Fragmentation of fractal random structures

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We analyze the fragmentation behavior of random clusters on the lattice under a process where bonds between neighboring sites are successively broken. Modeling such structures by configurations of a generalized Potts or random-cluster model allows us to discuss a wide range of systems with fractal properties including trees as well as dense clusters. We present exact results for the densities of fragmenting edges and the distribution of fragment sizes for critical clusters in two dimensions. Dynamical fragmentation with a size cutoff leads to broad distributions of fragment sizes. The resulting power laws are shown to encode characteristic fingerprints of the fragmented objects.

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Breakup phenomena of solid and liquid particulate matter are ubiquitous in nature and technology \[1\]. They span a vast range of time and length scales, including polymer degradation through the breaking of individual chemical bonds \[2\] as well as collision induced fragmentation of asteroids \[3\]. In geology, fragmentation phenomena result in the distribution of grain sizes observed in soils as well as rock sizes in boulder fields. Against the limitation of surface tension, fluids break up into droplets; in turbulent flow, one observes fragmentation of eddies and vortices, such that the flow field itself breaks up \[4\]. On the subatomic scale, excited atomic nuclei break up into fragments in a process known as nuclear multifragmentation reactions \[5\]. Practical applications ask for the adaptation and optimization of fragmentation processes according to technological requirements and efficiency considerations. This applies to mineral processing, where ore processing machinery needs to be optimized for energy efficiency \[1\]. In a more general socio-economic context, a wide range of structures from transport systems to social connections are described by complex networks, whose degree of resilience and pathway of fragmentation under the gradual removal of nodes or links is a recent subject of intense scrutiny \[6\] \[7\].

Due to this broad relevance, considerable effort has been invested in defining and analyzing tractable models of fragmentation processes, for a review see Ref. \[1\]. Much of this work is based on studying rate equations for the fragment size distribution. For the simplest case of binary break-up, where each fragmentation event results in exactly two fragments, the time dependent distribution \(n(s, t)\) of fragments of size \(s\) follows

\[
\frac{\partial n(s, t)}{\partial t} = - \int_0^s n(s, t) a(s) b(s, s') ds' + 2 \int_s^\infty n(s', t) a(s') b(s', s) ds',
\]

where \(a(s)\) denotes the fragmentation rate of clusters of mass \(s\) and \(b(s, s')\) is the conditional probability for an \(s\) break-up event to result in a fragment of size \(s'\).

Here, the first term on the r.h.s. describes the loss of fragments at size \(s\) due to break-up, whereas the second term corresponds to the gain from the break-up of clusters of mass larger than \(s\). A description of this type implies several drastic simplifications: the break-up kernel \(c(s, s') = a(s) b(s, s')\) is taken to be time independent; furthermore, the break-up is assumed to be spatially homogeneous and independent of fragment shape. Under these and further simplifying assumptions, a scaling theory has been developed which describes rather well a number of important aspects, including limiting behaviors \[8\] \[9\].

Much less progress has been made in terms of results beyond this mean-field approximation, however. For the fragmentation of objects resulting from shocks and collisions, there is a wealth of experimental observations (see, e.g., Refs. \[10\] \[13\]) as well as some degree of modeling of fracturing processes \[14\]. In terms of stylized models allowing to understand the relation between the structure of clusters and their fragmentation properties, the random disintegration of loop-free structures, such as intervals \[15\] \[16\] and trees \[17\], can be understood in some detail. Yet, for non-trivial shapes the only notable development has been a number of studies on the fragmentation of percolation clusters \[18\] \[21\]. It was shown there that the fragmentation rate \(a(s)\) as well as the conditional break-up probability \(b(s, s')\) exhibit power-law scaling, and the corresponding exponents were determined from simulations and exact enumeration for systems in two and higher dimensions.

In the present Letter we discuss fragmentation within a generalization of the percolation model with bond weight \(v\) and additional cluster weight \(q\), and partition function

\[
Z_{\text{RC}} = \sum_{G' \subseteq G} v^{b(G')} q^{k(G')}, \quad v, q > 0
\]

known as the random-cluster (RC) model \[22\]. Here, \(b(G')\) denotes the number of active edges and \(k(G')\) the resulting number of connected components in the subgraph \(G' \subseteq G\). Particular choices of \(q\) correspond to uniform spanning trees and random resistor networks \((v, q \to 0\)}
s.t. $q/v \to 0$), percolation ($q \to 1$), and the Ising model ($q = 2$). The connection to the corresponding expression for bond percolation [23] becomes more transparent noting that $v$ is related to the bond occupation probability $p$ as $v = p/(1-p)$. As $v$ is increased, a giant or percolating cluster appears in the system. For sufficiently large $q$, this transition is of first order, while for small $q$ it is continuous. For the square lattice exact results are available, and the transition occurs at coupling $v_c = \sqrt{q}$, remaining continuous up to (and including) $q_c = 4$ [24].

