Unifying the Percolation and Mean-field Descriptions of the Random Lorentz Gas

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The random Lorentz gas (RLG) is a minimal model of both transport in heterogenous media and structural glasses. Yet these two perspectives are fundamentally inconsistent, as the dynamical arrest is continuous in the former and discontinuous in the latter. This hinders our understanding of either, as well as of the RLG itself. By considering an exact solution of the RLG in the infinite-dimensional $d \to \infty$ limit as well as numerics in $d = 2 \ldots 20$ we here resolve this paradox. Our results reveal the importance of instantonic corrections, related to rare cage escapes, in unifying glass and percolation physics. This advance suggests a starting point for a first-principle description of hopping processes in structural glasses.

I. INTRODUCTION

The random version of the venerable Lorentz gas (RLG) consists of a tracer navigating within a collection of Poisson-distributed hard spherical obstacles. Despite the apparent simplicity of this model, its phenomenology is quite rich. As the density of obstacles increases, tracer diffusion is first delayed and then suppressed altogether. In physical dimensions $d = 2, 3$, the localization transition coincides with the percolation of void space $[1,2]$, hence it is continuous and accompanied by a marked sub-diffusive regime $[3,5]$. This minimal, real-space model for transport in heterogenous media has thus been widely used to describe systems ranging from electrons in impurities $[6]$ to proteins in cells $[7,8]$. The RLG plays a key role in the theory of glasses as well. Its consideration was an important step toward formulating the mode-coupling theory (MCT) of glasses $[9–12]$, and it has provided key insight into the role of pinning particles in deeply supercooled liquids $[13,16]$. The RLG is also related to a special limit of the non-convex perceptron, which is a minimal model for glasses and jamming $[17]$. Further insight into the glass problem arise from noting that the RLG can be construed as a special limit of a hard sphere binary mixture $[18,20]$, with one component—the obstacles—being infinitely smaller than the infinitely-dilute other—the tracer. (Exchanging obstacle and tracer sizes recovers Fig. [1a] $[12]$.) The RLG model should thus be part of the hard sphere glass universality class, and thus similarly undergo a discontinuous dynamical caging transition $[21]$. Interestingly, while in finite-dimensional glass formers this transition is avoided because various activated processes intervene, including nucleation and facilitation $[22]$, the RLG, which by construction eliminates all many-body effects, could exhibit this transition more sharply.

A paradox, however, lies at the root of this inference (Fig. [3a]). On the one hand, the exact mapping of the RLG to a percolation transition should give rise to a continuous localization transition $[3,5,24]$; on the other hand, the analogy to glass formation should give rise to a discontinuous caging transition, at least in the high dimensional, $d \to \infty$ limit where such description is understood to be exact. The simplest possible resolution, namely that the nature of the percolation transition changes in the $d \to \infty$ limit, was recently ruled out $[23]$. Could it then be that the large asymmetry limit of binary hard spheres is singular? Or that the $d \to \infty$ limit is pathological in some unexpected way?

In this letter, we answer these questions and resolve the underlying paradox. We first formulate a mean-field-theory (MFT) description of RLG independent of the hard sphere analogy to validate its premise, and then numerically obtain accurate percolation thresholds as well as static and dynamical descriptions of caging. Most importantly, by considering spatial dimensions high enough for our results to be comparable with the $d \to \infty$ limit, we uncover the basis for microscopic processes that are expected to play a key role in glass formation and yet have thus far eluded theoretical grasp.

II. MEAN-FIELD THEORY DERIVATION

The MFT of all glass-forming liquids predicts a dynamical (MCT) transition, at which the long-time limit of the scaled mean squared displacement, $\hat{\Delta} = d\Delta$, jumps from diverging diffusively to a finite value. Because the infinitely-asymmetric binary fluid mixture that coincides with the RLG in the $d \to \infty$ limit might however...
be singular, we here side-step this reasoning by solving the model directly using a cavity reconstruction scheme. Writing the explicit partition function for the RLG and using the replica symmetric construction of Refs. [21 and 24] (Detailed in Appendix B), one then obtains a self-consistent expression for $\hat{\Delta}$

$$\frac{1}{2\hat{\Delta}} = -\hat{\Delta} \int_{-\infty}^{\infty} dh \text{e}^h \log q(\hat{\Delta}/2, h) \frac{\partial q(\hat{\Delta}/2, h)}{\partial \hat{\Delta}},$$

