Structural and dynamical properties of the percolation backbone in two and three dimensions

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We study structural and dynamical properties of the backbone of the incipient infinite cluster for site percolation in two and three dimensions. We calculate the average mass of the backbone in chemical space, \( M_B(r) \), where \( d_B \) is the chemical dimension. We find \( d_B = 1.45 \pm 0.01 \) in \( d = 2 \) and \( d_B = 1.36 \pm 0.02 \) in \( d = 3 \). The fractal dimension in \( r \) space \( d_f \) is obtained from the relation \( d_f = 0.03 \), where \( d_{\text{min}} \) is the fractal dimension of the shortest path. The distribution function \( P_B(r, \ell) \) is determined, giving the probability of finding two backbone sites at the spatial distance \( r \) connected by the shortest path of length \( \ell \), as well as the related quantity \( \ell_{\text{min}}(r, N_{av}) \), giving the length of the minimal shortest path for two backbone sites at distance \( r \) as a function of the number \( N_{av} \) of configurations considered. Regarding dynamical properties, we study the distribution functions \( P_B(\ell, t) \) and \( P_B(r, t) \) of random walks on the backbone, giving the probability of finding a random walker after \( t \) time steps, at a chemical distance \( \ell \), and Euclidean distance \( r \) from its starting point, respectively, and their first moments \( \langle \ell_B(t) \rangle = t d_{\ell B} \) and \( \langle r_B(t) \rangle = t d_{r B} \), from which the fractal dimensions of the random walk \( d_{\ell B} \) and \( d_{r B} \) are estimated. We find \( d_{\ell B} = 2.28 \pm 0.03 \) and \( d_{r B} = 2.62 \pm 0.03 \) in \( d = 2 \) as well as \( d_{\ell B} = 2.25 \pm 0.03 \) and \( d_{r B} = 3.09 \pm 0.03 \) in \( d = 3 \).

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I. INTRODUCTION

Percolation represents a useful model for a variety of systems in many fields of science displaying both structural disorder and self-similarity, i.e., fractal behavior, within some range of length scales [1–3]. In many circumstances, a detailed knowledge of the internal structure of percolation clusters is required. In particular, for studying transport processes near the percolation threshold \( p_c \), a crucial role is played by the complex topology of the available conducting paths [4–7].

It is known that at \( p_c \), the incipient infinite cluster exhibits a variety of self-similar substructures and consequently a rich scenario of transport properties [4–7]. A prominent role is played by the backbone of the cluster, defined as the subset of cluster sites carrying the current when a voltage difference is applied between two sites (see [8] and references therein). Thus, the backbone structure solely determines the conductivity of the whole percolation network between both sites. The backbone of a percolation cluster is also useful as a model of a porous medium containing long polymer chains [9]. So far, much is known about structural and dynamical properties of percolation clusters, but little is known about the corresponding properties of the backbone.

In this paper, we report a detailed study of structural and dynamical properties of the backbone of the incipient infinite cluster at \( p_c \) in two and three dimensions. Actually, many of the exponents characterizing the structural and dynamical properties of the backbone are presently poorly known, in particular, in three dimensions. To obtain accurate results, we study the backbone in topological or chemical space [3,5]. The topological or chemical distance \( \ell \) between two points on the cluster is defined as the length of the shortest path connecting them via nearest-neighbor cluster sites. Since our clusters are generated in chemical space (see below), this is the natural metric for measuring critical exponents. To this end, we first calculate the fractal dimension of the backbone in chemical space (\( \ell \) space) \( d_{\ell B} \), and obtain the fractal dimension in Euclidean space (\( r \) space) \( d_r B \), from the relation \( d_r B = d_{\ell B} / d_{\text{min}} \), where \( d_{\text{min}} \) is the fractal dimension of the shortest path [3,5]. We next study the distribution function \( P_B(r, \ell) \), giving the probability that two backbone sites at distance \( r \) from each other are connected by a shortest path of length \( \ell \), as well as the related quantity \( \ell_{\text{min}}(r, N_{av}) \), giving the length of the minimal shortest path for backbone sites at distance \( r \) from each other as a function of the number \( N_{av} \) of configurations considered. To the best of our knowledge, these quantities have not been studied so far for the backbone. It is therefore interesting to calculate \( P_B(r, \ell) \) and compare it with the corresponding structural function \( P(r, \ell) \) for the whole cluster, which is now known quite accurately (for a recent work see Ref. [10]). From the additional information obtained by studying \( P_B(r, \ell) \), we expect to better understand the structural properties of the whole cluster as well.