Starting from a configuration with all bonds activated, corresponding to $p = 1$, the successive random removal of bonds describes a fragmentation process. Deleting any given bond can result in a break-up. Since this is a bond removal, the break-up is binary and creates exactly one extra fragment. If removal leads to a break-up, the bond is called a bridge, otherwise it is internal or a non-bridge. We can imagine that in a comminution process energy is injected at a constant rate into the system and there is hence a spatially homogeneous probability of structurally damaging the fragments; not every such weakening leads to fragmentation, however, only parts with sufficiently fragile connections break off. In a similar way, this model can describe the breaking of chemical bonds in a polymeric system. The structural resilience under the removal of randomly chosen bonds then depends on the density $B$ of bridges among all remaining bonds $N$. Figure 1 shows the relative bridge density $\langle B/N \rangle$ for the RC model on the square lattice for different values of the cluster weight $q$. Incidentally, it is seen that the change of the relative bridge density and hence the change in fragility of the configuration becomes maximal at the critical coupling $p_c = \sqrt{q}/(1 + \sqrt{q})$. This is when a significant fraction of fragmentation events first appears; this effect can be understood in terms of the self-entanglement of critical clusters [26]. In particular, as will be shown below, the behavior of $\langle B/N \rangle$ near $p_c$ is governed by the specific-heat exponent $\alpha$, which implies a divergent slope for $q \geq 2$ [33].

We are hence interested in understanding the fragmentation kernel $a(s)b(s,s')$ of Eq. 2 specifically in the vicinity of the critical point. A scaling form $a(s) \sim s^\lambda$ is typically assumed in the context of the rate equation (1) and, indeed, this ansatz is found to describe well the behavior observed in a number of experimental situations [1]. From such data, there appears to be evidence for a range of different values $\lambda \leq 1$ for the homogeneity index, with a theoretically interesting shattering transition occurring as one crosses over to negative $\lambda$ [27]. To determine $\lambda$ for the critical RC model, consider the total number of bridges,

$$\sum_s s n_c(s) a(s) \sim \int s^{-\tau+1+\lambda} e^{-\kappa s} ds \sim L^{(\tau-\lambda)/(\sigma \nu)}, \quad (3)$$

where we have used the scaling form of the critical cluster size distribution, $n_c(s) \sim s^{-\tau} e^{-\kappa s}$ as well as the relations $c \sim |p - p_c|^{1/2}$ and $|p - p_c| \sim L^{-1/2}$ valid in the scaling regime [25], where $L$ is the linear dimension. From Fig. 1...
it appears that the density of bridges is asymptotically non-vanishing. This is seen more clearly in our results for the critical bridge-density shown in Fig. 2(a). Hence the average number of bridges in (3) must grow as $L^d$, implying $d = (\tau - \lambda)/\sigma \nu$. With the exponent identities $\sigma \nu = 1/d_F$ and $\tau = 1 + d/d_F$, where $d_F$ is the critical cluster fractal dimension, this shows that

$$\lambda = 1,$$

independent of $q$. Hence the breakup is spatially homogeneous. This confirms previous numerical results for the percolation limit $q \to 1$ [20, 28].

