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Hamiltonian approach for explosive percolation

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We present 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 D. Achlioptas *et al.* [Science **323**, 1453 (2009)]. We show that the following two ingredients are sufficient 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 treelike graphs can be used to obtain an exact solution of our model that displays a first-order transition. Finally, the presented mechanism can be viewed as a generalization of standard percolation that discloses a 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 [4,5], as well as epidemic spreading [6] and network failure [7–10]. 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.* [11] 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 is chosen randomly. From these two, only the one with minimum weight becomes occupied. In Ref. [11], 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 two-dimensional square lattices, random networks, as well as scale-free networks [12–16].

In this Rapid Communication we investigate what are the sufficient conditions 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 sufficient 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 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

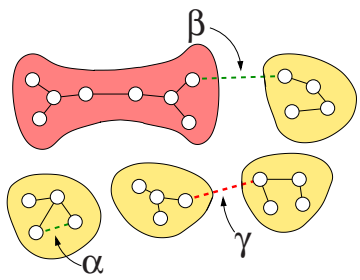

FIG. 1. (Color online) Two ingredients for explosive percolation. Here we show a possible configuration for a growth process where, at each step, any unoccupied bond can be introduced in the graph. For instance, in this figure we show three bonds that could be added in the next step, namely, α, β, and γ. The two ingredients for obtaining a sharp transition are the following: (i) bonds that keep the clusters approximately at the same size are favored over bonds that result in larger size discrepancies; and (ii) bonds that connect vertices in the distinct clusters (*merging bonds*) are favored over bonds that connect vertices in the same cluster (*redundant bonds*). Thus, among the bonds indicated, α has the smallest probability due to condition (ii), β is not accepted due to condition (i), and the most probable is the γ bond.

$Z=\Sigma_G \exp[-\beta H(G)]$. A simple form for a Hamiltonian that includes the two ingredients is

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

where the sum is over the entire set of clusters $\mathbf{C}$, s_i is the number of vertices in cluster i, and ℓ_i is the number of redundant bonds added to this cluster. If the number of bonds in the cluster is b_i, we have $\ell_i=1+b_i-s_i$. The parameter α controls the probability of redundant bonds being added to the system. Note that without redundant bonds the clusters are loopless trees; thus, for α large enough one should reach a state of treelike percolation.

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 $\Pi_b \sim \exp(-\beta \Delta H_b)$, where ΔH_b is the energy change after including this bond. The implementation of the present model is substantially different from the Achlioptas process since at each step all unoccupied connections can potentially be chosen, albeit some with much larger probabilities than others. Such a growth model emulates equilibrium configurations of graphs following 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.

In order to determine whether or not redundant bonds will be included in the system we should first investigate the asymptotic behavior in the two different scenarios. For small values of α, redundant bonds are favored over merging bonds, and 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 β high enough, all clusters have about the same size S. We also assume that clusters are fully connected subgraphs with $S(S-1)/2$ bonds, and $\ell=(S-1)(S-2)/2$. 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, $\Delta H_m=2S^2+(S-1)(S-2)(2^\alpha-1)S^\alpha$. For any value of α, in the asymptotic limit of very large clusters, $S \to \infty$, 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 α is large and redundant bonds are not included. 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 $\alpha>2$.

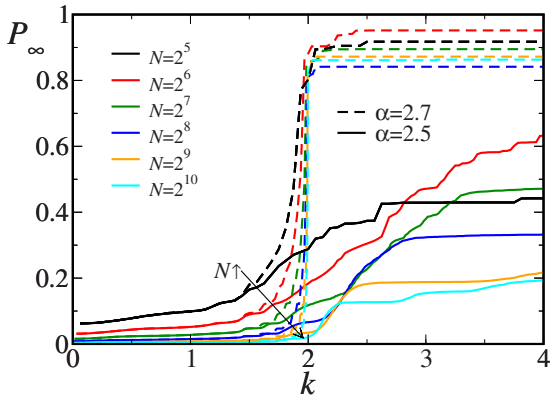

FIG. 2. (Color online) Transition to explosive percolation. When the process favors redundant bonds, $\alpha=2.5$, the largest cluster follows a slow continuous growth for the largest cluster. When the merging bonds are favored, $\alpha=2.7$, the system displays an abrupt transition around a critical connectivity $k=2$. In this case the transition becomes sharper as the system size increases, suggesting a first-order transition type of behavior. The inset shows the total number of redundant bonds divided by the number of vertices in the network, $N_r=N_b/N$. For $\alpha=2.7$, redundant bonds are not included before $k=2$. In all simulations, we use $\beta=1.0$ and take an average over 1000 realizations of the growth process.

The evolution of the system toward treelike 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 α to a slow continuous growth for the smaller value. Note also that the threshold value for α 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 treelike 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_∞ 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 $S=NP_\infty$. 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 about 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

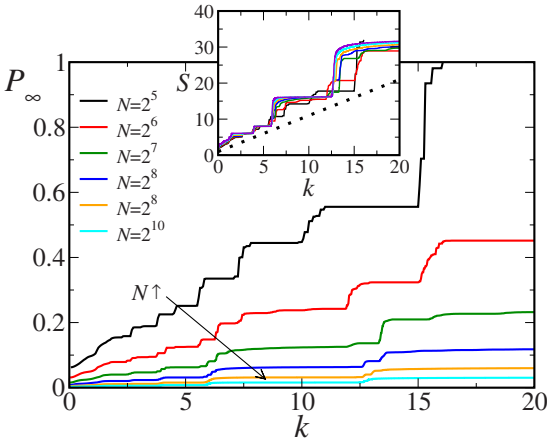

FIG. 3. (Color online) Growth process when redundant bonds are favored. Here we show results for $\beta=1.0$ and $\alpha=2.0$. Since in this situation merging bonds are less likely to be included, the graph has to reach states where it splits in several fully connected subgraphs, before a new merging bond is introduced. When the merging bond is included, a new and larger cluster is created. This explains the presence of discontinuous jumps in the size of the largest cluster. Assuming that the system consists of only fully connected clusters of the same size, we obtain the dotted line shown in the inset, $S=k+1$. This condition corresponds to the minimum bound for the simulation results, that approximately follows this theoretical prediction. Since the largest cluster S is finite for any finite connectivity k, the system does not display a percolation transition.

