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Cluster aggregation model for discontinuous percolation transitions

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The evolution of the Erdős-Rényi (ER) network by adding edges is a basis model for irreversible kinetic aggregation phenomena. Such ER processes can be described by a rate equation for the evolution of the cluster-size distribution with the connection kernel $K_{ij} \sim ij$, where ij is the product of the sizes of two merging clusters. Here we study that when the giant cluster is discouraged to develop by a sublinear kernel $K_{ij} \sim (ij)^{\omega}$ with $0 \leq \omega < 1/2$, the percolation transition (PT) is discontinuous. Such discontinuous PT can occur even when the ER dynamics evolves from proper initial conditions. The obtained evolutionary properties of the simple model sheds light on the origin of the discontinuous PT in other nonequilibrium kinetic systems.

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Irreversible cluster aggregations are widespread phenomena occurring in a diverse range of fields, including dust and colloid formation, aerosol growth, droplet nucleation and growth, gelation transition, etc. [1]. The Smoluchowski coagulation equation [2–4] can successfully describe such cluster aggregation processes. In linear polymerization, molecules with two reactive ends can react to form long chains. In this case, the reaction kernel is given as $K_{ij}=1$, where i and j are the masses of the two reactants. For the aggregation of branched polymers, the reaction kernel has the form $K_{ij}=(ai+b)(aj+b)$, where a and b are constants. When clusters have a compact shape, the reaction kernel has the form $K_{ij} \sim (ij)^{1-1/d}$, where d is the spatial dimension. Intensive studies have been carried out using the Smoluchowski coagulation equation with such different kernel types [1,5–8], and it is known that sol-gel transitions can occur at either finite or infinite transition points. They are continuous transitions.

During the past decade, the evolution of complex networks has been of much interest to the science communities in multidisciplinary fields. To study percolation transition (PT) during network evolution, the branching process approach [9,10] and the Potts model formalism [11] have been used. Such complex network evolution can also be viewed as a cluster aggregation phenomenon and can be studied by the rate-equation approach [6]. For example, in the evolution of the classical random network, called the Erdős-Rényi (ER) model [12], an edge is added at each time step, thereby either connecting two separate clusters (intercluster edge) or increasing the edge number in one cluster without changing cluster numbers (intracluster edge). Figure 1 shows that the frequency of intercluster connections is dominant until the percolation threshold. Thus, the cluster aggregation picture of the ER network evolution comes in naturally. In this Rapid Communication, we extend the cluster aggregation dynamics in networks to more general cases. Specifically, the model is as follows: in a system composed of N vertices, we perform the following tasks at each time step:

(i) Two clusters of sizes i and j are chosen with probabilities q_i and q_j, respectively. The two clusters can be the same. Probability q_i is given as $k_i/\Sigma_s k_s n_s$, where k_i and n_i are the weight and density of an i-sized cluster, respectively.

(ii) Two vertices are selected randomly one each from the selected clusters. If they are not yet connected, then they are connected by an edge. If they are already connected, we choose another pair of vertices in the same manner until a link can be added. Self-loop cases are excluded.

We repeat these simple steps until a given time $t \equiv L/N$, where L is the number of edges added to the system, is tuned. This model is called the cluster aggregation network model hereafter. In this model, the two selected clusters can be the same, and thus, the evolution can proceed even after one giant cluster remains. The ER network corresponds to the case $k_i=i$. Here, we show that when the weight is sublinear, as $k_i=i^{\omega}$ with $0 \leq \omega < 1/2$, a discontinuous PT occurs at a finite transition point. Moreover, under certain initial conditions, the ER dynamics also exhibits a discontinuous PT. This result is reminiscent of the explosive PT recently observed in the ER [13] and other networks [14–18] under the so-called Achlioptas process, in which the development of giant component is discouraged during the evolution process. Since the cluster aggregation network model evolves by single-edge dynamics, as compared with the ER network under the Achlioptas process, which involves a pair of edges at each time step, it motivates us to study the underlying mechanism of the discontinuous PT analytically via the cluster aggregation network model.