(1)

where $\hat{\Delta}$ denotes the dimensionally-rescaled packing fraction (See Appendix A for detail). Analyzing Eq. (1) gives that the dynamical transition takes place at $\hat{\varphi}_d = 2.4034 \ldots$, half that for hard spheres [24]. We similarly obtain that the cage size is twice that of hard spheres, i.e., $\hat{\Delta} = 2\Delta_{\text{HS}}(2\hat{\varphi})$, and thus upon approaching $\hat{\varphi}_d$ also presents a square-root singularity, $\Delta(\hat{\varphi}_d) - \Delta(\hat{\varphi}) \sim \sqrt{\hat{\varphi} - \hat{\varphi}_d}$. These results confirm that the RLG and hard spheres share a same MFT universality class. The MFT description of the RLG is therefore fundamentally incompatible with the continuous transition expected from simple percolation.

### III. PERCOLATION THRESHOLD

To explore the root of this inconsistency, we consider the scaling of the percolation threshold, $\hat{\varphi}_p$, with dimension to determine if it coincides with the MFT prediction in $d \to \infty$. In systems with $N$ Poisson-distributed obstacles in a $d$-dimensional box under the periodic boundary condition, we map the void percolation transition onto the bond percolation of a network built on the Voronoi tessellation of obstacles [25], and assign to each edge of that tessellation the smallest obstacle radius $\sigma$ that can block it, before using a disjoint-set forest algorithm adapted from continuum-space analysis to identify the percolated cluster [26, 27]. Optimizing the periodic boundary conditions [28] and the Voronoi tessellation [29, 30] enables us to obtain $\hat{\varphi}_p(N)$ up to 8 dimension (detailed in Appendix C). The thermodynamic $\hat{\varphi}_p$ is then extracted by fitting (Fig. 1(b))

$$|\hat{\varphi}_p(N) - \hat{\varphi}_p| \sim N^{-1/d\nu},$$

(2)

where $\nu$ is the percolation correlation length exponent [31].

Studying the void percolation in $d > 8$ this way is computationally intractable because the cost of the Voronoi tessellation grows exponentially with dimension. The smoothness of the $d = 2 \ldots 8$ results nonetheless suggests that extrapolating to higher $d$ is not unreasonable. We find that fitting the known $\hat{\varphi}_p$ values to a cubic form,

$$\hat{\varphi}_p = 3.40(5) - 10.0(6) \frac{1}{d} + 13(2) \left(\frac{1}{d}\right)^2 - 8(2) \left(\frac{1}{d}\right)^3,$$

(3)

captures the numerical result very accurately, and gives $\hat{\varphi}_p(d \to \infty) = 3.40(5)$, which differs significantly from the MFT prediction, $\hat{\varphi}_d = 2.4034 \ldots$ in that same limit (Fig. 1(c)). In other words, the percolation and the dynamical transitions remain distinct in the $d \to \infty$ limit.

Most remarkably, the order of the two switches between $d = 8$ and 9. While for $d < 8$ the tracer is localized on both sides of $\hat{\varphi}_d$, and hence echoes of the dynamical transition may be too faint to detect, a densifying system in $d > 8$ might first encounter (imperfect) local cages that collectively percolate, before being properly localized at the percolation threshold. Because local cage escapes are reminiscent of activated processes [32, 33], one possible resolution of the paradox could be that the discrepancy between the MFT and percolation descriptions in $d \to \infty$ is due to the systematic suppression of activated processes in that limit.

### IV. CAGE SIZES

In order to ascertain this scenario, the MFT description of caging needs first to be assessed. To do so, we implement a cavity reconstruction scheme adapted from Refs. [32, 33] (detailed in Appendix D), which can be viewed as the continuum-space generalization of the

![Fig. 1.](image-url)
Leath algorithm [34]. Specifically, we define a hyper-spherical shell, centered at the origin, of inner radius $\sigma$ and outer radius $r_{\text{max}}$, and pick a number of obstacles $N$ from the Poisson distribution $p(N) = N^Ne^{-N}/N!$ with $N_0 = d\phi(r_{\text{max}}^d - \sigma^d)$, which are then distributed uniformly at random within that shell. (The choice of $r_{\text{max}}$ is such that the cavity containing the origin is closed.) This algorithm guarantees that the probability of obtaining a cavity containing the origin, $C$, exactly tracks the distribution of cavities at that same $\phi$ in an infinitely large system. A set of randomly distributed points $\{S_i\}$, within $C$ can then be used to compute the second moment of the coordinates,

