A real-space renormalization group for jamming

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Abstract Jamming occurs in granular materials, as well as in emulsions, dense suspensions, and other amorphous, particulate systems. When the packing fraction $\phi$, defined as the ratio of particle volume to system volume, is increased past a critical value $\phi_c$, a liquid-solid phase transition occurs, and grains are no longer able to rearrange. Previous studies have shown evidence of spatial correlations that diverge near $\phi = \phi_c$, but there has been no explicit spatial renormalization group (RG) scheme that has captured this transition. Here, I present a candidate for such a scheme, using a block-spin-like transformation of a randomly vacated lattice of grains. I define a real-space RG transformation based on local mechanical stability. This model displays a critical packing fraction $\phi_c$ and gives estimates of critical exponents in two and three dimensions.

Keywords Jamming · Renormalization group · Phase transition

Introduction

Jamming [1,2,3,4] describes a liquid-solid phase transition that occurs as amorphous, athermal systems are compressed from a dilute state. Jamming is often used to analyze dense granular materials [5,6,7], as well as foams [8], emulsions [9], and colloids [10]. Additionally, jamming is used to study glassy dynamics more broadly [11]. The canonical model system for jamming is an ensemble of soft, frictionless spheres, where the packing fraction $\phi$, defined as the ratio of total volume of the particles to total system volume, is varied. Disordered solid-like states can form at and above a packing fraction $\phi_c$, which is

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smaller than the density of a close-packed crystal, $\phi_{\text{xtal}}$. In three dimensions, $\phi_{\text{xtal}} = \pi/3\sqrt{2} \approx 0.74$ and $\phi_c \approx 0.64$. Several studies \cite{2,4,10,12,13,9,14} have shown evidence for a diverging length scale, $\xi \propto |\phi - \phi_c|^{-\nu}$, that controls the mechanical response near $\phi \approx \phi_c$, suggesting that jamming is a kind of non-equilibrium critical transition.

There is currently no real-space renormalization group (RG) scheme \cite{15,16,17} that captures this diverging length scale. The disordered nature of solid-like states near $\phi_c$ makes a block-spin approach \cite{15} impossible, since there is no lattice on which to define a block-spin-like coarsening and rescaling. One possible way around this problem is to consider a specially prepared state of a randomly vacated lattice (RVL) of repulsive spheres, where each site is occupied with some probability. If this system is then compressed or thermalized, the spheres may rearrange locally, based on whether their neighbors are occupied. These local mechanical instabilities can couple together spatially and lead to global relaxation to a liquid-like state. This should occur at some $\phi = \phi_c$ such that $0 < \phi_c < \phi_{\text{xtal}}$.

Most importantly, the RVL system retains the necessary lattice symmetry to allow a block-spin-like RG transformation. Here, I propose such a transformation and solve it in both two (2D) and three (3D) dimensions. Blocks of lattice sites are coarse-grained into a super-lattice, and each super-site is either “occupied” or “unoccupied” based on mechanical stability of the underlying spheres that make it up. If the super-sites are assumed to interact with each other in the same way as the original sites, then this process is repeatable. This model yields a value for $\phi = \phi_c$, corresponding to the packing fraction at which the lattice appears statistically unchanged after an RG transformation, as well as a critical exponent $\nu$. The values of $\phi_c$ and $\nu$ are similar to the accepted values for jamming in 2D and 3D.

The RVL model and RG

The RVL model consists of repulsive spheres (or disks) arranged on a close-packed lattice with some fraction of the spheres removed randomly, such that a single lattice site is occupied with probability $p = \phi/\phi_{\text{xtal}}$. Local mechanical instability occurs when multiple neighboring sites are unoccupied \cite{18,19,20}. For example, a single missing particle in the 2D hexagonal lattice (see Fig. 1) is still stable (solid-like), since the six neighbors block each other from entering the unoccupied site. If two neighboring sites are unoccupied, then the nearby region will be liquid-like, and particles on either side of this missing pair can move into the void \cite{19}. In the 3D face-centered cubic (FCC) lattice, local instability requires a “missing triad” of unoccupied sites, with three unoccupied neighboring sites forming an equilateral triangle \cite{18}.