Regarding dynamical properties, we consider random walks on the backbone and calculate the mean square displacements of the walker as a function of time, in both \( \ell \) and \( r \) spaces. Finally, we consider the corresponding distribution functions \( P_B(\ell, t) \) and \( P_B(r, t) \), giving the probability density that the walker is, at time \( t \), at the distance \( \ell \) and \( r \), respectively, from its starting point at \( t = 0 \). Following the study of \( P(r, t) \) for the whole cluster [11], we also discuss the question of the dependence of \( P_B(r, t) \) on the number \( N_{av} \) of backbone configurations taken into account in the average.

The paper is organized as follows. In Sec. II, the fractal dimensions in chemical and Euclidean space are determined,
II. STRUCTURAL PROPERTIES

We generate large percolation clusters at criticality with the well-known Leath algorithm [12] on square and simple cubic lattices. The Leath algorithm generates in every step \( \ell \) the whole set of sites having a chemical distance \( r = \ell \) from the seed, i.e., in the first step all sites with \( r = 1 \) are generated, in the second step all sites with \( r = 2 \) and so on. The corresponding backbone is obtained using an improved version of the “burning” algorithm [8] described in detail in Appendix A. To perform the averages, we grow clusters up to a maximum chemical distance \( r_{\text{max}} = 2000 \) from the seed, with \( r_{\text{max}} = 1000 \) in two dimensions and \( r_{\text{max}} = 10000 \) in three dimensions. To minimize the computer memory needed for the calculations, we estimate the minimum lattice sizes \( L \) required to generate such large clusters from a relation given in [11] (see Appendix B for details). We use \( L = 2801 \) in \( d = 2 \) and \( L = 685 \) in \( d = 3 \), which in both cases are much smaller than \( L' = 2r_{\text{max}} + 1 \). Nevertheless, none of the generated clusters reached the lattice boundaries. This more efficient use of computer memory, as well as the improved burning algorithm, enables us to study much larger systems than before, leading to more accurate estimates for the critical exponents and the fractal dimensions.

A. Fractal dimensions

Because the clusters are generated in chemical space, no boundary effects occur when looking at properties that depend on the chemical distance \( r \), in contrast to Euclidean space (\( r \) space), where strong boundary effects are present. Thus, the fractal dimension \( d_B^r \) of the backbone, defined by \( \langle M_B(r) \rangle \sim r^{d_B^r} \), is not determined directly, but instead we study the mass-distance relation in \( r \) space according to

\[
\langle M_B(r) \rangle \sim r^{d_B^r},
\]

where \( d_B^r \) is the fractal dimension of the backbone in chemical space. The two fractal dimensions are related by \( d_f^r = d_B^r d_{\text{min}} \), where \( d_{\text{min}} \) is the fractal dimension of the shortest path and describes the scaling between \( r \) and \( \ell \), i.e., \( \langle r \rangle \sim r^{d_{\text{min}}} \), with \( d_{\text{min}} = 1.130 \pm 0.004 \) in \( d = 2 \) [13,14] and \( d_{\text{min}} = 1.374 \pm 0.004 \) in \( d = 3 \) [15].

The results for \( d_B^r \) are displayed in Fig. 1 for \( d = 2 \), and in Fig. 2 for \( d = 3 \), where the successive slopes of \( \ln M_B(r) \) vs \( \ln r \) as a function of \( 1/\ell \) are shown. The open symbols correspond to the case in which the backbone is defined between the seed and one randomly chosen site on the last grown chemical shell. Clearly, in this case the value of \( d_B^r \) tends to decrease when \( \ell \to r_{\text{max}} \), since close to \( r_{\text{max}} \) the backbone grows nearly linear. This provides us with a numerical lower bound for the actual value of \( d_B^r \). A numerical upper bound can be obtained by defining the backbone between the seed and all sites on the last grown chemical shell.

![FIG. 1. Plot of the chemical dimension \( d_B^r \) as a function of \( 1/\ell \) for \( d = 2 \) [obtained from successive slopes of \( \ln M_B(r) \) vs \( \ln r \)]. The backbone is determined using one site on the last grown chemical shell (open symbols) and all sites on the last grown chemical shell (full symbols). The plots are based on averages of \( M_B(r) \) over 80 000 cluster configurations, with a maximum chemical distance \( r_{\text{max}} = 2000 \) (open and full circles) and \( r_{\text{max}} = 400 \) (open and full triangles). The results are summarized in Table I.](Image 52x104 to 292x758)