While this result appears to depend on the numerical observation of finite asymptotic bridge densities on the square lattice, it is in fact far more general. Using probabilistic percolation theory, it is possible to show that for the RC model on an arbitrary graph the bond and bridge densities $\langle B \rangle$ and $\langle N \rangle$, respectively, are related as [20]

$$\langle B \rangle = \frac{\langle N \rangle - p}{(1 - p)(1 - q)}$$

such that, in general, the bridge density is non-vanishing whenever the edge density is positive. The singular case $\langle N \rangle = p$ corresponds to the percolation limit $q \to 1$, for which a closer analysis shows that $\langle B \rangle$ still is finite. Hence the result (4) holds for the RC model on any graph for any bond probability $0 < p < 1$, on or off criticality. For the square lattice, the edge density of the critical RC model is $\langle N \rangle_c = 1/2$ [24], such that for this case we find the exact expression

$$\langle B \rangle_c = \frac{1}{2} \frac{1}{1 + \sqrt{q}},$$

generalizing a recent result for percolation [25]. Figure 2(a) shows our simulation data together with the asymptotic result (6). Relation (5) shows that the finite-size corrections to $\langle B \rangle$ are given by the corrections to the edge density $\langle N \rangle$, which in turn is related to the average number of bridges in (3) must grow as $L^d/\sigma \nu$. Standard scaling arguments lead to

$$u_L = u_\infty + A u L^{-\kappa} + o(L^{-\kappa}),$$

where $\kappa = (1 - \alpha)/\nu = d - 1/\nu$. Our data for the finite-size corrections to the density of bridges are in perfect agreement with these calculations, see the fit results in Fig. 2(b). As a consequence of the relation (5) between bridge and edge density, it is straightforward to show that the $p$-derivative of $\langle B \rangle(p)$ has a power-law singularity at the critical point $p_c = \frac{1}{\sqrt{q}/(1 + \sqrt{q})}$. This singularity is governed by the specific-heat exponent $\alpha$ which, for the square-lattice model is given by $\alpha/\nu = (4q - 12)/q$ with the Coulomb gas coupling $q = 4 \cos^2(\pi g/4)$. Similar results can be derived for the density $\langle C \rangle$ of non-bridges [20].

Cluster break-up rates are hence proportional to the cluster size. The typical size of fragments created in a break-up is encoded in the probability $b(s', s)$ of creating a fragment of size $s'$ on fragmenting a cluster of size $s$. The scale-free nature of the critical RC model suggests a large-$s$ scaling form

$$b_{s', s} \sim s^{-\phi} \mathcal{G}\left(\frac{s'}{s}, \frac{s}{L^{d_F}}\right),$$

which is compatible with exact results for percolation in 1D and on the Bethe lattice [18]. The value of $\phi$ can be related to recently established critical exponents. To this end, we first multiply Eq. (6) by $s'$ and then integrate to find that $\mu_s \sim s^{2-\phi} \mathcal{H}(s/L^{d_F})$ and then use a finite-size scaling form of the overall cluster-size distribution [30] to conclude that the scaling of the ensemble average daughter cluster size is

$$\langle s' \rangle \sim L^{d_F(3 - d / d_F - \phi)}.$$
shown that \( C_{\text{min},2} \sim L^{d-v-x_2} \), which implies

\[
\phi = 2 + (x_2 - d)/d_F = 2 - d_R/d_F,
\]

where \( d_R = d - x_2 \) is known as the red-bond fractal dimension. Again, this confirms and generalizes previous results for bond percolation \([19, 28]\). Another special case concerns the uniform spanning tree ensemble \( v, q \to 0 \) with \( q/v \to 0 \) for which \( \phi \to 11/3 \), in agreement with results in Ref. \([21]\). As the data in Fig. 4(a) show, our extensive numerical simulations for the full range \( 0 \leq q \leq 4 \) are in perfect agreement with these arguments. More generally, Fig. 4(a) demonstrates the validity of the scaling form of Eq. (8), showing an excellent collapse of data for different cluster and system sizes onto scaling functions depending on universality classes parameterized by the cluster coupling \( q \). Notably, in contrast to recent claims in Ref. \([32]\), it is found here for the RC model that a break-up into segments of equal size is the least likely event.

This completes our analysis of the fragmentation properties of critical clusters of the RC model. We now turn to the investigation of kinetic fragmentation processes to understand the relevance of these results for dynamic fragmentation. Consider such a process starting from a configuration with macroscopic structures, i.e., at or above the percolation threshold in the RC model. Successive random bond removal then drives the system through the critical point, and ultimately into a configuration where all fragments only consist of one vertex. For real fragmentation processes, it is more realistic to assume the existence of a critical particle size \( s_c \) below which there is no further break-up \([1]\). This could come about, for instance, through the flow conditions for the break-up of droplets in liquids or through the chosen geometry in a milling setup. Limited fragmentation has been studied for simpler geometries such as intervals and trees \([15, 16]\). The final distribution of fragment sizes below the cutoff \( s_c \) found for the two-dimensional RC model is shown in Fig. 4(a) for fragmentation processes starting from the giant component of a critical percolation configuration \( (q \to 1) \). Over a range of fragment sizes increasing with \( s_c \), the data clearly follow a power-law. Additionally, the dependence on \( s_c \) is only via the ratio \( s/s_c \), resulting in a scaling form