The cluster aggregation processes in the model are described via a rate equation for the cluster density, which takes the following form in the thermodynamic limit:

$$\frac{dn_s(t)}{dt} = \sum_{i+j=s} \frac{k_i n_i}{c(t)} \frac{k_j n_j}{c(t)} - 2\frac{k_s n_s}{c(t)}, \tag{1}$$

where $c(t)=\Sigma_s k_s n_s(t)$. The connection kernel $K_{ij} \equiv k_i k_j / c^2$. The first term on the right-hand side represents the aggrega-

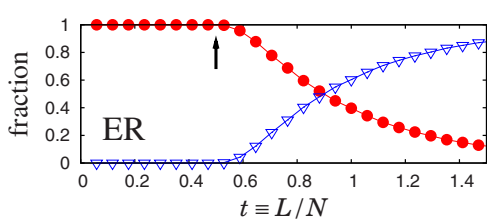

FIG. 1. (Color online) The fraction of each type of attached edges, intercluster (●) or intracluster (▽) edges for the ER model. Arrow indicates percolation threshold at $t_c=1/2$.

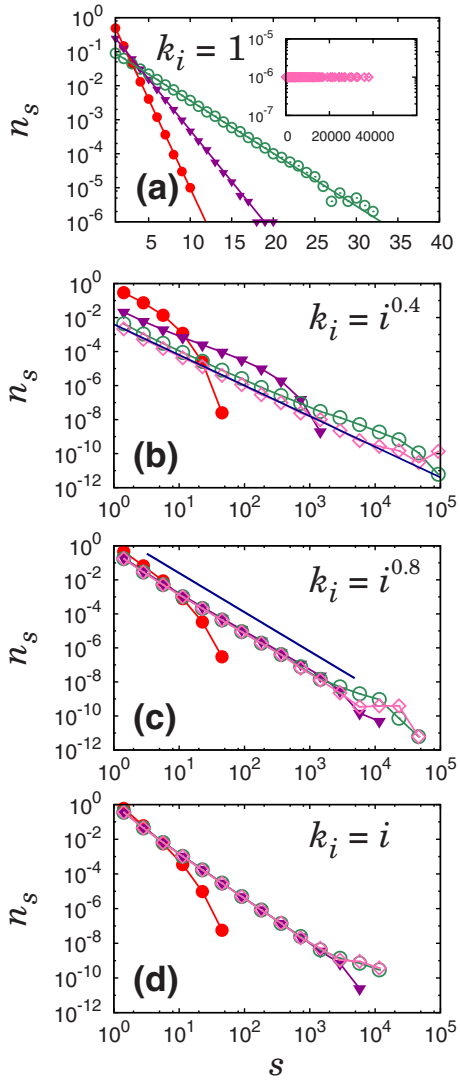

FIG. 2. (Color online) The cluster-size distributions of the cluster aggregation network models with (a) $k_i=1$, (b) $k_i=i^{0.4}$, (c) $k_i=i^{0.8}$, and (d) $k_i=1$ (ER model) with monodisperse initial condition. (a) is drawn in semilogarithmic scale, while the others are in double-logarithmic scales. Data points in (a) are at $t/t_c=0.3$ (●), 0.5 (▽) and 0.7 (○), and in (b)–(d) they are obtained at $t/t_c=0.50$ (●), 0.95 (▽), 0.998 (○), and 1.003 (◇). Data points in the inset of (a) are at $\delta=1-t=10^{-4}$. In (b), there exists a hump for data points (○). The system size N is taken as 10^6 for (a) and 10^5 for (b)–(d). Solid lines in (b) and (c) represent analytic formulas (4).