![FIG. 2. Plot of the chemical dimension \( d_B^r \) as a function of \( 1/\ell \) for \( d = 3 \) [obtained from successive slopes of \( \ln M_B(r) \) vs \( \ln r \)]. The backbone is determined using one site on the last grown chemical shell (open symbols) and all sites on the last grown chemical shell (full symbols). The plots are based on averages of \( M_B(r) \) over 80 000 cluster configurations, with a maximum chemical distance \( r_{\text{max}} = 1000 \) (open and full circles) and \( r_{\text{max}} = 200 \) (open and full triangles). The results are summarized in Table I.](Image 57x524 to 292x758)
The full symbols correspond to this case, where now the value of $d_B^r$ tends to increase when $\ell/\ell_{\text{max}}$ is close to $\ell_{\text{max}}$, since close to $\ell_{\text{max}}$ the so-defined backbone coincides with the cluster itself. Our estimated asymptotic values, obtained by fitting two straight lines for both the lower and upper sets of points, and extrapolating $1/\ell \rightarrow 0$, are reported in Table I. The reported exponents $d_B^r$ are the averages of these extrapolations, while the extrapolated values allow us to estimate the error bars. The obtained values are consistent with previously published results, see, e.g., [8].

### B. Distribution functions

Next, we consider the structural distribution function $\Phi_B(r,/r)$, giving the probability that two backbone sites connected by a shortest path of length $\ell$ are at spatial distance $r$ from each other. We assume for $\Phi_B(r,/r)$ a similar scaling form as for the entire cluster (see e.g., [5,10,14]), i.e.,

$$\Phi_B(r,/r) = \frac{1}{\ell^d f_B(x)},$$

with the scaling variable $x=r/l^{\tilde{v}}$ and $\tilde{v}=1/d_{\text{min}}$, and $\Phi_B(r,/r)=0$ for $l<\ell_{\text{min}}(r,N_m)$. The quantity $\ell_{\text{min}}(r,N_m)$ is discussed in detail in Sec. III. As for the entire cluster [10], we expect that the scaling function $f_B(x)$ cannot be fitted by a simple product of a power law and an exponential function, but displays a more general form

$$f_B(x) = \begin{cases} c_1 x^{g_1^B} & \text{for } x \ll 1, \\ c_2 x^{g_2^B} \exp[-a x^{\delta}] & \text{for } x \gg 1, \end{cases}$$

with two different exponents $g_1^B$ and $g_2^B$ in the regimes $r/l^{\tilde{v}} \ll 1$ and $r/l^{\tilde{v}} \gg 1$, respectively, and $\delta=(1-\tilde{v})^{-1}$. The normalization is given in the embedding $d$-dimensional space by $\int x^{d-1} \Phi_B(r,/r) dx = 1$. For convenience, we determine numerically the distribution function $\Phi_B(r,/r)$, related to $\Phi_B(r,/r)$ by

$$\Phi_B(r,/r) = r^{d-1} \Phi_B(r,/r) = \left(\frac{r}{\ell^{\tilde{v}}}\right)^d f_B(x),$$

which is normalized according to $\int \Phi_B(r,/r) dx = 1$. The function $r^{d-1} \Phi_B(r,/r)$ vs $r/l^{\tilde{v}}$ is shown in Fig. 3 for $d=2$ and $d=3$, from which the exponents $g_1^B$ and $g_2^B$ are determined, which are related to $g_1^B$ and $g_2^B$, by $g_1^B=g_1^B+d$ and $g_2^B=g_2^B+d$, respectively. The results for the fitting parameters are reported in Table II. We note that the corresponding distribution function $\Phi_B^{(\text{all})}(r,/r)$ for the backbone defined

<table>
<thead>
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<th>Fractal dimension</th>
<th>Lattice dimension</th>
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<tbody>
<tr>
<td>$d=2$</td>
<td>$d=3$</td>
</tr>
<tr>
<td>$d_B^r$</td>
<td>1.45±0.01</td>
</tr>
<tr>
<td>$d_B^f$</td>
<td>1.64±0.02</td>
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</tbody>
</table>

### FIG. 3. Scaling plots of the distribution function for percolation backbones $r \Phi_B(r,/r)$ vs $r/l^{\tilde{v}}$, for (a) $d=2$, $\ell=1000$ (circle), $\ell=1400$ (full diamond), and $\ell=1800$ (square), and (b) $d=3$, $\ell=400$ (circle), $\ell=600$ (full diamond), and $\ell=800$ (square). In both cases, the plots are based on averages over 80,000 cluster configurations, with a maximum chemical distance $\ell_{\text{max}}=2000$ in $d=2$ and $\ell_{\text{max}}=1000$ in $d=3$. The lines represent our fits for $r/l^{\tilde{v}} \ll 1$ (continuous line) and $r/l^{\tilde{v}} \gg 1$ (dashed line). The fitting parameters are summarized in Table II.