$$\Delta(C) = \langle (S_i - x_j)^2 \rangle = 2\langle S_i^2 \rangle - \langle S_i \rangle^2, \quad (4)$$

and then $\Delta = \mathbb{E}_C[\Delta(C)]$. Physically, this method provides the long-time limit of the mean squared displacement (MSD) of a tracer without explicitly running its dynamics, which is advantageous because it eliminates putative dynamical bottlenecks. However, because its computational cost increases exponentially with $d$, for $d \geq 8$ the explicit long-time limit of the tracer dynamics needs to be computed to estimate $\Delta$. The agreement between the two approaches at low and intermediate $d$, gives us confidence that bottlenecks can be confidently neglected in this regime.

For $\hat{\phi} \gg \hat{\phi}_d$, we find that the (scaled) cage size nicely converges to the MFT prediction as $d$ increases (Fig. 2), and that the dominant correction is perturbative in $1/d$. In this high density regime, the quantitative accordance with MFT is robust down to physical dimensions. A generalized MFT with perturbative corrections should thus offer accurate predictions in all $d$, a clear opportunity for future theoretical studies.

By contrast, for $\hat{\phi} \sim \hat{\phi}_d$, a regime dominated by percolation criticality—where $\Delta$ diverges at $\hat{\phi}_p$—is observed. The static cage size either crosses $\hat{\phi}_d$ smoothly or diverges before reaching $\hat{\phi}_d$ from above, depending on the relative order of $\hat{\phi}_d$ and $\hat{\phi}_p$. These strong discrepancies with respect to MFT found around $\hat{\phi}_d$ hint at a complex interplay between the dynamical and the percolation transitions, which we analyze below.

V. TRACER DYNAMICS

In order to disentangle the effect of the two transitions, we consider the dynamical counterpart of the above static description. We first consider the tracer dynamics, following the ballistic approach of Höfling et al. [33], but setting the microscopic timescale such that the short-time growth of the MSD scales as $\Delta = \ell^2$ when $\ell \to 0$ in all dimensions. As expected from percolation theory [4, 23], in the long-time limit either localization or diffusion is observed, for $\hat{\phi} > \hat{\phi}_p$ and $\hat{\phi} < \hat{\phi}_p$, respectively (Fig. 3(a,b)). An intermediate subdiffusive regime, which scales logarithmically with time for $d \geq 6$ [23], also develops around the percolation threshold, and diverges at $\hat{\phi} = \hat{\phi}_p$. Figure 3(c,d) shows the ballistic, logarithmic growth and localization regimes for systems in $d \geq 6$. These results are fully consistent with percolation phenomenology [4, 23]. In $d = 6$, no hint of MFT-like caging is observed, as expected since $\hat{\phi}_p < \hat{\phi}_d$. The logarithmic growth immediately follows the ballistic regime until plateauing when $\hat{\phi} > \hat{\phi}_p$. In $d = 10$, where instead $\hat{\phi}_p > \hat{\phi}_d$, dynamical slowdown seems to emerge at intermediate times for $\hat{\phi} \geq \hat{\phi}_d$, but the effect is weak. Determining whether this slowdown is a hint of MFT caging or a pre-asymptotic correction to percolation critically would require higher-dimensional systems than this computational scheme permits at the moment.

To resolve the matter, we instead consider an observable more sensitive to MFT-like caging. Recalling that the percolation criticality is dominated by rare large cages, while MFT is evaluated via a saddle point that extracts the typical cage size, we focus on the mode of the time-evolution distribution of displacements, $\Delta_{\text{mode}}(t)$ [24, 30]. This observable is further amenable to a dynamical version of the static cavity reconstruction. Although this setup misses finite-yet-large cages, it nonetheless provides a sufficiently broad span of the cage size distribution to reliably identify $\Delta_{\text{mode}}$ and further extends the accessible dimensional range in simulations. Results up to $d = 20$ and averaged over at least $2 \times 10^4$ independent samples with $\Delta_{\text{max}} = d \cdot (r_{\text{max}} - \sigma)^2 \geq 12$ can thus be reported in Fig. 4. We find that $\Delta_{\text{mode}}$ plateaus quickly after the ballistic regime, even near $\hat{\phi}_p$, and that this plateau steadily approaches the $d \to \infty$ MFT caging.
been debated in glass physics [37–39], but this particular process (by contrast to $1/d$ dynamics in any finite $d$) shows a correction of the order of $1/d$ that depends only weakly on the choice of cutoff for $d > 6$. At $d = 6$, the collapse form further suggests that near $\phi < \phi_p$, the onset of cage escape events is found to be exponentially delayed in time with increasing dimension for $d \geq 8$ (Fig. 4(c)). More precisely, the cumulative probability of escaped tracer, $P_{\text{esc}}(t)$, at fixed $\phi$ follows a scaling form