tion of two clusters of sizes i and j with $i+j=s$ and the second term represents a cluster of size s merging with another cluster of any size. The rate equation differs from the Smoluchowski coagulation equation in two aspects. First, the connection kernel is time dependent through $c(t)$ when $\omega \neq 1$. Second, the second term on the right-hand side of Eq. (1) includes the process of merging with an infinite-size cluster. Hence, Eq. (1) with $\omega=1$ and $c=1$ describes the ER process, while the conventional Smoluchowski coagulation equation with $\omega=1$ does not because only sol-sol reactions are taken into account. However, the case including the infinite-size cluster in the Smoluchowski coagulation equation was also considered in Ref. [6], which was called the F

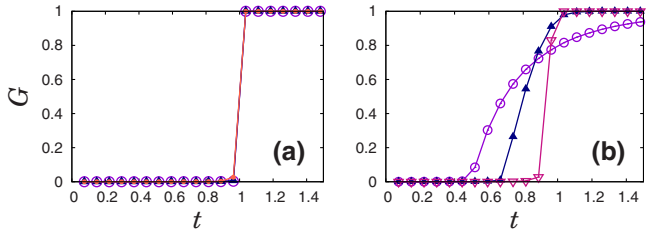

FIG. 3. (Color online) The giant cluster size G versus time t showing (a) discontinuous transitions in $k_i=1$ (○), $k_i=i^{0.2}$ (△), $k_i=i^{0.4}$ (●), and (b) continuous transitions in the cluster aggregation network model $k_i=i^{0.6}$ (▽), $k_i=i^{0.8}$ (△), and the ER network (○). $N=10^5$ in both (a) and (b). In (a), since data points for different ω cases overlap each other, one may not distinguish them to the eye.

model. Owing to the presence of $c(t)$, a PT occurs at a finite transition point even when a PT does not occur in the Smoluchowski coagulation equation, for example, when $\omega=0$. Here, we study the cases $k_i=1$ ($\omega=0$), $k_i=i^{\omega}$ with $0<\omega<1$, and $k_i=i$ ($\omega=1$), separately.

The case $\omega=0$: in this case, $c(t)=\Sigma_s n_s$ becomes the total density of the clusters, which decreases linearly with time. The generating function of $n_s(t)$ is defined as $f(z,t)=\Sigma_s n_s(t) z^s$, where z is the fugacity in the range $0<z<1$. Then, one can obtain the differential equation for $f(z,t)$ from Eq. (1) and solve in a closed form as $f(z,t)=(1-t)^2 z/(1-zt)$ for $t<1$ and 0 for $t>1$ in the thermodynamic limit. Expanding $f(z,t)$ as a series in z, we obtain

$$n_s(t) = (1-t)^2 t^{s-1} \tag{2}$$

for $t<1$. This formula shows that the cluster size distribution decays exponentially as s becomes large. Particularly, when $\delta \equiv 1-t$ is small, $n_s(\delta) \approx \delta^2 e^{-s/s^*}$ with $s^* \approx 1/\delta$. The characteristic size s^* diverges as $\delta \to 0$. As shown in the inset of Fig. 2(a), $n_s(t)$ is almost flat at $\delta=10^{-4}$ for $N=10^6$, indicating that large-size clusters are relatively abundant. The merging of these clusters causes a sudden jump in the giant cluster size, leading to a first-order transition.

We find the giant cluster size $G(t)$ by using the relation, $G(t)=1-f'(1,t) \equiv 1-\Sigma_s' s n_s(t)$, where the summation excludes an infinite-size cluster. We find that

$$G(t) = \begin{cases} 0 & \text{if } 0<t<1 \\ 1 & \text{if } t>1 \end{cases} \tag{3}$$

in the thermodynamic limit [Fig. 3(a)]. Thus, the PT is first order at $t_c=1$. This result differs from what we obtain from the Smoluchowski coagulation equation, in which the transition point $t_c=\infty$.

