How Generic are the Robust Theoretical Aspects of Jamming in Hard Sphere Models?

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In very recent work the mean field theory of the jamming transition in infinite dimensional hard spheres models was presented. Surprisingly, this theory predicts quantitatively numerically determined characteristics of jamming in two and three dimensions. This is a rare and unusual finding. Here we argue that this agreement in non-generic: only for hard sphere models it happens that sufficiently close to jamming the effective interactions are in agreement with mean-field theory, justifying the truncation of many body interactions (which is the exact protocol in infinite dimensions). Any softening of the bare hard sphere interactions results in effective interactions that are not mean-field all the way to jamming, making the discussed phenomenon non generic.

Models of hard sphere fluids and solids provided useful insights in condensed matter physics and in statistical mechanics for many decades $[1,2]$. In the last two decades hard spheres played a particularly important role in the investigation of the jamming transition, modeling the solidification of compressed granular matter $[3]$. The jamming transition is a critical phenomenon, characterized by a number of critical exponents whose values are typically irrational. Careful numerical simulations in 2 and 3 dimensions could determine these exponents quite precisely, with three to five digits accuracy $[4,5]$. Direct theoretical calculations in finite dimensions are not available, but a theory in infinite dimensions is available, providing exact predictions as $d \to \infty$ for these critical exponents. It turned out that the predictions at $d \to \infty$ appear to actually agree quantitatively with simulations results in $d = 2$ and 3 $[7,8]$. In the words of Ref. $[10]$, “One of the most remarkable features of the $d \to \infty$ solution is its agreement with both qualitative and quantitative aspects of jamming observed in numerical simulations. This outcome is especially stunning...”. Indeed stunning, and highly unusual: the critical exponents are usually strongly dependent on dimension, and in many cases turn into mean-field values above some critical dimension. For the jamming problem it was found that non-trivial exponents are $d$-independent from $d = 2$ to $d \to \infty$. The aim of this Letter is to explain this unusual phenomenon and to argue that it is non-generic, being fragile to any degree of softening of the hard sphere potential. The proposed answer is simple: the theory in infinite dimension is a perturbative approach that enjoys important simplifications by neglecting higher order terms that are hard to deal with in finite dimensions $[11]$. Below we demonstrate that near jamming, this is also the situation for hard spheres in 2 and 3 dimensions $[12]$, but only for hard spheres. Softening the hard sphere potential introduces unavoidable complications that mar the correspondence between low and infinite dimensions.

A key concept that underlies the discussion below is that of effective forces. These must be distinguished from the bare forces. For example in hard spheres the bare forces are zero when there is no contact and infinity upon contact. In a thermal ensemble particles collide and impart momenta, from which one can compute the effective forces $[12]$. If the bare potential is a function of the distance between particles, the effective force can be measured simply as an integral over the force, divided by the total interaction time. Another way to determine the effective forces, which is only appropriate for a glassy system, is to compute the time-averaged positions of the particles $\{\mathbf{r}_i\}^N_{i=1}$, and ask which effective forces stabilize these averaged positions to make them time independent. The second method $[13,14]$ is more appropriate for experiments in which the momentum transfer or the actual time dependent bare force are hard to measure. In the simulations below we employ the first method.

To find the effective interactions in hard disks we executed event driven 2-dimensional simulations for systems with fixed area $A$, a given number of disks $N = 400$ at temperature $T = 1$. The area is square with periodic boundary conditions and all the disks have the same mass $m$. The disk radii $R$ are slightly poly-dispersed around a binary 50:50 distribution with mean values and standard deviations of $\langle R_A \rangle = 0.5$, $\sigma_{R_A} = 0.0081$, $\langle R_B \rangle = 0.7$ and $\sigma_{R_B} = 0.0123$. All the hard disk simulations started by determining accurately the area $A_{in} \equiv L^2_{in}$ for which the system jams, and see Supplemental Material. Then we choose a density $\rho$ for the unjammed systems by expanding the system size according to

