A Hamiltonian approach for explosive percolation

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We introduce a cluster growth process that provides a clear connection between equilibrium statistical mechanics and an explosive percolation model similar to the one recently proposed by Achlioptas et al. [Science 323, 1453 (2009)]. We show that the following two ingredients are essential for obtaining an abrupt (first-order) transition in the fraction of the system occupied by the largest cluster: (i) the size of all growing clusters should be kept approximately the same, and (ii) the inclusion of merging bonds (i.e., bonds connecting vertices in different clusters) should dominate with respect to the redundant bonds (i.e., bonds connecting vertices in the same cluster). Moreover, in the extreme limit where only merging bonds are present, a complete enumeration scheme based on tree-like graphs can be used to obtain an exact solution of our model that displays a first-order transition. Finally, the proposed mechanism can be viewed as a generalization of standard percolation that discloses an entirely new family of models with potential application in growth and fragmentation processes of real network systems.

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The second-order critical point of percolation [1, 2] has been successfully used to describe a large variety of phenomena in Nature, including the sol-gel transition [3], or incipient flow through porous media [4], as well as epidemic spreading [5] and network failure [6–9]. A long standing question of practical interest has been since, how the transition could be made more abrupt and in the limit become even of first-order. In other words, what ingredient must be tuned in the basic model of random percolation to change the order of the transition?

Recently Achlioptas et al. [10] proposed a new mechanism on random graphs which they termed “explosive percolation” that exhibits first-order phase transition. Their process takes place in successive steps, with bonds being added to the system in accordance to a selection rule. At each step, a set of two unoccupied bonds are chosen randomly. From these two, only the one with minimum weight becomes occupied. In Ref. [10], the weight is defined as the product of the sizes of the clusters connected by this bond (this is called “product rule”). Importantly, if the bond connects two sites that already belong to the same cluster, the weight is proportional to the square of the cluster size. Since unoccupied bonds connecting vertices in the largest cluster have the largest possible weight, these bonds will become occupied only if two of them are randomly chosen. Thus, this selection rule hinders the inclusion of bonds connecting vertices that already belong to the largest cluster. As a consequence, bonds merging two smaller clusters will be selected more frequently, resulting in the fast growth observed. Their model was then implemented on a fully connected graph, however, it was shown that the same effect takes place on 2D square lattices [11] as well as scale-free networks [12, 13].

In this letter we investigate what are the basic principles that lead to the first-order phase transition observed in the explosive percolation model. First we name merging bonds those edges that connect vertices in distinct clusters, while redundant bonds are edges connecting vertices in the same cluster. We show that two conditions are necessary for obtaining a first-order transition in a growth process where bonds are included one by one, namely, the process has to favor the inclusion of bonds that keep all the clusters at about the same size, and the process has to preclude the introduction of redundant bonds, at least below the critical point. More precisely, merging bonds must be introduced with much higher

FIG. 1: Two ingredients for explosive percolation. Here we show a possible configuration for a growth process where, at each step, any unoccupied bond can be introduced in the graph. For instance, in this figure we show three bonds that could be added in the next step, namely, α, β, and γ. The two ingredients for obtaining a sharp transition are the following: (i) α is not accepted due to condition (ii), β is not accepted due to condition (i), and the most probable is the γ bond.
probability than redundant bonds. In Fig. 1 we show a pictorial description of these two ingredients.

In order to validate our hypothesis, we propose an extension of the percolation model that describes a general growth process in the space of graphs. For this, we define a Hamiltonian that depends on the graph $G$ describing the network. The probability of finding the system in a certain state $G$ will be given by $P(G) = Z^{-1} \exp(-\beta H(G))$, where $Z = \sum_G \exp(-\beta H(G))$. A simple form for a Hamiltonian that includes the two ingredients is

$$H(G) = \sum_{i \in C} s_i^2 + \ell_i s_i^\alpha,$$  \hspace{1cm} (1)

where the sum is over the entire set of clusters $C$, $s_i$ is the number of vertices in cluster $i$, and $\ell_i$ is the number of redundant bonds added to this cluster. If the number of bonds in the cluster is $b_i$, we have $\ell_i = 1 + b_i - s_i$. Note that each time one includes a redundant bond, one also closes a new loop in the cluster, thus $\ell_i$ is also a measure for the number of loops in the cluster.