The case $0<\omega<1$: for this case, while exact solution for $n_s(t)$ is not obtained, $n_s(t_c)$ is done under certain assumptions. To proceed, we define the generating function $g_\omega(\mu,t) \equiv \Sigma_s s^\omega n_s(t) e^{\mu s}/c(t)$ ($\mu<0$) and presume that $n_s(t_c) \sim s^{-\tau}$. Next, we use the assumption made in Refs. [5,7] for the Smoluchowski coagulation equation that $n_s(t)=n_s(t_c)/[1+b(t-t_c)]$ near $t=t_c^+$, where b is an s-independent constant. Then, comparing the most singular terms in the series of the generating functions $f(e^\mu,t_c)$ and $g_\omega^2(\mu,t_c)$ in μ, we find that

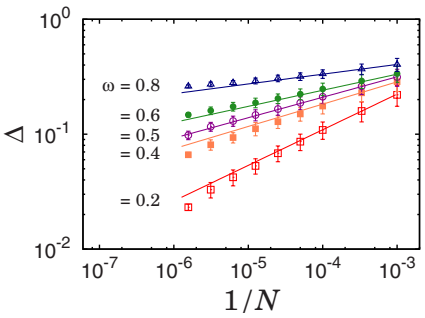

FIG. 4. (Color online) Test of the discontinuous or continuous PT for the cluster aggregation network models with various ω values. When $0<\omega<0.5$, Δ decays with increasing N; however, when $0.5<\omega<1$, it converges to a finite value. The straight lines are guidelines for eyes.

$$\tau = \begin{cases} 1+2\omega & \text{if } 0<\omega<1/2 \\ 3/2+\omega & \text{if } 1/2<\omega<1. \end{cases} \tag{4}$$

This result is confirmed numerically in Fig. 2. When $t<t_c$, $n_s(t)$ follows a power-law function with an exponential cutoff for $1/2<\omega<1$, but it exhibits a hump in a large-size region for $0<\omega<1/2$ [Fig. 2(b)].

We examine $G(t)$ as a function of time for various ω cases. $G(t)$ exhibits a transition at finite t_c, which is continuous for $1/2<\omega\leq 1$, discontinuous for $0\leq\omega<1/2$ (Fig. 3) and marginal for $\omega=1/2$. The first-order transition is tested in Fig. 4 using the scaling approach introduced in Ref. [13]. We define $\Delta\equiv t_1-t_0$, where t_0 and t_1 are chosen as the times at which the value of $G(t)$ reaches $1/\sqrt{N}$ and 0.8 for the first step, respectively. We find numerically that for $0\leq\omega<0.5$, Δ decays as $N\to\infty$, while for $0.5<\omega\leq 1$, Δ converges to a finite value. This result suggests that the transition is discontinuous (continuous) for $0\leq\omega<0.5$ $(0.5<\omega\leq 1)$.

The case $\omega=1$: this case is exactly solvable as the case of the Smoluchowski coagulation equation [6]. We consider an arbitrary initial condition of $n_s(0)$. In this case, $c(t)=\Sigma_s s n_s(t)$ is conserved as $c(t)=1$, but the first moment $M_1(t)=\Sigma_s' s n_s(t)$, with the sum excluding the largest cluster, is not. The generating function $g_1(\mu,t)=\Sigma_s n_s(t)\exp(\mu s)$ satisfies the relation

$$\dot{g}_1 = 2(g_1-1)g_1', \tag{5}$$

where the dot (prime) is the derivative with respect to time t (μ). Then, g_1 is the solution of

$$g_1(\mu,t) = 1 - H\{-\mu - 2t[g_1(\mu,t)-1]\}, \tag{6}$$

where $H(\mu)\equiv 1-g_1(-\mu,0)$ is fixed by the initial conditions of $n_s(0)$. The giant cluster size $G(t)$, defined as $G=1-g_1(0^-,t)$, can be solved by the self-consistent equation $G=H(2tG)$. The obtained $G(t)$ has the form near t_c as

$$G(t) = \frac{2M_2^2(0)}{M_3(0)}[2M_2(0)t-1], \tag{7}$$

where $M_n(0)=\Sigma_s' s^n n_s(0)$ is the initial nth moment. Also, one finds that the second moment $M_2(t)\equiv\Sigma_s' s^2 n_s(t)$ obtained from $g_1'(0^-,t)$ behaves as

