nonoverlap constraints will also satisfy the exact (nonlinear) constraints. Thus, to obtain the densest packing we apply these displacements, recalculate \( \mathbf{A} \), and then repeat the process until no further displacement
of the disks will reduce the length. For our minimum-length configurations with strict zigzag order, we find that there is no room for disks to “rattle”: the system has reached a jammed state. Our stopping criterion was chosen as $\Delta L < 10^{-8}\sigma$, as this is a typical observed order of magnitude for changes when the algorithm is applied to a known stable configuration, such as the buckled crystal. When a state is stable the final state is, of course, the same as the initial state, to within the numerical precision of the calculation.

The sandwich states, with and without the insertion of extra pairs of disks at positions $\pm y_1$, were compressed using the iterative algorithm described above. In the main text we have shown the result of compressing the $N=24$ sandwich state containing no extra disks at $\pm y_1$: see Fig. 3(c,d). Another example for which the sandwich state is found to be unstable is shown in Fig. 8 for the case $N=32+10$, which contains the maximum number of insertions of disks at $\pm y_1$ into a sandwich state of 32 disks. The configuration is unstable when only one unit cell of buckled crystal is included (as shown in Fig. 8(a)), but becomes stable if two unit cells of buckled crystal are present.

FIG. 8. Before, (a), and after, (b), the compression of an unstable configuration of $N=42$ disks that contains the maximum possible number of 1–1 insertions in a sandwich state of 32 disks. The packing fraction of state (a) is $\phi = 0.80652$, which increases to 0.80721 on compression to the state (b).

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