Cluster aggregation model for discontinuous percolation transition

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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 sub-linear 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 non-equilibrium kinetic systems.

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Irreversible cluster aggregations are widespread phenomena 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, 3] 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, 2, 4, 5], 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 [6, 7] and the Potts model formalism [8] 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 [2]. For example, in the evolution of the classical random network, called the Erdős-Rényi (ER) model, an edge is added at each time step, thereby either connecting two separate clusters (inter-cluster edge) or increasing the edge number in one cluster without changing cluster numbers (intra-cluster edge). Fig. [4] shows that the frequency of inter-cluster connections is dominant until the percolation threshold. Thus, the cluster aggregation picture of the ER network evolution comes in naturally. In this paper, 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.

- 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 $k_i / \sum_s k_s n_s$, where $k_i$ and $n_i$ are the weight and density of an $i$-sized cluster, respectively.
- 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 $t = L/N$, 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 sub-linear, 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 observation is remarkable, because a discontinuous PT has rarely been discovered in irreversible kinetic systems, except for recent observations in the ER [9] and other networks [10, 11] under the so-called Achlioptas process [12]. On the other hand, it is noteworthy that 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. Thus, this cluster aggregation network model allows us to study the underlying mechanism of the discontinuous PT analytically for some cases, which is shown later.

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:

$$\frac{dn_i(t)}{dt} = \sum_{i+j=s} \frac{k_i n_i k_j n_j}{c(t) c(t)} - 2 \frac{k_i n_i}{c(t)},$$

where $c(t) = \sum_s k_s n_s(t)$. The connection kernel $K_{ij} \equiv k_i k_j / c^2$. The first term on the right hand side represents the aggregation of two clusters of sizes $i$ and $j$ with
图 1: (Color online) The fraction of each type of attached edges, inter-cluster (●) or intra-cluster (○) edges for the ER model. Arrow indicates percolation threshold at $p_c = 1/2$.

Let $i + j = s$ 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. [3], which was called the F-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, $c(t) = \sum_s n_s(t)$ becomes the total density of the clusters, which decreases linearly with time. The generating function of $n_s(t)$ is defined as $f(z, t) = \sum_s n_s(t) z^s$, 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 $f(z, t) = (1 - t)^2(z/(1 - z))$ for $t < 1$ and 0 for $t > 1$ in the thermodynamic limit. Expanding $f(z, t)$ as a series in $z$, we obtain

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

for $t < 1$. This formula shows that the cluster size distribution decays exponentially as $s$ becomes large. Particularly, when $\delta = 1 - t$ is small, $n_s(\delta) \approx \delta^2 e^{-s/\delta}$ with $s^* \approx 1/\delta$. The characteristic size $s^*$ diverges as $\delta \to 0$. As shown in the inset of Fig. (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,

$$G(t) = 1 - f'(1/t) \equiv 1 - \sum_{s} s n_s(t),$$

where the summation excludes an infinite-size cluster. We find that

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

in the thermodynamic limit (Fig. (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 cer-
tain assumptions. To proceed, we define the generating function \( g_0(\mu, t) = \sum_s s^n n_s(t)e^{\mu s}/c(t) \) (\( \mu < 0 \)), and presume that \( n_s(t_c) \sim s^{-\tau} \). Next, we use the assumption made in Ref. [13] 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 \( g_0^2(\mu, t_c) \) in \( \mu \), we find that

\[
\tau = \begin{cases} 
1 + 2\omega & \text{if } 0 < \omega < 1/2, \\
3/2 + \omega & \text{if } 1/2 < \omega < 1.
\end{cases}
\] (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 \( \omega \) cases. \( G(t) \) exhibits a transition at finite \( t_c \), which is continuous for \( 1/2 < \omega < 1 \), discontinuous for \( 0 < \omega < 1/2 \) (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 time, respectively. We find numerically that for \( 0 < \omega < 0.5 \), \( \Delta \) decays as \( N \to \infty \), while for \( 0.5 < \omega < 1 \), \( \Delta \) converges to a finite value. This result suggests that the transition is discontinuous (continuous) for \( 0 < \omega < 0.5 \) \((0.5 < \omega \leq 1)\).