### TABLE II. The fitting parameters describing the scaling function $f_B(x)$ (see Fig. 3) for the backbone of percolation clusters at criticality, where $f_B(x)=c_1 x^{g_1^B}$ for $x \ll 1$ (continuous line) and $f_B(x)=c_2 x^{g_2^B} \exp[-a x^{\delta}]$ for $x \gg 1$ (dashed line), with $\delta=(1-\tilde{v})^{-1}$. The measured exponents $g_1^B$ and $g_2^B$ are related to $g_1^B$ and $g_2^B$ by $g_1^B=g_1^B+d$ and $g_2^B=g_2^B+d$.

<table>
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<td>0</td>
</tr>
<tr>
<td>$c_1$</td>
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<td>4.02±0.20</td>
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</tr>
<tr>
<td>$c_2$</td>
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<td>3.59±0.20</td>
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</tr>
<tr>
<td>$d_B^r$</td>
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<td>$a_B$</td>
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between the seed and all sites on the last grown chemical shell is identical to $\Phi_B(r,\phi)$ within the current numerical accuracy.

### C. Minimal shortest path

We discuss next the behavior of the minimal shortest path $r_B^{\text{min}}(r,N_{av})$ determining the values of $\phi$ at which $\Phi_B(r,\phi)=0$. This quantity plays a very important role for determining transport properties: The fact that the minimal shortest path $r_B^{\text{min}}(r,N_{av})$ shows an explicit dependence on the number of configurations $N_{av}$ considered has important consequences for dynamical properties as, e.g., random walks, fractions or electronic wave functions [11]. In this paper we restrict ourselves to the discussion of the effect on random walks, see Sec. III.

We expect a scaling behavior of $r_B^{\text{min}}(r,N_{av})$, as a function of the Euclidean distance $r$ and the number of configurations $N_{av}$ considered, similar to that on the entire cluster [11], i.e.,

$$r_B^{\text{min}}(r,N_{av}) = \begin{cases} r & \text{for } r < r_B^{\text{c}}(N_{av}), \\ \alpha_{\text{min}}^B(N_{av}) r^{d_{\text{min}}} & \text{for } r > r_B^{\text{c}}(N_{av}). \end{cases}$$

Notice that below the crossover distance $r_B^{\text{c}}(N_{av})$, the minimal chemical distance $r_B^{\text{min}}(r,N_{av})$ is independent of the number of configurations $N_{av}$ considered, while for $r > r_B^{\text{c}}(N_{av})$ it depends explicitly on $N_{av}$. To obtain the crossover distance $r_B^{\text{c}}(N_{av})$ analytically, we consider the probability $W_B^{\text{av}}$ to find a shortest path of length $\phi = r = r_B^{\text{c}}$ within $N_{av}$ backbone configurations, where $W_B^{\text{av}} = N_{av}^{-1}$ holds. For the entire cluster the relation $W_B^{\text{av}} = z_{p_z}^{r_B^{\text{c}}}$ used in [11], where $z$ is the coordination number of the lattice. For the backbone we expect a similar relation $W_B^{\text{av}} = z_{\text{eff}} p_z^{r_B^{\text{c}}}$, where $z_{\text{eff}}$ is replaced by an effective coordination number $z_{\text{eff}}$ which incorporates the probability that the considered site belongs to the backbone. Since the backbone is more dilute than the whole cluster, we have in average a smaller connectivity, i.e., $z_{\text{eff}} < z$. This yields

$$r_B^{\text{c}}(N_{av}) = \frac{\ln z_{\text{eff}} + \ln N_{av}}{\ln(1/p_z)},$$

where $z_{\text{eff}}$ is not known analytically and must be determined a posteriori.