$$L = L_{in} \times (1 + \epsilon) \ .$$

After expanding the system size from the jammed state by the desired $\epsilon$, the simulation is first equilibrated for $2 \times 10^6$ collisions and then run for $10^8$ collisions. This long run is examined manually to ascertain that it has a section of at least $n_c = 10^7$ collisions in which there are no transitions between meta-basins. Disk positions were measured and averaged-over with the maximal resolution possible (i.e. after each collision). Given a value of $\epsilon$ the effective forces $f_{ij}$ were measured by computing the momentum transfer $\Delta_k \mathbf{p}(i,j)$ during every $k^{th}$ collision between particles $i$ and $j$, followed by averaging according
The velocity-Verlet algorithm with time step $\Delta t$ is used to test the accuracy of the forces $f_{ij}$ is the requirement that they uphold force balance, or

$$f_i = \sum_j f_{ij} = 0.$$  \hspace{1cm} (3)

For hard disks this sum rule was obeyed in our numerics to better than 1 part in $10^3$ in units of the mean inter-particle force. The reader should notice that although we measure $f_{ij}$ by tracking interactions between particles $i$ and $j$ it is not generally a function of only $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. Even in mean-field theory one expects that the effective forces between particles $i$ and $j$ depend on some characteristic of the cages in which they move, in addition to $\vec{r}_{ij}$. In correspondence with the mean field theory of spin glasses we can expect a dependence on the mean-squared fluctuations in the respective two cages. Defining $K_i \equiv \sqrt{\langle (\vec{r}_i(t) - \vec{r}_i)^2 \rangle}$ we expect that

$$f_{ij} = g(K_i, K_j, \vec{r}_{ij}) \hspace{1cm} \text{in mean field theory}, \hspace{1cm} (4)$$

with $g$ being an a-priori unknown function. In finite dimensions multiple collisions and the effect of successive collisions cause the effective forces to depend also on the averaged positions of other particles. In other words the effective forces are not in general mean-field, and see below for more details. We will show however that for hard disks sufficiently close to jamming the effective forces are binary, and even independent of $K_i$ and $K_j$.

To underline the difference between hard spheres and more generic potentials we study here a system of softer disks. Here the system consists of a 50:50 mixture of ‘small’ (A) and ‘large’ (B) particles, with diameter ratio of $\lambda_B/\lambda_A = 1.4$. This system has been used extensively in numerical simulations to create jammed configurations. The bare interaction potential between particles $i$ and $j$ is given by

$$U(\vec{r}_{ij}) = \frac{V_0}{2} \left( 1 - \frac{\vec{r}_{ij}}{\lambda_{ij}} \right)^2 \Theta \left( 1 - \frac{\vec{r}_{ij}}{\lambda_{ij}} \right),$$ \hspace{1cm} (5)

where $r_{ij}$ is the distance between the center of masses of the particle $i$ and $j$, $\lambda_{ij} = (\lambda_i + \lambda_j)/2$ is the average diameter, $V_0$ is the strength of interaction, and $\Theta$ is the Heaviside step function. To remain close to the hard sphere limit we choose first a large value of $V_0 = 500000$. A second comparison to a softer interaction is achieved with $V_0 = 1000$. The comparison between the hard sphere limit and these two softer potentials is shown in Fig. 1. The units for energy and length are $V_0$ and $\lambda_A$ respectively. We integrate the equations of motion for this system using a standard velocity-Verlet algorithm with time step $\Delta t = 0.001$ for $V_0 = 1000$ and $\Delta t = 0.0002$ for $V_0 = 500000$. The Nose-Hoover chain thermostat was used to maintain the desired temperature. After expanding the system size from the jammed state by the desired $\epsilon$, we first equilibrate the system for time $\tau_1 = 10^6$ in reduced units) (For more details see Supplemental Material). The simulation is then run at constant $T = 10^{-3}$ for a further time of $\tau_2 = 10^6$. All the results pertaining to the soft disks are extracted as described above from a time segment of length $\tau_2/10$. This is again done to avoid transitions between meta-basins. The upshot of this choice is that the average positions were determined using averaging times that are well below the time for which particle diffusion destroys their meaning. In practice this constrains the values of the expansion $\epsilon$. For values of $\epsilon \geq 5.5 \times 10^{-2}$ for hard disks and $\epsilon > 10^{-2}$ for soft disks we could not determine the mean positions of the particles with sufficient accuracy. The average position of the particles are denoted as above as $\{\vec{r}_i\}_{i=1}^N$. In the present case the effective forces are computed from the dynamics according to

$$f_{ij} \equiv -\frac{1}{t} \int_0^t dt' \left( \frac{\partial U}{\partial \vec{r}_{ij}} \right), \hspace{1cm} \text{for differentiable bare potential}, \hspace{1cm} (6)$$

with $t$ being the time of integration of the dynamics. The sum rule was well obeyed for the soft disks to better than 1 part in $10^6$ (in units of the mean inter-particle force). Again the main question below will be whether these effective forces are mean field as in Eq. (4), or whether they exhibit many-body interactions.