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, \( c(t) = \sum_s sn_s(t) \) is conserved as \( c(t) = 1 \), but the first moment \( M_1(t) = \sum_s sn_s(t) \), with the sum excluding the largest cluster, is not. The generating function \( g_1(\mu, t) = \sum_s sn_s(t)e^{\mu s} \) satisfies the relation

\[
g_1 = 2(g_1 - 1)g_1',
\] (5)

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

\[
g_1(\mu, t) = 1 - H(-\mu - 2t(g_1(\mu, t) - 1)),
\] (6)

where \( H(\mu) = 1 - g_1(-\mu, 0) \) 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 \( G = H(2G) \). The obtained \( G(t) \) has the form near \( t_c \) as

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

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

\[
M_2(t) = \frac{M_2(0)}{|1 - 2M_2(0)t|}
\] (8)

for \( t < t_c \), and \( t > t_c \), 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 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 $s_m$, the size of the largest cluster at $t = 0$, depends on $N$ as $s_m = N^n$. Then, $n_0 = 2N^{-2n}$, $M_2(0) \propto N^n$, and $M_3(0) \propto N^{2n}$. Then, a PT takes place at $t_c(N) = 1/2M_2(0) \propto N^{-n}$, and $G(t) \sim t(2M_2(0)t - 1)$ 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 $G = H(3t'G)$, where $H(x) = 2\sum_{n=1}^{\infty} (-1)^{n+1} x^n/(n(n + 2))$ 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 $\mathcal{O}(N^{-\eta})$. Thus, we have a first-order transition as $N \to \infty$ (Fig. 2(a)).

Second, we suppose that the initial condition is given as $n_s(0) = A s^{-\tau}$ in the range $0 < s < s_m$, where $A$ is the normalization constant determined by the condition $\sum_s n_s = 1$. $A$ is given in Table I for various ranges of $\tau$, 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 continuous when $2 < \tau < 4$. This difference originates from the fact that the ratio $M_2(0)/M_3(0)$ is finite for the former, while it vanishes for the latter. For $\tau > 4$, 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 $M_2(0)/M_3(0)$ 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].

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Note added.—After the submission of this paper, we became aware of a work [21], which starts from the same motivation as ours.

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**Table I:** When the number of cluster sizes at initial time obeys a power law $n_s(0) = A s^{-\tau}$ 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.

| $\tau$ | $A$ | $M_2(0)$ | $t_c$ | $G(t > t_c)$ | type of PT |
|---------|-----|----------|------|-------------|------------|
| (i)     | $0 \leq \tau < 2$ | $\frac{2}{s_m}$ | $\frac{2(\tau-1)}{3-\tau}$ | 0 | $1$ | discontinuous |
| (ii)    | $\tau = 2$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | 0 | $1$ | discontinuous |
| (iii)   | $2 < \tau < 3$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | 0 | $\propto \frac{1}{2(\tau-1)}$ | continuous |
| (iv)    | $\tau = 3$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | 0 | $\propto \frac{1}{2(\tau-1)}$ | continuous |
| (v)     | $3 < \tau < 4$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | $\frac{1}{2(\tau-1)}$ | $\propto (t - t_c)^{-2}$ | continuous |
| (vi)    | $\tau = 4$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | $\frac{1}{2(\tau-1)}$ | $\propto \frac{t - t_c}{\ln(t - t_c)}$ | continuous |
| (vii)   | $\tau > 4$ | $\frac{1}{s_m}$ | $\frac{1}{s_m}$ | $\frac{1}{2(\tau-1)}$ | $\propto t - t_c$ | continuous |

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