We can now simulate a process of cluster growth controlled by the Hamiltonian of Eq. (1). This is performed by starting with a network of $N$ vertices without bonds, so each vertex initially belongs to a different cluster. At each step, a new bond can be placed between any pair of vertices not yet connected. The probability of including a particular bond $b$ is given by $P_b \sim \exp(-\beta \Delta H_b)$, where $\Delta H_b$ is the energy change after including this bond. Such a growth model emulates equilibrium configurations of graphs following the Eq. (1) and having a given number of bonds $N_b$. However, since the removal/rewiring of bonds is not considered during growth, this corresponds to an out-of-equilibrium process. Consequently, some differences should be expected between the observed results and the actual thermal equilibrium.

For small values of $\alpha$, redundant bonds are favored over merging bonds, while for large values of $\alpha$ the opposite takes place. Let us investigate the asymptotic behavior in the two different scenarios. If redundant bonds are favored, one might expect that a new merging bond will be included only after the addition of all possible redundant bonds. Since clusters of equal size minimize Eq. (1), we can assume that, for low temperatures, all clusters have about the same size $S$, so that fully connected sub-graphs with $S(S-1)/2$ bonds are formed with $\ell = (S-1)(S-2)/2$. After adding the next bond, two of these clusters shall merge to form a new largest cluster, into which redundant bonds can be included. At this point we can calculate the energy variation for a redundant bond, $\Delta H_r = (2S)^\alpha$, and for a merging bond between pair of clusters, $\Delta H_m = 2S^2 + (S-1)(S-2)(2^\alpha - 1)S^\alpha$. Surprisingly, for any value of $\alpha$, in the asymptotic limit of very large clusters, $S \rightarrow \infty$, merging bonds have higher energy variation than redundant bonds, and the growth process with fully connected clusters is stable.

The situation becomes quite different when the presence of merging bonds is favored. As before, we use that all clusters have approximately the same size $S$. However, without redundant bonds, the clusters are all treelike with exactly $S-1$ bonds, and $\ell = 0$. At this point, we have $\Delta H_r = S^\alpha$, and $\Delta H_m = 2S^2$. Thus, for large $S$, the inclusion of merging bonds will lead to smaller energy variations, as long as $\alpha > 2$. We then conclude that, in the large cluster limit, $S \gg 1$, both scenarios are stable for $\alpha > 2$.

The evolution of the system towards tree-like or fully connected clusters is determined at the beginning of the growth process. Considering that $S = 3$ represents the minimal size necessary for the inclusion of a redundant bond, we obtain $\Delta H_r = 3^\alpha$ and $\Delta H_m = 2 \times 3^2 = 18$. Thus, merging bonds become more probable when $\alpha > \ln(18)/\ln(3) = 2 + \ln(2)/\ln(3) \approx 2.63$, which corresponds to a threshold condition above which the system exhibits an abrupt transition. One should note that this is an approximate result, since we do not account for fluctuations in the cluster size distribution. However, as shown in Fig. 2, the results for $\alpha = 2.5$ and 2.7 indeed confirm the change in behavior from a sharp transition for the larger value of $\alpha$ to a slow continuous growth for the smaller value. Note also that the threshold value for $\alpha$ is not universal and could be readily changed by adding a multiplicative constant to any of the two terms constituting the Hamiltonian of Eq. (1). In the inset of Fig. 2, we show the dependence of the fraction of redundant bonds $N_r = N_b/N$ on the average connectivity of the network $k$. As one can see, for $\alpha = 2.7$, the inclusion of redundant bonds is delayed up to $k \approx 2$, confirming that the system
is in the tree-like regime.

Let us examine in more detail the scenario for a small value of $\alpha = 2.0$. In Fig. 3 we show that the fraction occupied by the largest cluster $P_\infty$ systematically increases with the average connectivity $k$, with a growth rate that decreases with system size $N$. The inset of Fig. 3 shows the same results, but for the size of the largest cluster $S = N P_\infty$. One can see that $S$ follows approximately a linear growth with the connectivity $k$. In this scenario, a merging bond is expected to be placed only when all clusters become saturated with redundant bonds. If we now use that all clusters have the same size $S$, we obtain $k = S - 1$, which corresponds to the dotted line in the inset. The deviations of the numerical results from this prediction should be expected. In the growth model, the merging of two clusters can only double the value of $S$, so that the values of $S$ at the plateaus observed in the curves are approximately powers of two. However, we see that the curves always approach the dotted line before doubling $S$. This linear growth for $P_\infty$ with a slope that decays with the system size $N$, indicates that, in the thermodynamic limit, this system does not undergo a percolation transition, namely, $P_\infty = 0$ for any finite value of $k$.