$$P_{\text{esc}}(t; \phi) \sim \bar{f}(e^{-C\Delta\phi \Delta_0^d}; \phi),$$

with master functions $\bar{f}(x; \phi)$ and prefactor $C(\Delta_{\text{esc}}) \approx 0.5$ that depend only weakly on the choice of cutoff for $\Delta_{\text{esc}}/\Delta_{\text{mode}} \sim O(1)$. We can now properly understand the logarithmic drift of the MSD that appears at intermediate times when $\phi > \phi_d$ (Fig. 4(d)) as being due to imperfect caging. As dimension increases, the MFT prediction is recovered because the prefactor of the logarithm slowly vanishes. Geometrically, most cages are open for $\phi < \phi < \phi_p$, thus giving rise to void percolation, but escape paths out of open cages steadily shrink with increasing $d$, giving rise to stronger dynamical caging. This collapse form further suggests that near $\phi_d$, cage escape is so prevalent that they dominate the dynamics in any finite $d$. Such exponentially suppressed processes (by contrast to $1/d$ perturbations) have long been debated in glass physics [37–39], but this particular instantonic correction to the MFT of glasses was previously unknown. More than a mere correction, it is here found to give rise to new physics that connects the glass problem with that of percolation.

**Conclusion.**—Combining these points together, we have unified the two descriptions—MFT and percolation—of caging in the RLG, and have shown quantitative evidence of finite dimensional correction to MFT. Specifically, the static cage size in high density shows a correction of the order of $1/d$ to the MFT prediction, while the dynamical cage escape events is suppressed exponentially with $d$. In RLG, these finite-dimensional corrections become dominant in physical dimensions, therefore revealing in a precise and concrete way the important role of activated processes in the dynamical transition of glasses in real world.

Our results provide guidelines to develop a theory of activated processes for glassy dynamics, and more broadly of non-perturbative corrections to MFT for finite-dimensional disordered systems. They also offer a putative first-principle pathway for relating local structure and dynamics in glass-forming liquids [40].

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Appendix A: Notation

In order to unify the mean-field theory and percolation descriptions of the RLG, we first need to reconcile the two set of notations. The central quantity for both is the number density of obstacles, \( \rho \), which allows to define a unitless volume fraction of obstacles \( \Phi = \rho V_d \sigma^d \), where \( V_d \) is the \( d \)-dimensional volume of a unit sphere and \( \sigma \) is the obstacle radius. For the RLG, the obstacle radius is \( \sigma = 1 \) while the tracer radius \( \sigma_{\text{tracer}} \) is infinitesimal, and hence naturally we can define \( \Phi = \rho V_d \). Without loss of generality, and by analogy to the Mari-Kurchan model [12, 32, 33], we can equivalently choose \( \sigma = \sigma_{\text{tracer}} = 1/2 \), which naturally defines \( \varphi = \Phi 2^{-d} \). For high-dimensional scaling convenience, we further define the rescaled packing fraction

\[
\hat{\varphi} = \Phi / d = 2^d \varphi / d. \tag{A1}
\]

Similarly, the cage size, \( \Delta \), defined as the infinite-time limit of mean-square displacement of the tracer, can be rescaled as \( \hat{\Delta} = d^{1/2} \Delta \). For reference, Table I provides the correspondence between notations commonly used in the scientific literature about the RLG.

| Quantity | Equivalence |
|----------|-------------|
| \( \rho \) | \[12\] \[12\] |
| \( \Phi \) | \[12\] \[12\] |
| \( \varphi \) | \[12\] \[21\] \[32\] |
| \( \hat{\varphi} \) | \[12\] \[21\] \[32\] |
| \( \Delta \) | \[32\] \[32\] |
| \( \hat{\Delta} \) | \[32\] \[21\], \( Ad^2 \) \[41\] |