The analysis is easier in the case of hard disks with which we begin. In this case we find that near jamming the effective forces trivialize to binary interactions. To show this we follow two steps: (i) finding for each con-

![FIG. 1. Comparison between the hard and the soft potentials used in this Letter to underline the fragility of the hard sphere limit. The vertical black line is the hard disk potential and the two others illustrates Eq. (5) with $V_0 = 500000$ (red dashed line) and $V_0 = 1000$ (green continuous line).](image-url)
In Fig. 2 upper panel we show typical data for $f_{ij}$ as a function of $h_{ij}$ for $\epsilon = 10^{-3}$. We see that the data do not form a function. Next we calculated standard deviation $\sigma_h(\epsilon)$ around the compensated data $f_{ij} \times h_{ij}/T$. This quantity was averaged over different initial configurations for each expansion $\epsilon$. The lower panel of Fig. 2 shows $\sigma_h$ for different values of $\epsilon$ in a log-log plot. The red error bars in this figure stem from standard deviation between different configurations. The blue error bars represent the accuracy in determining the inter-particle forces from Eq. 8. The deviation from purely binary interactions decreases upon approaching jamming:

$$\langle \sigma_h(\epsilon) \rangle \sim \epsilon^\zeta, \quad \zeta \approx 0.15 \pm 0.04 . \quad (9)$$

It remains to be seen whether this critical exponent can be derived from known exponents of the jamming criticality or is this a new exponent for the problem at hand.
the normalized forces a polynomial of degree 4. The new fit is denoted as $g_2(h_{ij})$. Next we considered, as seen in Fig. 3, the function $f_{ij}/g_1 - g_2$ and determined the standard deviation $\sigma_s$ of the data scatter around zero. Finally we averaged $\sigma_s$ among the 3 interactions, for each expansion parameter $\epsilon$ [20]. Fig. 4 shows this $\langle \sigma_s \rangle$ vs. $\epsilon$ in a log-log plot. For both values of $V_0$ the difference between the behavior of the hard and soft disks is glaring. In the latter case the importance of the many-body interactions is not decreasing upon approaching jamming, becoming quite independent of $\epsilon$. In hindsight this is not surprising: even when almost touching, two soft colliding spheres $i$ and $j$ which are in the range of interaction of other soft spheres $k, \ell$ etc. should feel their influence; the momentum transferred by the $i,j$ interaction is not determined only by their bare forces, but also by the pull and push of adjacent other disks. In colloquial terms ‘when push comes to shove it is important who are your neighbors’.

It is interesting to notice that in absolute values the degree of non-mean-field many-body contributions increases when the range of interaction increases (the spheres get softer). The above stated intuition is the obvious reason for that. But also one should note that the constant value of many-body contributions for the softer spheres is of the same order as the maximal value of the same contribution for the hard spheres. There is really very little effect on the proximity of the jamming density on the relative importance of higher-order forces in the case of softer potentials. One cannot expect that a truncation of the many-body forces would provide an accurate theory for the critical behavior near jamming.

In summary, it was demonstrated that the hard sphere force-law conforms with mean-field expectation Eq. 4. We acknowledge support by the Minerva foundation with funding from the Federal German Ministry for Education and Research, the Israel Science Foundation (Israel Singapore Program) and the Italy-Israel joint laboratory funded by the Ministry of Foreign affairs. IP is grateful to the Simons Fellowship under the auspices of the Niels Bohr International Academy.
Supplemental Material to “How Generic are the Robust Theoretical Aspects of Jamming in Hard Sphere Models?”