Each local instability will affect its neighbors over some length scale, and these instabilities can couple together over many length scales to yield global liquid-like behavior \cite{21}, suggesting the need for an RG approach. The technique of a real-space RG transformation, pioneered by Kadanoff \cite{15} and later
fully developed by Wilson [16,17], consists of two essential steps. First, the system is coarsened over some length scale $b$, and degrees of freedom on length scales smaller than $b$ are averaged out. Second, the resulting system is spatially rescaled (i.e., zoomed out) by a factor $b$ such that the rescaled system has the same microscopic length scale as the original system. For jamming, these two steps would be represented by a transformation $\phi' = R_b(\phi)$, where $R_b$ relates the effective packing fraction $\phi'$ of the system after the RG transformation to the packing fraction $\phi$ of the original system. At the critical packing fraction $\phi_c$, the system is correlated over infinitely large distances. Thus, at $\phi = \phi_c$ the system should be statistically invariant under an RG transformation, i.e., $\phi_c = R_b(\phi_c)$.

In the block-spin system, Kadanoff assumed that the coarse-grained Hamiltonian has the same form as the original Hamiltonian and that super-sites interact with each other in the same way as the underlying spins. In reality, there is a more complicated rule that relates the coarse-grained Hamiltonian and interactions to the original, but Kadanoff’s approximation showed how, if such a rule was known, the full RG picture could be formalized. Here, I make similar assumptions: I define a block-spin-like RG transformation by grouping the lattice into super-sites consisting of $b^D$ individual sites, where $D$ is the dimensionality. Each super-site is mechanically stable or unstable depending on the criteria outlined above. After coarse-graining, mechanically stable super-sites are denoted as occupied, and the procedure can be repeated at the next level. Thus, super-sites are assumed to interact in the same way as individual particles. Ideally, the super-sites should fill space in the same way as the initial lattice, since the procedure should be repeatable.
Using these assumptions, I define a rule \( R_b \) relating the occupation probability \( p' \) of the super-site to \( p \):

\[
p' = R_b(p)
\]

The critical occupation probability \( p_c \) corresponds to the non-trivial state (i.e. not completely occupied or unoccupied) at which the RG transformation leaves the system statistically unchanged.

\[
p_c = R_b(p_c)
\]

Assuming that there is a diverging length scale \( \xi \propto |\phi - \phi_c|^{-\nu} \propto |p - p_c|^{-\nu} \) and that \( R_b \) reduces the correlation length \( \xi \) by a factor of \( b \), i.e., \( \xi' = \frac{\xi}{b} \propto |p' - p_c|^{-\nu} \), one can write:

\[
|R_b(p) - p_c|^{-\nu} = \frac{|p - p_c|^{-\nu}}{b}.
\]

Rearrangement combined with Eq. (2) yields an expression for \( \nu \):

\[
\nu = \frac{\log b}{\log \frac{|R_b(p) - p_c|}{|p - p_c|}} = \frac{\log b}{\log \frac{|R_b(p) - R_b(p_c)|}{|p - p_c|}}.
\]

In the limit of \( p \to p_c \), this becomes:

\[
\nu = \frac{\log b}{\log \frac{dR_b(p)}{dp}|_{p=p_c}}.
\]

So, any choice of \( R_b \) yields a value of the critical point, \( p_c \), and the value of the critical exponent, \( \nu \).

**Solution in two dimensions**

For the 2D lattice, I define super-sites as four-site diamond shapes, shown in Fig. 1. Upon application of the RG transformation, each four-site cluster would be represented by a single super-site which would be stable (occupied) or unstable (unoccupied). Since instability requires two neighboring sites to be unoccupied, stability for a cluster can then be determined by simply looking at possible configurations and applying this rule. Figure 1(a) shows an RVL system in 2D, and Fig. 1(b) shows the same system evolved with molecular dynamics for some time. Note that regions with missing pairs have become liquid-like, but single missing sites remain solid-like, unless they are near a missing pair.

To explicitly write \( R_b(p) \), I consider a four-particle cluster and all nearest neighbors (i.e. particles which could move into the cluster’s lattice sites), as shown in Fig. 1(c). The central cluster particles are labeled either A or B, and the neighboring particles are labeled 1-3 (here, referred to as N1, N2, and N3). Also, note that \( b = 2 \) for this configuration, since our two-dimensional...
super-site contains four particles. If all four sites are occupied, which occurs with probability $p^4$, then the super-site is stable. If only three sites are occupied, then these configurations can either be stable or unstable depending on whether the nearest-neighbor sites are occupied. A single unoccupied A-site occurs with probability $2p^3(1-p)$, and stability requires all four associated N1 and N2 sites to be occupied, which occurs with probability $p^4$. A single unoccupied B-site occurs with probability $2p^3(1-p)$, and stability requires the N3 and both N2 sites to be occupied, which occurs with probability $p^3$. Next, the configuration with two occupied B-sites and two unoccupied A-sites occurs with probability $p^2(1-p)^2$. Stability for this configuration requires all N1 and N2 sites to be occupied, which occurs with probability $p^4$. No other configurations can be stable. The total probability of stability is thus:

$$p' = R_b(p) = p^4 + 2p^3(1-p)(p^4 + p^3) + p^2(1-p)^2p^8$$  \quad (6)