Appendix B: Mean-field Theory Derivation

As mentioned in the main text, the cage size of the RLG in the \( d \to \infty \) limit is obtained by applying the replica technique to a cavity computation. We here provide details about this derivation. The setup consists of \( N \) hard spherical obstacles of radius \( \sigma \) placed uniformly at random at positions \( R_i \) within a volume \( V \) centered around the origin. The free volume available to a tracer placed at the origin is thus

\[
Z = \int \mathcal{D}x \prod_{i=1}^N \theta(|x - R_i| > \sigma), \tag{B1}
\]

where \( \theta(x) \) denotes the Heaviside function. The replicated partition function in the thermodynamic, \( N \to \infty \), limit at fixed obstacle density \( \rho = N/V \) is

\[
\overline{Z^n} = \int \mathcal{D}r \left[ \frac{\int_{|R| > \sigma} dR \prod_{a=1}^n \theta(|x_a - R| > \sigma)}{\int_{|R| > \sigma} dR} \right]^N, \tag{B2}
\]

and the free energy is

\[
F = -\log \overline{Z} = - \lim_{n \to 0} \partial_n \overline{Z^n}. \tag{B3}
\]

For this system, we expect two phases:

- In the liquid phase, the (replicated) tracers are not confined close to the origin. Each replica thus decorrelates over the whole volume and

\[
\overline{Z^n} \sim V^n \left( \frac{V - (n + 1)V_\sigma}{V - V_\sigma} \right)^N \sim V^n e^{-n \rho V_\sigma}, \tag{B4}
\]

where \( V_\sigma \) is the volume of a sphere of diameter \( \sigma \).

- In the glass phase, with high probability the origin is contained within a cage. Many other cages exist in the volume, but a tracer starting at the origin remains confined within that cage. (Note that the cage at the origin is metastable, because far-away cages thermodynamically dominate the measure, hence our choice for a cavity computation.)

In the glass phase, we can write, after introducing a fictitious coordinate \( x_0 = 0 \),

\[
\overline{Z^n} = \int \mathcal{D}r \left\{ \frac{\int dR \prod_{a=0}^n \theta(|x_a - R| > \sigma)}{V - V_\sigma} \right\}^N
\]

\[
= \int \mathcal{D}r \left\{ 1 + \frac{\int dR \prod_{a=0}^n \theta(|x_a - R| > \sigma) - 1}{V - V_\sigma} + V_\sigma \right\}^N
\]

\[
= \int \mathcal{D}r e^{-\rho} \int \mathcal{D}r \theta(\min_{a} |x_a - R| < \sigma) + V_\sigma \right\}^N
\]

\[
= e^{\rho V_\sigma} \int \mathcal{D}r e^{-\rho} \int \mathcal{D}r \theta(\min_{a} |x_a - R| < \sigma) \left( \int \mathcal{D}q e^{d_n} \right)
\]

\[
= e^{\rho V_\sigma} C_{n+1,d} \int \mathcal{D}q e^{d_n} \log \det \hat{q} + \rho \hat{q} T_{n+1,0}(0, \mathcal{F}), \tag{B5}
\]

where we have changed to overlap variables that are rotationally invariant, \( q_{ab} = x_a \cdot x_b \) as in Ref. [21] Eq.(2.96), and we defined

\[
\mathcal{F}_n(x) = -\int \mathcal{D}r \theta(\min_{a \in [1,n]} |x_a - R| < \sigma), \tag{B6}
\]
as in Ref. [45], Eq. (30).

Following the approach of Refs. [21] and [24] for evaluating $Z^\infty$ by saddle point integration for $d \to \infty$, we obtain

$$
\log Z^\infty = \text{cst} + \frac{d}{2} \log \det \tilde{q} + d \tilde{\varphi} \tilde{g}_n
$$

$$
= \text{cst} + \frac{d}{2} \log \left( \left( n \tilde{\Delta} - (n - 1) \frac{\tilde{\Delta}}{2} \right) \left( \frac{\tilde{\Delta}}{2} \right)^{n-1} \right)
$$

$$
+ d \tilde{\varphi} \left( \tilde{f}_{n+1}(\tilde{\Delta}, \tilde{\Delta}) + 1 \right),
$$

(B7)

where irrelevant constants have been dropped, and the rescaled square displacement and density, $\tilde{\Delta}$ and $\tilde{\varphi}$, respectively, are defined as in Section A. By taking the replica symmetric solution, $\tilde{\Delta} = \tilde{\Delta}$, the expression can then be reduced to a one-dimensional integral [21], such that

$$
f_{n+1}(\tilde{\Delta}) = \int_{-\infty}^\infty dh \exp \left( q(\tilde{\Delta}/2, h)^{n+1} - 1 \right),
$$

(B8)

where $q(\tilde{\Delta}, h) = (1 + \text{erf}(h/\sqrt{2\tilde{\Delta}}))/2$. Note that in the original hard sphere derivation, in which all particles oscillate, the large variance term has the form $\Delta = (\Delta_{\text{tracer}} + \Delta_{\text{obstacle}})/2$. By contrast, obstacles are fixed in the RLG, and hence $\tilde{\Delta} = \Delta_{\text{tracer}}/2$.