I. INTRODUCTION

In this document we offer Supplementary Information to the main text. In Sect. II we describe in detail the creation of jammed configurations of hard disks and their inflation to a wanted density away from jamming. The next Sect. III provides similar details for the jamming of the soft disks. In Sect. IV we describe the manual procedure employed to guarantee that the mean positions of the particles do not change during our runs. Sect. V shows that selecting particles with very close-by cage fluctuations does not lead to an elimination in Sect. VII we show that selecting particles with very close-by cage fluctuations does not lead to an elimination of the importance of contributions to the effective forces that cannot be approximated by the mean-field form.

II. HARD DISKS SIMULATIONS

To create jammed configurations of hard disks we follow the following steps:

1. Create systems of harmonic disks at a packing fraction \( \phi = 0.86 \).

2. Implement the FIRE minimization algorithm \([21]\) coupled to a Berendsen barostat to bring the pressure to \(10^{-6} - 10^{-7}\), depending on the system size.

3. Use 128-bit numerics from here: impose increments of expansive strain that are proportional to the current pressure, and follow each of these increments by a minimization using the FIRE algorithm (without the barostat, i.e. at constant volume). Repeat until the pressure approaches \(10^{-10}\) or below.

4. Find the maximal overlap \(-h_{ij}\) between any two particles, and expand L precisely to eliminate this maximal overlap.

Having determined the system volume as close to the jammed state as possible, we expand the system size from the jammed state by the desired \(\epsilon\), cf. Eq. I in the main text. (Note that the value of \(L_{\text{in}}\) fluctuated from realization to realization in our finite size samples). Then the simulation is first equilibrated for \(2 \times 10^6\) collisions and then run for \(n_c = 10^8\) collisions more. As described in section IV for each simulation only a section of \(n_c/10\) collisions is used for computing the average positions. This is in order to avoid transitions between meta-basins.

For each value of \(\epsilon\) the deviation of the force law from the 2-body putative interaction was averaged over 20-32 configurations, each taken from a different simulation starting from a different initial condition.

III. HARMONIC DISKS SIMULATIONS

We use velocity-Verlet algorithm with time steps \(\Delta t = 0.001, 0.0002\) for \(V_0 = 1000, 500000\) respectively to integrate the equation of motion. The Nosé-Hoover chain thermostat was used to maintain the desired temperature.

A. Setup of Jammed Configurations:

To create the jammed configurations, we follow the protocol as described in Refs. [3, 18]. Starting with a random configuration in a square box at a temperature \(T = 0.01\) and low packing fraction of \(\phi = 0.65\) the system is allowed to equilibrate. Subsequently the system is quenched to a low temperature \(T = 10^{-12}\), at a rate of \(T = 10^{-4}\). Finally the energy is minimized (using the conjugate gradient technique).

After reaching the local minimum at initial low packing fraction \(\phi_i\), we apply the “packing finder” algorithm \([3, 18]\) to obtain the nearest static packing with infinitesimal particle overlaps. The system is compressed or de-compressed, followed by conjugate-gradient energy minimization at each step. Compression is chosen when the total energy is zero after minimization while decompression is performed when the total energy is nonzero even after energy minimization, due to overlapping particles. This procedure is terminated when the total potential energy per particle satisfies \(U/N < 10^{-16}\) at which point we consider the configuration as jammed. Note that the two methods described for hard and soft disks appear different but for all practical purposes are in fact equivalent and could be interchanged.

B. Procedure

As described in section IV for each simulation only a section of \(\Delta \tau = \tau_2/10\) is used for computing the average positions. The aim is to avoid transitions between meta-basins. For each value of \(\epsilon\) data was taken from 77-92 configurations each taken from a different simulation starting from a different initial condition.