Figure 4 shows results for $\alpha = 3.0$. Here we are in the scenario where the clusters grow as loopless trees. In this case, the system undergoes a transition that becomes sharper as the number of vertices $N$ increases. Again, if we assume that the system is divided in trees of the same size $S$, we obtain $S = 2(2 - k)$, as indicated by the dotted line in the inset. As before, the size $S$ increases in steps due to the out-of-equilibrium nature of the growth process. Strikingly, the theoretical relation for the equilibrium state still provides a consistent prediction for the lower bound of the largest cluster size. Since $S$ remains finite for any $k < 2$, and at the critical point $k = 2$ a tree that spans all the system is formed, it follows that the order parameter $P_\infty$ displays a first-order transition in the thermodynamic limit.

As already mentioned, this growth process bears some differences with a thermal equilibrium state of graphs with the proposed Hamiltonian Eq. (1) at low temperatures. In fact, for $k \to 2$ there is always an energy gain in breaking large trees in smaller highly connected graphs. One may then ask whether the sharp transition observed in the simulations is just a feature of the ir-
reversible growth process or could be reproduced in an equilibrium statistical framework. We now show that in the limit of large $\alpha$ we can obtain an exact equilibrium solution that exhibits a first-order transition.

If we impose that all clusters in the system are loopless trees, $\alpha \to \infty$, it is possible to enumerate all possible ways in which the network can be divided in a set of clusters of a given size. Let $\Omega$ represent the number of ways that a fully connected graph can be divided in trees with $n_i$ trees of size $i = 1, 2, 3...$ We then have

$$\Omega = N! \prod_s \left( \frac{T_s}{s!} \right)^{n_s} \frac{1}{n_s!},$$

(2)

where $N$ is the total number of vertices in the network, and $T_s$ is the number of trees that span a fully connected graph of size $s$, given by Cayley’s formula, $T_s = s^{s-2}$ [14]. Since all clusters are trees, we can relate the number of clusters $N_c$ with the system size $N$ and the average connectivity $k$ as $N_c = N(1 - k/2)$. Therefore, given a fixed value of $k$, the values of $n_s$ obey the following two constraints: $\sum n_s = N_c$ and $\sum s n_s = N$, where the sum is over all possible cluster sizes $s$. In our generalized percolation model, we still need to impose a fixed energy value, $\sum E_s n_s = E$, where $E_s = s^2$ is the energy of a tree with size $s$. Using Lagrange multipliers, $\eta$, $\lambda$, and $\beta$ to deal with each of these constraints, we can find the cluster size distribution that maximizes $\Omega$,

$$n_s = e^{\eta - \beta s^2 - \lambda s^{s-2} - \lambda},$$

(3)

The critical condition takes place when the distribution Eq. (3) diverges. One can verify that, for $\beta = 0$, this happens when $\lambda = \lambda_c (\beta = 0) = 1$. The critical connectivity can then be determined as

$$k = 2 \left( 1 - \frac{N_c}{N} \right) = 2 \left( 1 - \frac{\sum n_s}{\sum s n_s} \right),$$

(4)

yielding $k_c = k(\lambda_c = 1, \beta = 0, \eta \to \infty) = 1$. Note that, at the critical condition $n_s \sim s^{-3/2}$, the fraction occupied by the largest cluster follows $P(\infty) = k - k_c$, thus reproducing the known critical properties of the standard Erdos-Renyi model [15].

For $\beta > 0$, the distribution always converges unless $\lambda \to -\infty$. From Eq. (4), we obtain that $k_c = k(\lambda \to -\infty, \beta, \eta \to \infty) = 2$. For $k < k_c$ all clusters are finite trees, therefore occupying a vanishing fraction of the network. At $k = k_c = 2$, a giant tree spans the entire network, characterizing a first-order transition. Of course, this simple approach to the problem is only possible due to the imposition of tree-like clusters. The general enumeration of connected graphs with any number of redundant bonds is not a simple task [16], and the cluster size distribution in this generalized condition might be quite different. However, at least in the situation where redundant bonds are not present, explosive percolation can be duly explained within the framework of equilibrium statistical mechanics.

In summary, we have shown that two simple conditions, namely, the absence of loops and the imposition of clusters of similar sizes, are the only necessary ingredients for a percolation process to display first-order transition in the size of the infinite cluster as function of the average degree of the network. We argue that both conditions are implicitly present in the explosive percolation model proposed in Ref. [10]. We emphasize that these conditions are essentially non-local, namely, the probability of adding a particular bond depends on the global structure of the graph. Moreover, our model provides a simple connection between explosive percolation and equilibrium statistical physics, leading to a clear interpretation of the mechanisms behind this growth process. Finally, other possibilities for the energy function can also be investigated in different contexts, revealing a whole new family of percolation-like models.