To determine $\alpha_{\text{min}}^B(N_{av})$, we assume, as for the entire cluster, the scaling behavior $r_B^{\text{min}}(r,N_{av}) = r_B^{\text{c}}(N_{av}) g_B[r/r_B^{\text{c}}(N_{av})]$. To fulfill Eq. (5), the scaling function $g_B(x)$ must behave as $g_B(x) = x$ when $x < 1$ and $g_B(x) \sim x^{d_{\text{min}}}$ when $x > 1$. This yields

$$\alpha_{\text{min}}^B(N_{av}) = \alpha_B^B [r_B^{\text{c}}(N_{av})]^{1-d_{\text{min}}},$$

where the prefactor $\alpha_B$ remains to be determined. Results for $r_B^{\text{min}}(r,N_{av})/r_B^{\text{c}}(N_{av})$ versus $r/r_B^{\text{c}}(N_{av})$ for different values of $N_{av}$ are shown in Fig. 4 for $d = 2$ and $d = 3$. The shown lines indicate the predicted exponents, 1 for $r/r_B^{\text{c}}(N_{av}) < 1$ and $d_{\text{min}}$ for $r/r_B^{\text{c}}(N_{av}) > 1$. The values of $z_{\text{eff}}$ are determined such that the best data collapse is achieved, and $\alpha_B = x_{\text{c}}^{1-d_{\text{min}}}$.

### III. DYNAMICAL PROPERTIES

In the following, we consider dynamical properties of the backbone by studying random walks, both in Euclidean and chemical space. To this end, we employ the exact enumeration method [5]. For the present purposes, clusters are grown on square and simple cubic lattices up to a maximum chemical distance $r_{\text{max}} = 1000$ in $d = 2$ and $r_{\text{max}} = 400$ in $d = 3$. Clusters which have not reached the chemical shell $r_{\text{max}}$ are

| TABLE III. Structural constants, defined in Eqs. (6) and (7) and obtained from the data collapse shown in Fig. 4. |
|-----------------|-----------------|-----------------|
| Structural constant | Lattice dimension |
|-----------------|-----------------|-----------------|
| $z_{\text{eff}}$ | $\alpha_B$      |
| $d = 2$         | $d = 3$         | $d = 6$         |
| $2.1 \pm 0.2$   | $1.2 \pm 0.2$   | $1$             |
| $1.02 \pm 0.05$ | $0.95 \pm 0.07$ |                 |
successive slopes of $\ln r_B(t)$ and $\ln r_0(t)$ vs $\ln t$, respectively. The backbone is determined using one site on the chemical shell $\langle x \rangle_{\text{max}}$ (open circles) and all sites on the chemical shell $\langle x \rangle_{\text{max}}$ (full circles). The plots are based on averages of $r_B(t)$ and $r_0(t)$ over 10 000 cluster configurations, with a maximum chemical distance $\langle x \rangle_{\text{max}} = 1000$ and $t_{\text{max}} = 4000$ time steps. The results are summarized in Table IV.

discarded. Again, the lattice sizes are estimated with the method discussed in Appendix B. In our simulations, we consider random walks of $t_{\text{max}} = 4000$ and $t_{\text{max}} = 1600$ time steps in $d = 2$ and $d = 3$, respectively.

A. Mean displacements

The mean displacements after $t$ time steps in chemical and Euclidean metric are given by

$$\langle x_B(t) \rangle \sim t^{1/d_w^{B'}}$$

and

$$\langle r_B(t) \rangle \sim t^{1/d_w^{B}}$$

from which the fractal dimensions of the random walk $d_w^{B'}$ and $d_w^{B}$ are determined. The results for $d_w^{B'}$ and $d_w^{B}$ are displayed in Fig. 5 for $d = 2$ and Fig. 6 for $d = 3$, where the successive slopes of $\ln r_B(t)$ and $\ln r_0(t)$ vs $\ln t$, respectively, are shown. The open circles correspond to the case in which the backbone is defined between the seed and one randomly chosen site on the chemical shell $\langle x \rangle_{\text{max}}$, and the full circles to the case in which the backbone is defined between the seed and all sites on the chemical shell $\langle x \rangle_{\text{max}}$. Both sets of points coincide as long as the random walker mainly explores regions of the backbone where both algorithms yield similar structures. This provides us with numerical upper and lower bounds for the actual values of $d_w^{B'}$ and $d_w^{B}$. Our estimated asymptotic values, obtained by fitting two straight lines for both the lower and upper sets of points, and

extrapolating $1/t \to 0$, are reported in Table IV. The reported exponents $d_w^{B'}$ and $d_w^{B}$ are the averages of these extrapolations, while the extrapolated values allow us to estimate the error bars. The obtained values are consistent with previously published results, see, e.g., [16].