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_∞ 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 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_∞ 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 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 irreversible growth process or could be reproduced in an equilibrium statistical framework.

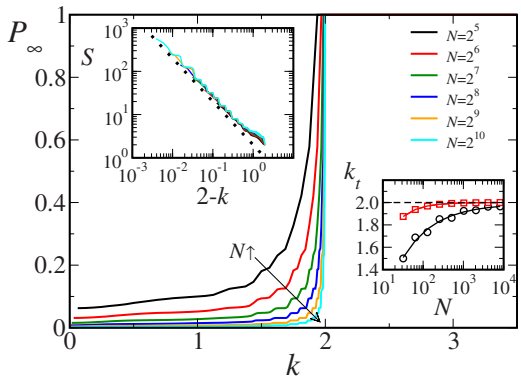

FIG. 4. (Color online) Growth process when merging bonds are favored. For $\beta=1.0$ and $\alpha=3.0$, the system does not include redundant bonds and all clusters remain treelike until the critical point $k_c=2$ is reached. Supposing that the system comprises only clusters of the same size S, we have that $S=2/(2-k)$ for the case of trees. This relation works as a minimum bound for the simulation results, as shown in the inset on the left. Thus we have the critical condition $k_c=2$, where the size of the largest cluster diverges to occupy the whole network. For $k<k_c$ the largest cluster remains finite and its occupation fraction P_∞ goes to zero as the system size grows, characterizing a typical first-order transition. The inset on the right shows the threshold connectivity k_t to obtain a largest cluster greater than the square root of the system size, $S>N^{1/2}$ (black circles), and greater than half the system size, $S>N/2$ (red squares). The red line follows $k=2-4/N$, the expected behavior for the connectivity where $S=N/2$. The black line is a fit of the form $k=p_1+p_2\times N^{-p_3}$, with $p_1=1.99\pm0.03$, $p_2=3.14\pm0.02$, and $p_3=0.53\pm0.05$. In the limit $N\to\infty$ both curves converge to $k\approx 2$, that is in the thermodynamic limit we observe at $k=2$ a discontinuous transition in the order parameter from a vanishing fraction, $P_\infty\sim N^{-1/2}$, to a finite fraction, $P_\infty=1/2$, confirming the approach to a first-order transition.

We now show that in fact in the limit of large α 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 Ω represent the number of ways that a fully connected graph can be divided in trees with n_i trees of size $i=1,2,3\ldots$ We then have

$$\Omega = N!\prod_s \left(\frac{T_s}{s!}\right)^{n_s}\frac{1}{n_s!}, \tag{2}$$

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, $T_s=s^{s-2}$ [17]. 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: $\Sigma n_s=N_c$ and $\Sigma s n_s=N$, where the sum is over all possible cluster sizes s. In our generalized percolation model, we still need to impose a fixed energy value, $\Sigma E_s n_s=E$, where $E_s=s^2$ is the energy of a tree with size s. Using Lagrange multipliers, η, λ, and β to

deal with each of these constraints, we can find the cluster size distribution that maximizes Ω,

$$n_s = e^{\eta - \beta s^2 - \lambda s} \frac{s^{s-2}}{s!}. \quad (3)$$

The critical condition takes place when 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

$$k = 2\left(1 - \frac{N_c}{N_s}\right) = 2\left(1 - \frac{\sum n_s}{\sum s n_s}\right), \quad (4)$$

yielding $k_c=k(\lambda_c=1,\ \beta=0,\ \eta\to\infty)=1$. Note that, at the critical condition $n_s \sim s^{-5/2}$, 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 [18].

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 treelike clusters. The general enumeration of connected graphs with any number of redundant bonds is not a simple task [19], 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.

Finally, it is important to consider the effect of lower dimensionalities in the growth process. We performed simulations of our model with the vertices placed on a square lattice and with connections allowed only between nearest neighbors. For large values of the parameter α, the results are essentially the same, implying that independent on the dimensionality of the underlying lattice, an abrupt transition is observed at $k_c=2$, and the size of the largest cluster diverges as $(k_c-k)^{-1}$ (data not shown). For lower values of α we also obtain results similar to those of a fully connected graph, however, on a square lattice, there is an upper limit for the connectivity $k_{\max}=4$. Therefore, the size of the largest cluster remains finite until the saturation is reached at $k=4$, where all bonds are included in the lattice.

In summary, we show that two simple conditions, namely, the absence of loops and the selection of graphs divided in clusters of similar sizes, are sufficient ingredients for a percolation process to display first-order transition in the size of the infinite cluster as a function of the average degree of the network. We argue that both conditions are implicitly present in the explosive percolation model proposed in Ref. [11]. However, the present process bears relevant differences with Achlioptas' product rule. In particular the cluster size distribution in Achlioptas' process displays a heavy tailed power-law behavior [15], that would normally be a signature of a second-order transition, and is not reproduced in our model unless in the trivial case $\beta\to0$. We emphasize that the sufficient conditions are essentially nonlocal; 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 family of percolationlike models.

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