IV. TESTING CHANGES IN META-BASINS

In order to get reliable average positions, we must guarantee that there are no transitions to different meta-
measurements. To clean the data from such outliers we consider three different time-correlation functions: (i) the self-intermediate scattering function, (ii) the mean square displacement, and (iii) the maximal distance traveled by any single particle. The time-correlations are measured every 1000 collisions in the hard disks simulations and at each time-step in the harmonic disks simulation. For hard disks, the values of these correlations mostly fluctuate around a constant value (apart from some initial decay/growth) with infrequent sharp drops/jumps (see Fig. 5). Such a sharp drop/jump in one of these correlation functions indicates a transition between meta-basins. We divide the simulation into 10 temporal sections (with equal number of collisions/time-steps), and for each simulation analyze a single section in which such transitions were not observed. All the average positions are computed within such transition-free sections. This is a stricter criterion than the one used in Ref. [13]. Such sharp drops are observed mostly for the larger expansions \( \epsilon \geq 10^{-4} \). For smaller expansions the simulation time is too short for transitions to occur. For the soft harmonic disks, the values of the correlation functions can also change smoothly and we choose simulation sections where these values fluctuate around constant values without observable decay or growth.

V. CLEANING THE DATA FROM INFREQUENT COLLISIONS

Hard Disks: Configurations of hard disks involve “rattlers” that collide only infrequently compared to typical disks. This introduces errors in the effective force measurements. To clean the data from such outliers we identify the range of \( h_{ij} \) that can be trusted. To this aim we plot a histogram of \( \log_{10}(h_{ij}) \) and bin it into 50 bins, cf. Fig. 6. The value of \( h_{ij} \) in the bin with the highest weight is denoted as \( \tilde{h}_{ij}^{freq} \). We then include only effective forces \( f_{ij} \) for which \( h_{ij} \leq 3 \times \tilde{h}_{ij}^{freq} \).

Harmonic Disks: In the case of harmonic disks the “gaps” \( h_{ij} \) can be negative, and the cleaning of the data is a bit more tricky. Instead of using the gap \( \tilde{h}_{ij} = r_{ij} - \sigma_i - \sigma_j \), we used \( \tilde{h}_{ij} = r_{ij} - r_{ij}^{min} \) where \( r_{ij}^{min} \) is the minimal \( r_{ij} \) of the relevant interaction. We then followed the same procedure as for the hard disks: We plotted a histogram (50 bins) of \( \log_{10}(h_{ij}) \), found the largest bin \( \tilde{h}_{ij}^{freq} \) and considered effective forces associated with \( h_{ij} \leq 3 \times \tilde{h}_{ij}^{freq} \). Besides cleaning the data from pairs having very large values of \( h_{ij} \), one should also consider for both soft and hard disks some rare configurations that include particle pairs with extremely small and negative values of \( h_{ij} \) that deviate strongly from the typical behavior, exhibiting abnormally small forces \( f_{ij} \). These abnormally small \( f_{ij} \) were not considered in the analysis. This rare phenomenon disappears when the definition of \( h_{ij} \) is changed in favor of a scalar average, and see Sect. VI below. At any rate these rare events do not change the general conclusions of the study, as is shown explicitly in Sect. VI.

To get an impression of the data before the clean-up of negative \( h_{ij} \) we present in Fig. 7 some of the effective forces computed for the hard disk case as a function of \( h_{ij} \). It is visually clear that the problematic points are rare.

VI. ANALYSIS WITH SCALAR AVERAGING OF DISTANCES \( r_{ij} \)

Instead of using the definition of \( h_{ij} \) in which \( \bar{r}_{ij} \equiv \frac{1}{\tau} \int_0^\tau dt \, r_{ij}(t) \) which is computed as a vector average, one could employ a scalar definition of the mean distance...
FIG. 7. The effective forces in the hard sphere case with $\epsilon = 10^{-3}$. The data is shown only for small $h_{ij}$ to provide higher resolution around the rare events with negative $h_{ij}$. The few negative values of $h_{ij}$ are real, stemming from dynamics in which the difference in average positions are indeed negative.

FIG. 8. The standard deviation from the mean field binary force law for soft spheres as a function of the distance from jamming. Here $V_0 = 1000$. Here we used the scalar definition of the distance between pairs and particles and we show the results for each type of interaction (AA, BB and AB) separately for extra care.

between particles,

$$\tilde{h}_{ij} = \tilde{r}_{ij} - R_i - R_j ; \quad \tilde{r}_{ij} \equiv \frac{1}{\tau} \int_0^\tau dt \ r_{ij}(t) .$$

(10)

For the case of soft spheres we checked carefully whether this definition may lead to a different conclusion. The answer is negative. As an example we show in Fig. 8 the computed contribution of many body interactions as a function of $\epsilon$. The overall order of magnitude of the standard deviation reduces compared to the vector definition of the distances, but still there is no indication for approaching the binary limit when $\epsilon \to 0$.