B. Distribution functions

The probability of a random walker to be at chemical distance $x$ and Euclidean distance $r$ after $t$ time steps is given by the distribution functions $P_B(x,t)$ and $P_B(r,t)$, respectively. The mean displacement $\langle x_B(t) \rangle$ and $\langle r_B(t) \rangle$ discussed above are the first moments of these distributions. For the distribution function in chemical space we expect a form similar to that for the entire cluster [5,6], i.e.,

$$P_B(x,t) \sim \exp \left[-\left(\frac{x}{\xi_B}\right)^{\nu_B}\right],$$

where

<table>
<thead>
<tr>
<th>Diffusion exponent $d$</th>
<th>Lattice dimension $d=2$</th>
<th>$d=3$</th>
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<tr>
<td>$d_w^{B'}$</td>
<td>2.28 ± 0.03</td>
<td>2.25 ± 0.03</td>
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<tr>
<td>$d_w^{B}$</td>
<td>2.62 ± 0.03</td>
<td>3.09 ± 0.03</td>
<td>4</td>
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</table>
with \( \xi^B \sim \langle /B(t) \rangle \) and \( P_B(0,t) \sim \xi^B \), where \( \langle /B(t) \rangle \) is the mean displacement in chemical metric defined above.

The distribution is normalized as \( \int d^{d-1}P_B(\xi,t)d\xi=1 \). To obtain the exponent \( \nu_B \), we plot \(-\ln[P_B(\xi,t)/P_B(0,t)]\) vs \( \xi/B \) in double logarithmic form in Fig. 7 for \( d=2 \) and \( d=3 \). Similar to the entire cluster, we find \( \nu_B=d_B^B/2 \) for \( \xi/B<1 \) and \( \nu_B=d_B^B/d_B^B-1 \) for \( \xi/B>1 \).

To analytically calculate the distribution function \( P_B(r,t;N_{av})=(P_B(r,t))_{N_{av}} \) for a random walker in Euclidean space, averaged over \( N_{av} \) configurations, we follow Refs. [6,11] and write \( P_B(r,t;N_{av}) \) as a convolution integral of the distribution of a random walker in \( \xi/B \) space, \( P_B(\xi,t) \), and the structural function \( \Phi_B(\xi) \), i.e.,

\[
P_B(r,t;N_{av}) = \int_{\xi_{\min}(r,N_{av})}^{\infty} \Phi_B(\xi) d\xi \int_{\xi_{\min}(r,N_{av})}^{\infty} d^{d-1}\Phi_B(\xi,t) d\xi,
\]

where \( \xi_{\min}(r,N_{av}) \) is the length of the minimal shortest path discussed in Sec. II. The dependence of the lower integration limit \( \xi_{\min}(r,N_{av}) \) on the number of configurations \( N_{av} \) considered introduces a second crossover distance \( r_\times(N_{av}) \) and causes a dependence of \( P_B(r,t;N_{av}) \) on \( N_{av} \). The distribution \( P_B(r,t;N_{av}) \) is normalized on the backbone by \( \int r^{d_B^B-1}P_B(r,t;N_{av})dr=1 \). Following the procedure described in [11,17], we obtain, in full analogy to the results for percolation clusters,

\[
P_B(r,t;N_{av}) / P_B(0,t;N_{av}) \sim \begin{cases} 1 - c \left( r / \xi^B \right)^{d_B^B+d_B^B-1} & \text{for } r < r_1^B, \\ \exp \left[ -c' \left( r / \xi^B \right)^{d_B^B/(d_B^B-1)} \right] & \text{for } r_1^B \leq r < r_\times^B(N_{av}), \\ \exp \left[ -c'' \left[ (r(B(N_{av})) / \xi^B \right)^{d_B^B/(d_B^B-1)} \right] & \text{for } r > r_\times^B(N_{av}) \end{cases}
\]
for the regime \( r < r^B_1 \) see also [18,19]). The crossover distances \( r^B_1 \) and \( r^B_\infty(\Naw) \) are given by

\[
r^B_1 = \xi^B r \left[ (g^B r d)(d_{\min}^{-1}-1) \right]^{(d_{Bw}^{-1}/d_B)^{+}}
\]

and

\[
r^B_\infty(\Naw) = \xi^B r d^{-1} \left[ (d_{\min}^{-1}-1)(d_{Bw}^{-1}-1) \right] ^{ [r^B_\infty(\Naw)]^{d_{Bw}^{-1}/d_B} }
\]

with \( \xi^B = \langle r_B(t) \rangle \), where \( \langle r_B(t) \rangle \) is the mean displacement in the Euclidean space defined above. Hence, for large distances \( r \), the relevant length scale increases logarithmically with the number \( \Naw \) of configurations. Below \( r^B_\infty(\Naw) \), \( P_B(r,t) = P_B(\Naw) \) is independent of \( \Naw \); while above \( r^B_\infty(\Naw) \), the self-averaging hypothesis breaks down and \( P_B(\Naw) \) depends logarithmically on \( \Naw \). The so-called typical average \( \langle P_B(r,t) \rangle_{typ} \) is equivalent to the case \( \Naw = 1 \), i.e., \( \langle P_B(r,t) \rangle_{typ} = P_B(r,t) \).