Solving for $R_b(p_c) = p_c$ numerically yields:

$$p_c \approx 0.9356,$$  \quad (7)

which yields

$$\phi_{c,2D} = p_c\phi_L \approx 0.8485,$$  \quad (8)

where $\phi_L = \pi\sqrt{3}/6$ is the packing density of a fully occupied lattice. This value is similar to the packing fraction $\phi_{J,2D} \approx 0.84$ where jamming occurs for frictionless disks in 2D. Equation (5) yields a value for the critical exponent, $\nu$.

$$\nu = \frac{\log b}{\log \frac{d\ln(p_c)}{dp}|_{p=p_c}} = \frac{\log 2}{\log 1.7942...} = 1.1857...$$  \quad (9)

Compare this value to the exponent obtained in 2D by Vågberg, et al. [13]. $\nu \approx 1$. This value was obtained by considering corrections to scaling (i.e., by considering irrelevant variables that only matter for small system sizes). Other studies have also found $\nu$ between 0.6 and 0.7 [2,4] in 2D when corrections to scaling were not considered.

**Solution in three dimensions**

In 3D, there are two ways to pack spheres with the highest possible density: face-centered cubic (FCC) and hexagonally close-packed (HCP). Both lattices consist of layers of hexagonally packed spheres stacked on top of one another. Here, I consider the FCC lattice, shown in Fig. 2(a). I group the lattice sites into super-sites as shown in Fig. 2(b). The super-sites have $2^3 = 8$ sites, so $b = 2$. The eight-cell super-site has 36 neighbors, as shown in Fig. 2(c).

Local instability requires a missing triad, as discussed above. If a state has a missing triad among the eight core sites, it is unstable. Otherwise, all the neighbors of unoccupied sites must be considered. Every stable configuration occurs with probability $p^n(1-p)^{(44-n)}$, where $n$ is the number of occupied sites in that particular configuration (and 44 is the total number of sites).
To simplify the problem, different combinations of unoccupied sites which do not share any neighbors can be factorized. For example, if both the top and bottom particles are missing, each with nine neighboring sites, this yields $2^{18}$ configurations to check. However, since the top and bottom sites do not share neighbors, the probabilities can be factorized ($2^9$ configurations each), and the probability of stability for both missing sites is equal to the square of the probability for one to be stable. There are eight irreducible configurations, shown in Fig. 2 with missing end (E), body (B), end-body (EB), body-body same level (BBs), body-body different level (BBd), body-body-body (BBB), end-body-body (EBB), and end-body-body-end (EBBE). Once these combinations are known, all possible configurations can be constructed from them.

The stability criteria for these eight configurations is then solved numerically by iterating through all possible neighbor configurations. This yields polynomials $f_E(p)$, $f_B(p)$, $f_{EB}(p)$, etc., for each different configuration from Fig. 2 which gives the probability that the neighbors of the unoccupied sites are occupied such that the whole configuration (all 44 sites) is stable (i.e. no missing triads). For example, the polynomial for one missing body site (with seven neighbors) is written:

$$f_B(p) = p^7 + 7p^6(1-p) + 11p^5(1-p)^2 + 3p^4(1-p)^3.$$  

(10)

This means that there is one stable configuration with (all) seven neighbors occupied, seven stable configurations with six occupied neighbors, eleven stable configurations with five occupied neighbors, and three stable configurations with four occupied neighbors. These can be more compactly represented by

$$N(a, b) = bp^a(1-p)^{N-a},$$  

(11)

where $a$ is the number of occupied neighbors, $b$ the number of stable configurations, and $N$ as the total number of neighbors under consideration. With
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Fig. 3 The eight irreducible combinations of missing core sites, with missing: (a) end (E); (b) body (B); (c) end-body (EB); (d) body-body same level (BBs); (e) body-body different level (BBd); (f) body-body-body (BBB); (g) end-body-body (EBB); (h) end-body-body-end (EBBE). The probability of stability of these eight configurations can be used to build the probability of stability for all other configurations.