VII. RULING OUT MEAN FIELD EFFECTIVE FORCES IN SOFT SPHERES

In order to determine whether in a given system the force-law conforms with mean-field expectations we need
to determine the cage fluctuations $K_i$. The probability distribution function (pdf) of $K_i$ was measured for soft spheres using some 77-92 configurations (depending on $\epsilon$). Next, we selected pairs of particles from a bin of $K_i$ value with decreasing width of the bin. If Eq. 4 of the main text pertains, we should expect that reducing the bin size and plotting the effective forces as a function of $h_{ij}$ must result in reducing the scatter around a functional behavior. In Fig. 9 we show that this is not the case. The data shown pertains to particle pairs whose $K_i \approx K_j$ up to the bin width, selected from the bin with highest weight. In the upper panel we show the histogram of $K_i$ with large bins, and in the middle panel with finer bins. Finally, in the lower panel we show that the contribution of non-binary interaction does not reduce when the bins of the histogram get finer and finer. The conclusion is that the mean-field expectation Eq. 4 of the main text is untenable in the case of harmonic spheres.

[1] J. Hansen and I. McDonald, in *Theory of Simple Liquids (Third Edition)* edited by J.-P. Hansen, , and I. R. McDonald (Academic Press, Burlington, 2006).
[2] D. Rapaport, *The Art of Molecular Dynamics Simulation* (Cambridge University Press, 1997).
[3] C. S. O’Hern, L. E. Silbert, A. J. Liu, and S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).
[4] L. E. Silbert, D. Ertas, G. S. Grest, T. C. Halsey, and D. Levine, Phys. Rev. E **65**, 031304 (2002).
[5] C. S. O’Hern, S. A. Langer, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. **88**, 075507 (2002).
[6] L. Berthier, D. Coslovich, A. Ninarello, and M. Ozawa, Phys. Rev. Lett. **116**, 238002 (2016).
[7] P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, and F. Zamponi, Nature Communications **5**, 3725 (2014).
[8] P. Charbonneau, E. Corwin, G. Parisi, and F. Zamponi, Phys. Rev. Lett. **114**, 125504 (2015).
[9] L. Berthier, H. Jacquin, and F. Zamponi, Phys. Rev. E **84**, 011305 (2011).
[10] P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, and F. Zamponi, Annual Review of Condensed Matter Physics **8**, 265 (2017).
[11] G. Parisi and F. Zamponi, Journal of Statistical Mechanics: Theory and Experiment **2006**, P03017 (2006).
[12] C. Brito and M. Wyart, EPL (Europhysics Letters) **76**, 149 (2006).
[13] O. Gendelman, E. Lerner, Y. G. Pollack, I. Procaccia, C. Rainone, and B. Riechers, Phys. Rev. E **94**, 051001 (2016).
[14] O. Gendelman, Y. G. Pollack, and I. Procaccia, Phys. Rev. E **93**, 060601 (2016).
[15] T. Pelka, Journal of Physics A: Mathematical and general **15**, 1971 (1982).
[16] A. Georges and J. Yedidia, Journal of Physics A: Mathematical and General **24**, 2173 (1991).
[17] In principle one can also consider a dependence on a tensorial quantity $K_{\alpha \beta} \equiv \sqrt{\langle (r_{i \alpha}^\ast(t) - \bar{r}_{i \alpha}^\ast)(r_{i \beta}^\ast(t) - \bar{r}_{i \beta}^\ast) \rangle}$.
[18] C. F. Schreck, C. S. O’Hern, and L. E. Silbert, Phys. Rev. E **84**, 011305 (2011).
[19] See in the Supplemental Material another, scalar definition of the average gap and its consequences.
[20] Note that in the case of soft spheres we computed the standard deviation from all the samples together, whereas in the hard spheres we averaged over individual configurations. Doing the same in the present introduces no difference.
[21] E. Bitzek, P. Koskinen, F. Gähler, M. Moseler, and P. Gumbsch, Phys. Rev. Lett. **97**, 170201 (2006).