To verify our predictions given in Eqs. (12)–(14), we plotted \(- \ln[\langle P_B(r,t) \rangle/ P_B(\Naw)]\) vs \( r/\xi^B \) in double logarithmic form in Fig. 8 for \( d = 2 \) and \( d = 3 \). The shown lines indicate our predicted exponents \( g^B_1 = d - d^B_1 \) for \( r < r^B_1 \), \( d^B / (d_{Bw}^{-1}) \) for \( r^B_1 < r < r^B_\infty(\Naw) \), and \( d^B_1 / (d_{Bw}^{-1}-1) \) for \( r > r^B_\infty(\Naw) \). The numerical data are well described by our analytical results.

### IV. SUMMARY

In this paper we present extensive numerical simulations concerning the structural and dynamical properties of the backbone of percolation clusters at criticality in two and three dimensions. An improved burning algorithm, introduced in this work, enables us to study much larger systems than before, therefore leading to improved estimates for the fractal dimensions of the backbone \( d^B_w \) and \( d^B \), as well as for the corresponding fractal dimensions of the random walk \( d^B_w \) and \( d^B \). We also calculate the structural distribution function \( \Phi_B(r,\ell) \), the length of the minimal shortest path \( \ell^B_{\min}(r,\Naw) \), and the distribution function of a random walker in chemical and Euclidean space \( P_B(\ell,t) \) and \( P_B(r,t;\Naw) \), respectively.

We note that from \( d^B_w \) and \( d^B \) the conductivity exponent \( \mu^* \), which describes the scaling behavior of the conductivity \( \sigma \) of a percolation system near criticality as a function of the system size \( L \), i.e., \( \sigma \sim L^{-\mu^*} \), can be calculated by \( \mu^* = d^B_w - d^B + d - 2 \) [5,6]. Our results for \( d^B_w \) and \( d^B \) yield \( \mu^* = 0.98 \pm 0.03 \) in \( d = 2 \) and \( \mu^* = 2.22 \pm 0.03 \) in \( d = 3 \). These results are in very good agreement with the values \( \mu^* = 0.97 \pm 0.01 \) and \( \mu^* = 2.2 \pm 0.1 \) for \( d = 2 \) and \( d = 3 \), respectively, obtained from other simulations [3].

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### APPENDIX A: IMPROVED “BURNING” ALGORITHM

The backbones studied in this paper are generated using an improved version of the burning algorithm. The basic burning algorithm was first introduced in [8]. We review the above algorithm and consider its improvement.

To use the burning algorithm, one has to find the chemical distances \( \ell \) to the starting site of the backbone and the sites where loops of cluster sites relative to the starting site close up (loop sites). Using the Leath method, the sites of the cluster are generated with increasing chemical distance \( \ell \) from the seed. Therefore it is convenient to define the backbone between the seed (starting site) and one randomly chosen site on the last grown chemical shell of the cluster (end site) [20]. In such a case the chemical distances \( \ell \) to the starting site are trivially identical to those obtained by Leath growth. By choosing the end site of the backbone on the last grown chemical shell we ensure that no sites with a larger chemical distance \( \ell \) to the starting site than the end site exists. In addition, the loop sites are easy to identify during Leath growth, as they occur with increasing chemical distance \( \ell \) from the seed.

The burning algorithm is divided into two parts. In the first part we start burning the end site, becoming a burning site. Then, its nearest-neighbor cluster sites are burnt, and become the new burning sites. This process is repeated from each burning site, with the condition that only nearest-neighbor sites are burnt which have a chemical distance \( \ell \) to the starting site smaller than the burning site itself. This part of the burning algorithm ends when the starting site is reached. The thus obtained burnt sites are located along the shortest path between the starting and the end site, and form the so-called skeleton or elastic backbone [8,21]; an example is shown in Fig. 9(a).

In the second part of the algorithm we deal with the loop sites. At the beginning all loop sites are considered as active and stored in a list sorted by increasing chemical distance \( \ell \) to the starting site. We start burning the first loop site, i.e., the one with the smallest chemical distance \( \ell \) to the starting site, and proceed in the same way as for the skeleton. If during this process two or more different sites are reached which are known to be part of the backbone, then the burnt sites (including the loop site) belong to the backbone, and the corresponding loop site is no longer active and is removed from the list. Otherwise it cannot be decided yet whether these sites belong to the backbone or not, and one has to
restore the previous state of the burnt sites including the loop site, which remains active. In both cases one can continue treating the next loop site (having a chemical distance \( \ell \) to the starting site equal or larger than the previous one) in the same way as described above. If the active loop site with the largest chemical distance \( \ell \) has been considered, one starts from the active loop site with the smallest \( \ell \). The algorithm ends when no new site has been found belonging to the backbone during a complete run through the list of active loop sites.