In this notation, one can write:

\[
\begin{align*}
    f_B &= 7(7, 1) + 7(6, 7) + 7(5, 11) + 7(4, 3) \\
    f_E &= 9(9, 1) + 9(8, 9) + 9(7, 21) + 9(6, 11) \\
    f_{EB} &= 14(14, 1) + 14(13, 12) + 14(12, 51) + 14(11, 94) + 14(10, 77) + 14(9, 26) + 14(8, 3) \\
    f_{BBs} &= 13(13, 1) + 13(12, 12) + 13(11, 50) + 13(10, 86) + 13(9, 61) + 13(8, 14) + 13(7, 1) \\
    f_{BBd} &= 12(12, 1) + 12(11, 10) + 12(10, 33) + 12(9, 40) + 12(8, 16) \\
    f_{EBB} &= 19(19, 1) + 19(18, 15) + 19(17, 87) + 19(16, 248) + 19(15, 367) + 19(14, 275) + 19(13, 95) + 19(12, 12) \\
    f_{BBB} &= 18(18, 1) + 18(17, 15) + 18(16, 87) + 18(15, 246) + 18(14, 355) + 18(13, 256) + 18(12, 82) + 18(11, 8) \\
    f_{EBBE} &= 26(26, 1) + 26(25, 20) + 26(24, 166) + 26(23, 746) + 26(22, 1989) + 26(21, 3244) + 26(20, 3229) + 26(19, 1918) + 26(18, 658) + 26(17, 120) + 26(16, 9)
\end{align*}
\]
Finally, the full probability of mechanical stability for the eight-particle cluster can now be constructed with consideration for all 36 neighbors. To do this, I organize by the number of occupied core sites, \( m \), which gives a prefactor of \( p^m (1 - p)^{8 - m} \) (i.e. the probability of \( m \) occupied sites). Then, all possible configurations can be constructed by combining the eight irreducible configurations. For example, the \( m = 7 \) term should account for two ways to have an end-particle missing (2\( f_E \)), plus six ways to have a body-particle missing (6\( f_B \)). The full RG transformation, \( p' = R_b(p) \) is written:

\[
p' = R_b(p) = p^8 + p^7 (1 - p)[2f_E + 6f_B] + p^6 (1 - p)^2[6f_E^2 + 6f_B^2 + 3(f_E f_B + 6f_B B_B + 6f_E B_B + 6f_B B_E + 12f_E B_E)] + p^5 (1 - p)^3[6f_E B_E + 12f_E B_B + 6f_B B_E + 6f_B B_B + 12f_E B_B] + p^4 (1 - p)^4[3(f_E B_E)^2 + 6f_E B_B E_E] \quad (12)
\]

This is a polynomial of order 34, which can be solved numerically for \( p_c = R_b(p_c) \). There is one solution for this equation between 0 and 1:

\[
p_c = 0.894622... \quad (13)
\]

As in two dimensions, multiplying by the packing density of an FCC lattice of spheres, \( \phi_L = \pi \sqrt{2}/6 \), yields the critical packing fraction:

\[
\phi_{c,3D} = p_c \phi_L = 0.66245... \quad (14)
\]

This value is similar to the random close packing value for monodisperse frictionless spheres in three dimensions, \( \phi_{J,3D} \approx 0.64 \).

For the divergence of the correlation length, equation 5 yields a value for the critical exponent, \( \nu \), in three dimensions. Again, note that \( b = 2 \) since there are \( 8 = 2^3 \) particles.

\[
\nu = \frac{\log b}{\log(d \phi(p)/d p) |_{p=p_c}} = \frac{\log 2}{\log 2.5077...} = 0.7539... \quad (15)
\]

This value is in agreement with O’Hern, et al. \[2\], \( \nu \approx 0.7 \).

**Discussion**

Here, I have shown how the a real-space renormalization group might be developed by considering a close-packed lattice of spheres with some percentage of the spheres randomly removed. The RG transformations I present here suffer from the same flaw as Kadanoff’s initial block-spin approach, in that they assume that the interactions among sites (before coarse graining) is the same as the interaction among super-sites (after coarse graining). Future work could
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improve upon the block-spin-like RG transformation I present here to find a more accurate way treat interactions at larger length scales.