\[
n_{s_c}(s, \infty) \sim s^{-\chi} F \left( \frac{s}{s_c} \right),
\]

with a dynamic fragmentation exponent \( \chi \). Figure 4(b) summarizes the result of power-law fits to the decay displayed in Fig. 4(a) for different cluster weights \( q \). For sufficiently large cutoffs, we find that \( \chi \) coincides with the exponent \( \phi = 2 - d_R/d_F \) characteristic of equilibrium fragmentation. The deviations for \( s_c/L^2 \ll 1 \) are an effect of the scaling function \( F \) of Eq. (10). Moreover, not only the power-law decay but the full scaling form (10) of the final fragment distribution is fully supported by our data, as is illustrated in the scaling collapse shown in the inset of Fig. 4(a).

While the close relation of a dynamical fragmentation protocol with critical equilibrium properties is at first surprising, it can be understood from the nature of the break-up process. Due to the shape of the breakup kernel shown in Fig. 3 the fragmentation process is dominated by “abrasive” events, i.e., daughter clusters that are small compared to the initial cluster. Representing the fragmentation events in a genealogical tree, we indeed typically find one long branch, related to the erosion of the giant component, with sub-branches of only a few steps \([24]\). In contrast, if the breakups occurred in a uniform way then one would obtain a statistically balanced genealogical tree as discussed in [10]. As a consequence, we find that the basic assumption in the mean-field model \([1]\), taking the break-up kernel \( c(s, s') = a(s)b(s, s') \) to be independent of time turns out to be a rather accurate description for iterative fragmentation of the critical RC model.

Studying the fragmentation properties of critical configurations in the random-cluster model, we have given a
rather complete description of the scaling behavior. The
density of fragmenting edges is independent of cluster
size, implying $\lambda = 1$. The daughter size function
assumes a scaling form with a scaling index connected to
the two-arm exponent of the model. A number of further
conclusions following from the general result [5] will be
discussed elsewhere [26]. Investigating the asymptotic
size distribution under fragmentation with a cutoff $s_c$
starting from fractal initial conditions, we find that this
non-equilibrium process is determined by the equilibrium
critical behavior with a final fragment size distribution
described by the equilibrium exponent $\phi$. The distribu-
tion of fragments hence reveals the structure of the ini-
tially fragmented object. The insensitivity to microscopic
details implied by the universality of critical phenomena
thus indicates that our results for dynamic fragmenta-
tion should be widely applicable also to the fragmenta-
tion of fractal structures in experiment. In fact, we find
that the size exponents found in experimentally observed
fragment distributions as referred in Ref. [1] are a sub-set
of the behavior described by the random-cluster model, cf.
the shaded area of Fig. 1(b).

The discussion above is restricted to the case of bi-
ary fragmentation effected through the removal of single
bonds. A more general situation occurs for the deletion of
vertices producing up to $z$ fragments in each break-up
event, where $z$ is the coordination number of the
lattice. For this situation we find that the binary branch is
still strongly dominant. Preliminary investigations indi-
cate a connection between the statistics of such break-up
events and generalizations of Eq. (8), where the scaling
exponents $\phi^k = 2 - (d - x_k)/d_F$ of break-ups with $k$
fragments are governed by the corresponding multi-arm
exponents $x_k$, discussed in Ref. [20].

Generalizations of the numerical results to three-
dimensional lattices are straightforward. In fact, we have
studied the fragmentation of clusters of Eq. (2) on the
simple cubic lattice and found $\lambda = 1$ as well as values of $\phi$
compatible with the few previous results for $d_F$ in the 3D
random-cluster model. For the dynamical fragmentation
process, we find that fragmenting solid instead of fractal
objects in two and three dimensions also leads to alge-
braically decaying size distributions, however governed
by a different set of exponents [25]. Beyond the impli-
cations of the present work for fragmentation processes
in nature and industry, an exciting extension concerns the
fragmentation of random graphs and networks with
promises of valuable conclusions concerning resilience.

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