However, this sequential algorithm described above generally produces erroneous results, such that sites not belonging to the backbone are added to it [see Fig. 9(c1) and (d1)]. To avoid such failures, one has to start again at the active loop site with the smallest chemical distance \( \ell \) to the starting site whenever adding a new part to the backbone, instead of proceeding sequentially. By doing this, the backbone is determined correctly [see Fig. 9(c2), (d2), and (e2)]. Unfortunately this “back-start” algorithm is very time consuming, since now the computing time depends quadratically on the number of loop sites [22].

The improvement of the algorithm is based on a simple observation: The reason for the erroneous outcome of the sequential version is due to the likely existence of so-called “tadpoles,” i.e., a group of sites which is linked to the actual backbone through a singly connected path. According to Fig. 9, the burning starting at the first loop site (denoted “1”) in the figure) reaches the so far known backbone in one point, which coincides with the starting site. Therefore, the burnt sites are not identified as backbone sites and are restored to their previous state. A new burning process, starting from the next loop site, (denoted “2”), as shown in Fig. 9(b), reaches the backbone in two points, one is the starting site and the second a skeleton site (nearest-neighbor site of “2” to the right), and these burnt sites are correctly identified as backbone sites. Proceeding sequentially in the list of active loop sites in such a situation, i.e., by starting a burning process from the site “3,” as shown in Fig. 9(c1), instead of starting again at the active loop site with the smallest chemical distance \( \ell \) to the starting site (i.e., site “1”), as shown in Fig. 9(c2), yield the erroneous result shown in Fig. 9(d1). This failure can be easily prevented, if it is realized during a burning process that only one site is burning during a burning step, reflecting the singly connected structure of the path, and the backbone has not yet been reached, see Fig. 9(c3).

In such a case, one can immediately stop the burning process from this loop site, keep the loop site active, and restore the previous state of the corresponding burnt sites. In addition, one can always proceed sequentially, even after adding a new part to the backbone, as shown in Fig. 9(c3), (d3), and (e3), and as a result the computing time scales only linearly with the number of loop sites.

**APPENDIX B: ESTIMATE FOR THE LATTICE SIZE FOR PERCOLATION CLUSTERS AT CRITICALITY**

To minimize the computer memory needed for the simulations, we estimate the minimum lattice size \( L = 2R + 1 \) required to generate a cluster of \( \ell_{max} \) shells, with the condition that its radial extent \( r_{max} \) will not exceed \( R \). To this end, we employ the relation \( \ell_{min}(r, N_{av}) = \alpha_{min} N_{av} \rho_{c}^\ell \) [cf. Eq. (5)] valid in the regime \( r > r_{c}(N_{av}) \), where \( \alpha_{min}(N_{av}) = \alpha[r_{c}(N_{av})]^{-a_{min}}, \alpha \equiv 1 \), and \( r_{c}(N_{av}) = (\ln z + \ln N_{av}) / \ln(1/p_c) \) [11]. From these relations one can estimate \( r_{max} \) for a typical \( N_{av} = 10^6 \) configurations, so that for determining, e.g., structural properties with \( \ell_{max} = 2000 \) and \( \ell_{max} = 1000 \) for \( d = 2 \) and \( d = 3 \), respectively, we estimate \( r_{max} \approx 1228 \) and \( r_{max} \approx 309 \). We have actually used \( R = 1400 \) and \( R = 342 \) in \( d = 2 \) and \( d = 3 \), respectively, which in both cases are much smaller than \( \ell_{max} \) and actually correspond to the value of \( r_{max} \) obtained with the above formula for more than \( 10^6 \) configurations.
Another possibility is to take all sites on the last grown chemical shell as end sites. In this case the method can be used in the same way as for a single end site, with the additional prescription that in the first part of the algorithm the burning starts simultaneously from all end sites.

It has been shown that the number of loop sites $N_{\text{loop}}$ scales as $N_{\text{loop}} \sim \nu_{d}$ [23]. If we start at the very beginning of the list whenever deleting a loop site out of it, the computing time is of the order $O(N_{\text{loop}}) = O(\nu_{d})$. For the improved version the time is only of order $O(N_{\text{loop}}) = O(\nu_{d})$.