It is not immediately obvious whether the RVL systems considered here will, even if they are unstable, relax to the same disordered states as in typical jamming studies. It is likely that the RVL model in 3D would “relax” (by whatever protocol is used) to a disordered state, while a 2D system of monodisperse disks will more likely form crystalline states. This is because the hexagonally packed lattice is both the locally and globally preferred packing in 2D. In 3D, this is not the case, since the locally preferred packing is an icosohedron with five-fold symmetry, which cannot form a lattice. However, recent work has shown that disordered 2D packings of monodisperse disks are possible. Preliminary simulations (not shown) using 3D soft spheres in a fully periodic cubic cell show that RVL systems with $\phi<\phi_J$ do relax to form jammed, amorphous packings as they are compressed. A complete characterization of these states, including a comparison to states generated via other jamming protocols, will be the subject of a future study. Finally, I note that, while the diverging length scale exponents $\nu \approx 1.19$ in 2D and $\nu \approx 0.75$ in 3D agree well with other studies on jamming, they also agree with previously given values for the yielding transition in amorphous media. Thus, there may be a connection between these two types of non-equilibrium critical transitions.

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Compliance with Ethical Standards

Conflict of Interest: The author declares that he has no conflict of interest. This research involved no human participants or animals.

References

1. H.M. Jaeger, S.R. Nagel, R.P. Behringer, Rev. Mod. Phys. 68(4), 1259 (1996)
2. C.S. Ohern, L.E. Silbert, A.J. Liu, S.R. Nagel, Phys. Rev. E 68(1), 011306 (2003)
3. A. Donev, S. Torquato, F.H. Stillinger, R. Connelly, J. Appl. Phys. 95(3), 989 (2004)
4. P. Olsson, S. Teitel, Phys. Rev. Lett. 99(17), 178001 (2007)
5. T. Majmudar, M. Sperl, S. Luding, R.P. Behringer, Physical review letters 98(5), 058001 (2007)
6. O. Dauchot, G. Marty, G. Biroli, Physical review letters 95(26), 265701 (2005)
7. R.P. Behringer, D. Bi, B. Chakraborty, A. Clark, J. Dijksman, J. Ren, J. Zhang, Journal of Statistical Mechanics: Theory and Experiment 2014(6), P06004 (2014)
8. D.J. Durian, Phys. Rev. Lett. 75(26), 4780 (1995)
9. J. Paredes, M.A. Michels, D. Bonn, Physical review letters 111(1), 015701 (2013)
10. K.N. Nordstrom, E. Verneuil, P.E. Arratia, A. Basu, Z. Zhang, A.G. Yodh, J.P. Gollub, D.J. Durian, Phys. Rev. Lett. 105, 175701 (2010)
11. L.E. Silbert, D. Ertaş, G.S. Grest, T.C. Halsey, D. Levine, Physical Review E 65(5), 051307 (2002)
12. P. Olsson, S. Teitel, Phys. Rev. E 83, 030302 (2011)
13. D. Vágberg, D. Valdez-Balderas, M.A. Moore, P. Olsson, S. Teitel, Phys. Rev. E 83(3), 030303 (2011)
14. C.P. Goodrich, A.J. Liu, J.P. Sethna, PNAS 113(35), 9745 (2016)
15. L.P. Kadanoff, Physics Physique Fizika 2(6), 263 (1966)
16. K.G. Wilson, Physical review B 4(9), 3174 (1971)
17. K.G. Wilson, Physical Review B 4(9), 3184 (1971)
18. S. Torquato, F. Stillinger, Journal of Applied Physics 102(9), 093511 (2007)
19. F.H. Stillinger, H. Sakai, S. Torquato, Phys. Rev. E 67, 031107 (2003)
20. A.R. Kansal, S. Torquato, F.H. Stillinger, Phys. Rev. E 66, 041109 (2002)
21. R.G. Palmer, D.L. Stein, E. Abrahams, P.W. Anderson, Phys. Rev. Lett. 53, 958 (1984)
22. P.M. Reis, R.A. Ingale, M.D. Shattuck, Phys. Rev. Lett. 96(25), 258001 (2006)
23. D.R. Nelson, F. Spaepen, in Solid State Physics, vol. 42 (Elsevier, 1989), pp. 1–90
24. S. Atkinson, F.H. Stillinger, S. Torquato, PNAS 111(52), 18436 (2014)
25. J. Lin, E. Lerner, A. Rosso, M. Wyart, Proc. Natl. Acad. Sci. 111(40), 14382 (2014)