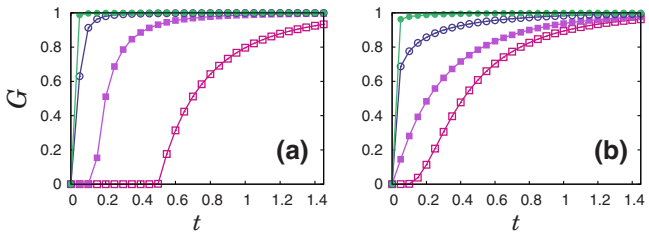

FIG. 5. (Color online) Plot of the giant cluster size G versus time for the ER network with different initial conditions. In (a), the cluster-size distribution $n_s(0)$ is flat with different cutoff values $s_m=N^\eta$, with $\eta=0$, 0.1, 0.2, and 0.3 from right to left. In (b), $n_s(0)$ decays according to a power law with exponent $\tau=3$, 2.5, 2, and 1.5 from right to left. For $\tau=2$ and 1.5, $s_m=\sqrt{N}$ at $t=0$ is taken. $N=10^7$ in both (a) and (b).

$$M_2(t) = \frac{M_2(0)}{|1-2M_2(0)t|} \tag{8}$$

for $t<t_c=1/[2M_2(0)]$ and for $t>t_c$ as $t\to t_c^+$.

These solutions for arbitrary initial conditions are used to study the first-order transition in the ER network below. For the cluster aggregation network model, the initial condition is $n_s(0)=\delta_{s,1}$. Then, $M_2(0)=M_3(0)=1$, and consequently, $t_c=1/2$, which is the well-known ER value. The giant cluster size exhibits a continuous transition at t_c with $n_s(t_c)\sim s^{-5/2}$.

It is often the case that starting from $n_s(0)=\delta_{s,1}$, the cluster-size distribution $n_s(t)$ exhibits a power-law behavior (or with hump) in s just before or at the transition point even when the dynamics is different from the ER (see Fig. 2). To see how such n_s evolves under the ER dynamics with different initial conditions from then on, we consider here two particular cases in which $M_2(0)$ and $M_3(0)$ depend on N. First, we assume that $n_s(0)$ follows a flat distribution, $n_s(0)=n_0$, in the range $0<s<s_m$, where s_m is the size of the largest cluster at $t=0$, depends on N as $s_m=N^\eta$. Then, $n_0=2N^{-2\eta}$, $M_2(0)\propto N^\eta$, and $M_3(0)\propto N^{2\eta}$. Then, a PT takes place at $t_c(N)=1/2M_2(0)\propto N^{-\eta}$ and $G(t)\sim r[2M_2(0)t-1]$ for $t>t_c(N)$ from Eq. (7), where r turns out to be in $\mathcal{O}(1)$. Thus, if time t is scaled as $t'=tM_2(0)$, then one can show that $G(t')$ is the solution of $G=\tilde{H}(3t'G)$, where $\tilde{H}(x)=2\Sigma_{n=1}^{\infty}(-1)^{n+1}x^n/[n!(n+2)]$ is a regular function qualitatively similar to $H(x)=1-e^{-x}$ of the standard ER problem. Hence, $G(t')$ has a mean field behavior similar to the original ER case. This scaling behavior implies that while $\delta G(t)\equiv G(t_1)-G(t_0)$ increases by $\mathcal{O}(1)$, $\Delta\equiv t_1-t_0$ does so by $\sim\mathcal{O}(N^{-\eta})$. Thus, we have a first-order transition as $N\to\infty$ [Fig. 5(a)].