Under the replica symmetric assumption, the free energy is then

$$
\log Z^\infty = \text{cst} + \frac{dn}{2} \log \tilde{\Delta}
$$

$$
+ d \tilde{\varphi} \left( \int_{-\infty}^\infty dh \exp \left( q(\tilde{\Delta}/2, h)^{n+1} - 1 \right) + 1 \right).
$$

(B9)

Solving for $\frac{\partial \log Z^\infty}{\partial \tilde{\Delta}} = 0$ provides the cage size that optimizes the free energy,

$$
\frac{n}{2\tilde{\Delta}} = -\tilde{\varphi} \int_{-\infty}^\infty dh \frac{d}{\partial \tilde{\Delta}} \exp \left( (n + 1)q(\tilde{\Delta}/2, h) \right) \frac{\partial q(\tilde{\Delta}/2, h)}{\partial \tilde{\Delta}}.
$$

(B10)

Noting that $\int_{-\infty}^\infty dh \frac{d}{\partial \tilde{\Delta}} \exp \left( (n + 1)q(\tilde{\Delta}/2, h) \right) = 0$ and taking the limit $n \to 0$, the cage size and the obstacle density are related by

$$
\frac{1}{2\tilde{\varphi}} = -\tilde{\Delta} \int_{-\infty}^\infty dh \log q(\tilde{\Delta}/2, h) \frac{\partial q(\tilde{\Delta}/2, h)}{\partial \tilde{\Delta}}.
$$

(B11)

Appendix C: Void Percolation Threshold Computation

This section details the algorithm used for detecting the void percolation threshold of the RLG. We first place $N$ obstacles uniformly at random within a $d$-dimensional box under periodic boundary conditions. Conventional cubic boxes, $Z^d$, are used in $d \leq 6$, while the Wigner-Seitz cell of the checkerboard, $D_7$, lattice and of the $E_8$ lattice are used in $d = 7$ and $8$, respectively. A Voronoi tessellation of the obstacles allows us to map the void percolation problem onto that of the bond percolation of edges in that tessellation. Each edge is weighted by the circumscribed radius of the facet in the Delaunay triangulation that is dual to this edge, which defines the minimum radius of the obstacles that can block this edge. Because the number of Voronoi vertices and edges grows exponentially with dimension, memory use must be carefully handled. First, we build the tessellation point by point [16]. Specifically, for each obstacle, $p_i$, we calculate the convex hull [30] of the inverse coordinates of the other obstacles, after translating $p_i$ at the origin. The vertices of this convex hull then correspond to the neighbors of $p_i$ in the Voronoi tessellation [29]. Second, edges with a sufficiently small weight remain blocked in a percolation network and are dropped on-the-fly, while building the tessellation. Orders of magnitude in memory use are therefore gained, thus enabling the analysis of sufficiently large systems, even in the highest dimension considered.

The percolation threshold is then determined by an algorithm akin to that used for the continuum-space percolation of obstacles [26, 27]. This approach is applied on a disjoint-set forest data structure. A disjoint-set consists of a number of nodes, each of which corresponding to a Voronoi vertex. Each node maintains a parent pointer and the displacement vector to its parent, tracing back to a unique root node in the set. Each disjoint-set thus corresponds to a cavity in the system. Voronoi edges are first sorted in descending order, and then the neighboring vertices of each edge are iteratively considered. If the two vertices, $X_1$ and $X_2$, do not yet belong to same cavity, they are merged; otherwise, percolation is checked by:

1. Calculating the displacement vector between $X_1$ and $X_2$ (under minimal image convention) $r_0 = X_1 - X_2$;

2. Calculating the displacement vector from $X_1$ and $X_2$ to the root, $r_1$ and $r_2$, respectively;

3. Comparing if $r_1 - r_2 \neq r_0$.

If the displacements calculated from the two methods differ (necessarily, by integers), then the cavity must span across the periodic boundary and form a cycle. Percolation is deemed to take place when there exist such cycles in all dimensions, which reduces sample-to-sample variations compared to other percolation criteria [12]. From the standard percolation universality class [3], we know that the percolation threshold in a finite system of $N$ obstacles converges to the thermodynamic, $N \to \infty$, limit, with asymptotic scaling

$$
\Phi_p(N) - \Phi_p(\infty) \sim N^{-1/d\nu},
$$

(C1)

where $\nu$ is the correlation length exponent, $\nu = 4/3, 0.8774, 0.6852, 0.5723$ for $d = 2$ to $5$ [31] and $1/2$ for $d \geq 6$. Our percolation threshold detection algorithm increases the range of accessible system sizes by orders of
magnitude, which makes this fitting robust in all dimensions considered in this work. Empirically, we observe that the asymptotic fitting requires that half the system size (inscribed radius of the periodic box) must be greater than the maximum neighbor-distance of obstacles. The resulting percolation threshold are listed in Table II. Note that our results reveal a systematic bias in the numerical treatment of Ref. [12] for \(d \geq 4\), because it included pre-asymptotic system sizes in the fit.

### Algorithm 1 Sampling a cavity

```plaintext
for \(C_i\) in visited cells do
    \(V_i \leftarrow \text{SimplexVolume}(C_i)\)
    Increment \(V_{\text{cells}}\)
end for
for \(j = 1\) to \(N_{\text{samples}}\) do
    Randomly choose a simplex \(C_k\) in \(\{C_i\}\) with probability \(V_k/V_{\text{cells}}\)
    Place a random sample \(S \leftarrow \text{SampleSimplex}(C_k)\)
    if \(S\) in the void space then
        Add \(S\) to the void sample list and increment \(N_{\text{voids}}\)
    end if
end for
```

Note that the volume of a \(d\)-simplex defined by the vertices \(\{p_0, p_1, \ldots, p_d\}\) is

\[
V_{\text{simplex}} = \frac{1}{d!} \det(p_1 - p_0, p_2 - p_0, \ldots, p_d - p_0).
\]  

Obtaining uniform samples in a \(d\)-simplex is equivalent to generating \(d + 1\) random spanning with unit sum [38 p. 568]. To generate \(d + 1\) random spacings \(x_0, \ldots, x_d\), one first generates \(d\) independent and uniformly distributed random variables \(y_1, \ldots, y_d\) in \([0, 1]\) and sort them in place, in addition to \(y_0 = 0\) and \(y_{d+1} = 1\), then \(x_i = y_{i+1} - y_i\), and the random sample \(S = \sum_{i=0}^d x_i p_i\).

Determining whether \(S\) is in the void space requires a nearest-neighbor query of the obstacles. Although the nearest obstacle of \(S\) is most likely to be one of the vertices of \(C_i\), outliers are possible. To accelerate the computation, one may pre-compute the point-to-simplex distances of these possible obstacles other than the simplex vertices, and store those with distance less than \(\sigma\) as candidate nearest neighbors.

### Appendix D: Numerical Cavity Reconstruction Scheme

At high density, the RLG is amenable to cavity reconstruction, which allows to compute efficiently the properties of the localized regime within a spherical shell of radius \(r_{\text{max}}\). The number of obstacles \(N\) to be placed within that shell is first picked at random from the Poisson distribution

\[
p(N) = \frac{N^N e^{-N}}{N!},
\]

where \(N_0 = d\bar{\varphi}(r_{\text{max}}^d - \sigma^d)\) is the average number of obstacles for the system size and density considered. These \(N\) obstacles are then placed uniformly at random within a hypersphere shell of inner radius \(\sigma = 1\) and outer radius \(r_{\text{max}} > \sigma\). Because \(N\) is chosen in accordance to the fluctuation of the Poisson random field in a finite volume, this construction guarantees that the probability of obtaining a cavity containing the origin, \(C\), exactly tracks the distribution of cavities at that same \(\bar{\varphi}\) in an infinitely large system. The properties of this cavity can then be sampled using either static or dynamical algorithms.

#### 1. Static Sampling

For a purely geometric sampling of the cavity properties, a Delaunay triangulation (into \(d\)-simplicial cells) of the obstacles within that cavity is built using CGAL’s \(dD\) Triangulation library [47]. The cavity is then constructed by a graph search with cells as vertices and facets as edges. Starting from the cell that contains the origin, an edge (facet) is connected if the circumcenter of two cells are in same side, or the circumcenter are on opposite sides and the circumradius of the facet is greater than \(\sigma\). All visited cells are added to the cavity. The cavity is valid if the displacement of any sites in the cavity to the origin is less than \(r_{\text{max}} - \sigma\). Care must be taken choosing \(r_{\text{max}}\), such that this condition is met. Like in the Leath algorithm for lattice percolation [34], cavities are evenly sampled in a site base, that is, the probability of generating a cavity of volume \(V\) is proportional to \(V P(V)\), where \(P(V)\) is the probability of having a cavity of volume \(V\) in the thermodynamic limit.

Sastry et al. proved that the visited cells constructed in this way contain and only contain the void space that belongs to the same cavity [33]. They also introduced an exact algorithm to determine the cavity volume through a recursive division of \(d\)-simplices. Because the exact decomposition of a cavity into simple primitives is quite involved in general dimension, we consider instead a random sampling algorithm. The basic idea is to generate uniformly distributed random points (samples) within the cavity and to use these samples to approximate the cavity volume and other physical quantities. The high level description of the principal algorithm is as follows:

### Table II. Numerical estimates of the void percolation threshold

| \(d\) | \(\Phi_p\) | \(\varphi_p\) |
|------|------------|------------|
| 2    | 1.1276(9)  | 0.5638(5)  |
| 3    | 3.510(2)   | 1.1698(8)  |
| 4    | 6.247(3)   | 1.5618(6)  |
| 5    | 9.170(7)   | 1.834(1)   |
| 6    | 12.22(3)   | 2.037(5)   |
| 7 \((D_7)\) | 15.40(5) | 2.194(9)  |
| 8 \((E_8)\) | 18.6(1)  | 2.32(1)   |
As the obstacle density increases, the fraction and size of the voids become increasingly small, which makes this sampling approach inefficient. We then instead find the vertices of the cavity, build the triangulation over these vertices, and then run the cavity sampling algorithm in the new triangulation. Note that a simplex generated this way may lie completely in occupied space, or even contain the voids of other cavities. The later case should be rare and in fact is not observed in practice. One should nonetheless test for this case and drop occupied or invalid simplices from thus sampling. With this simple optimization, the fraction of void samples \((N_{\text{voids}}/N_{\text{samples}})\) typically varies from a half to nearly one.

From the \(N_{\text{voids}}\) samples out of \(N_{\text{samples}}\) within the cavity, we approximate the cavity volume

\[
V_{\text{cavity}} = V_{\text{cells}} \frac{N_{\text{voids}}}{N_{\text{samples}}},
\]

where \(V_{\text{cells}}\) is the total volume of visited cells. From the set of samples within the void space, \(\{S_i\}\), we can also approximate the infinite-time mean squared displacement of a tracer in this cavity as

\[
\Delta_{\text{cavity}} = \langle (S_i - S_j)^2 \rangle = 2\langle S_i^2 \rangle - \langle S_i \rangle^2.
\]

The self van Hove function, \(G_s(r,t)\), which is defined as the probability of finding a tracer at displacement \(r\) at time \(t\), can be computed in the \(t \to \infty\) limit, when every site is equally probable, for a single cavity as

\[
G_{s,\text{cavity}}(r) = G_{s,\text{cavity}}(r, t \to \infty) \sim \sum_{i \neq j} \delta(|S_i - S_j| - r)
\]

and is normalized as \(\int_0^\infty G_s(r)dr = 1\). Note that the summation is over sites \(i \neq j\), in order to eliminate the artificial peak at \(r = 0\) due to the discretization scheme. Finally, the expected \(V\), \(\Delta\) and \(G_s(r)\) are the arithmetic mean over all randomly generated cavities.

### 2. Dynamical Sampling

For the tracer dynamics, we implemented a high-dimensional generalization of the simulation scheme of Höfling et al. [3, 35]. For the cage escape analysis, obstacles are first generated according to the cavity reconstruction scheme, which allows the vicinity of \(\varphi_d\) in dimensions as high as \(d = 20\) to be reached. A tracer is then placed at the origin and ballistic dynamics is run. The simulation terminates when \(t_{\text{max}}\) is reached or when the tracer escapes the shell, i.e., \(r(t) > r_{\text{max}} - \sigma\), whichever comes first. For a given \(t\), multiple time intervals are sampled and averaged to obtain the dynamical cage size \(\Delta(t)\) for a specific realization of disorder. The escape event time, \(t_{\text{esc}}\) at \(\Delta_{\text{esc}}\) is calculated as the first-passage time of the tracer square displacement from the origin being \(\Delta_{\text{esc}}\).
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