Second, we suppose that the initial condition is given as $n_s(0)=As^{-\tau}$ in the range $0<s<s_m$, where A is the normalization constant determined by the condition $\Sigma_s s n_s=1$. A is given in Table I for various ranges of τ, together with the initial second moment for arbitrary s_m, the critical point, and the giant cluster size $G(t)$, obtained from Eq. (6).

In short, the PT occurs at $t=0$ for $\tau\leq 3$ and at finite t_c for $\tau>3$. This behavior is related to the divergence of the second moment $M_2(0)$ since time is scaled in the form $t'=2tM_2(0)$. The transition is discontinuous when $\tau<2$ but

TABLE I. When the number of cluster sizes at initial time obeys a power law $n_s(0)=As^{-\tau}$ for $s=1,\ldots,s_m$, listed are the amplitude A, the second moment at initial time $M_2(0)$, the critical point t_c, and the critical behavior of the giant cluster size $G(t)$. Type of PT is specified for each case. The listed t_c and G are the ones in the thermodynamic limit.

	τ	A	$M_2(0)$	t_c	$G(t>t_c)$	Type of PT
(i)	$0\leq\tau<2$	$\frac{2-\tau}{s_m^{2-\tau}}$	$\frac{(2-\tau)s_m}{3-\tau}$	0	1	Discontinuous
(ii)	$\tau=2$	$\frac{1}{\ln s_m}$	$\frac{s_m}{\ln s_m}$	0	1	Discontinuous
(iii)	$2<\tau<3$	$\frac{1}{\zeta(\tau-1)}$	$\frac{s_m^{3-\tau}}{\zeta(\tau-1)(3-\tau)}$	0	$\propto t^{(\tau-2)/(3-\tau)}$	Continuous
(iv)	$\tau=3$	$\frac{1}{\zeta(\tau-1)}$	$\frac{\ln s_m}{\zeta(2)}$	0	$\propto \frac{1}{2t}e^{-\zeta(2)/2t}$	Continuous
(v)	$3<\tau<4$	$\frac{1}{\zeta(\tau-1)}$	$\frac{\zeta(\tau-2)}{\zeta(\tau-1)}$	$\frac{\zeta(\tau-1)}{2\zeta(\tau-2)}$	$\propto(t-t_c)^{1/(\tau-3)}$	Continuous
(vi)	$\tau=4$	$\frac{1}{\zeta(\tau-1)}$	$\frac{\zeta(2)}{\zeta(3)}$	$\frac{\zeta(3)}{2\zeta(2)}$	$\propto \frac{t-t_c}{\ln(t-t_c)}$	Continuous
(vii)	$\tau>4$	$\frac{1}{\zeta(\tau-1)}$	$\frac{\zeta(\tau-2)}{\zeta(\tau-1)}$	$\frac{\zeta(\tau-1)}{2\zeta(\tau-2)}$	$\propto t-t_c$	Continuous

continuous when $2<\tau<3$. This difference originates from the fact that the ratio $M_2^2(0)/M_3(0)$ is finite for the former, while it vanishes for the latter. For $\tau>3$, both $M_2(0)$ and $M_3(0)$ are finite, resulting in the classical percolation behavior at a finite t_c.

In summary, we have introduced a cluster aggregation network model, in which discontinuous percolation transitions occur when the connection kernel is sublinear as $K_{ij}\sim(ij)^{\omega}$ with $0\leq\omega<1/2$. Even for the ER network, a discontinuous PT can also be obtained by using initial conditions where $M_2(0)$ diverges and $M_2^2(0)/M_3(0)$ remains finite. The simple model manifests explicitly the role of the abundance of large-size clusters just before a transition point as a mechanism of the discontinuous PT [17]. We expect that the cluster aggregation network model can be used to study underlying dynamics of the explosive percolation transition of random ER network under the Achlioptas process [13].

Note added. Recently, we became aware of a work [19], which starts from the same motivation as ours.

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