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Scale-free random graphs and Potts model

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Abstract. We introduce a simple algorithm that constructs scale-free random graphs efficiently: each vertex i has a prescribed weight $P_i \propto i^{-\mu}$ $(0 < \mu < 1)$ and an edge can connect vertices i and j with rate $P_i P_j$. Corresponding equilibrium ensemble is identified and the problem is solved by the $q \to 1$ limit of the q-state Potts model with inhomogeneous interactions for all pairs of spins. The number of loops as well as the giant cluster size and the mean cluster size are obtained in the thermodynamic limit as a function of the edge density. Various critical exponents associated with the percolation transition are also obtained together with finite-size scaling forms. The process of forming the giant cluster is qualitatively different between the cases of $\lambda > 3$ and $2 < \lambda < 3$, where $\lambda = 1 + \mu^{-1}$ is the degree distribution exponent. While for the former, the giant cluster forms abruptly at the percolation transition, for the latter, however, the formation of the giant cluster is gradual and the mean cluster size for finite N shows double peaks.

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1. Introduction

Graph theoretic approach is of great value to characterize complex systems found in social, informational and biological areas. Here, a system is represented as a graph or network whose vertices and edges stand for its constituents and interactions. A simplest model for such is the random graph model proposed by Erdős and Rényi (ER) [1]. In the ER model, N number of vertices are present from the beginning and edges are added one by one in the system, connecting pairs of vertices selected randomly. The degree distribution is Poissonian. However, many real-world networks such as the World-wide web, the Internet, the coauthorship, the protein interaction networks and so on display power-law behaviors in the degree distribution. Such networks are called scale-free (SF) networks [2]. Thanks to recent extensive studies of SF networks, various properties of SF network structures have been uncovered [3–5].

There have been several attempts to describe scale-free networks in the framework of equilibrium statistical physics, even though the number of vertices N grows with time in many real-world networks [6–18]. To proceed, one needs to define equilibrium network ensemble of graphs with appropriate weights, where one graph corresponds to one state of the ensemble. In the microcanonical ensemble approach, given a degree distribution $P_d(k)$, a degree sequence is given: that is $P_d(0)N$ vertices have 0 degree, $P_d(1)N$ vertices have degree 1, etc. so that the degree k_i of each vertex is fixed. Then those links emanating from each vertex are randomly joined with uniform weights [11]. In the canonical ensemble approach, the total number of links L is fixed but the links are rewired with certain weights so that the degree sequence is satisfied in the average sense.

A grandcanonical ensemble can be also defined, where the number of edges is also a fluctuating variable while keeping the SF nature of the degree distributions. The grandcanonical ensemble for SF random graphs is realized in various ways [13–18]. One of the simplest and elegant way is the static model introduced by Goh *et al.* [13] and analyzed by Lee *et al.* [19]. The name 'static' originates from the fact that the number of vertices is fixed from the beginning. Here each vertex i has a prescribed weight P_i summed to 1 and an edge can connect vertices i and j with rate $P_i P_j$. A chemical potential-like parameter K that can be regarded as "time" in the process of attaching edges controls the mean number of edges so that $\langle L \rangle$ increases with increasing K. The probability of vertex i and j being connected is then

$$f_{ij} = 1 - e^{-2NKP_iP_j}. \tag{1}$$

This is in marked contrast to other grandcanonical ensemble approaches where f_{ij} are expressed as a product of vertex weights. However, note that f_{ij} in Eq. (1) properly incorporates the "fermionic" constraint; $f_{ij} \to 1$ as $K \to \infty$.

As the parameter K increases, a giant cluster, or giant component, forms in the system. Here the giant cluster means the largest cluster of connected vertices whose size is $\mathcal{O}(N)$. Often such a giant cluster appears at the percolation transition point. In equilibrium statistical physics, the percolation problem can be studied through a spin model, the q-state Potts model in the $q \to 1$-limit [20]. Using the relation, in this paper, we study the evolution of SF random graphs from the perspective of equilibrium statistical physics.

The formulation in terms of the spin model facilitates explicit derivation of various properties of the SF network. Thus we derive the formula for the giant cluster size, the mean cluster size, and in particular, the number of loops and clusters. These quantities are explicitly evaluated analytically for the static model with $P_i \propto i^{-\mu}$, $(0 < \mu < 1)$ in the thermodynamic limit as a function of the edge density, and their critical properties are also studied. The degree exponent λ is related to μ by $\lambda = 1 + 1/\mu$. Moreover, their finite-size scaling behaviors are obtained using the *finite* largest cluster size for finite N that in turn is evaluated from the cluster size distribution. From these, we are able to elucidate the process of formation of the giant cluster. While for the case $\lambda > 3$, the giant cluster forms abruptly at the percolation transition point K_c, for the case $2 < \lambda < 3$ where most real world networks belong to, however, the formation of the giant cluster is gradual and the mean cluster size for finite N shows double peaks.

2. Static model: Random graphs with weighted vertices

The static model introduced in Goh *et al.* [13] is defined as follows:

1. The number of vertices N is fixed (static) and each vertex $i = 1, \ldots, N$ is given a probability P_i summed to 1. The ER model of random graphs corresponds to assigning $P_i = 1/N$ for all i. To construct a SF graph, we use for definiteness,

$$P_i = \frac{i^{-\mu}}{\sum_{j=1}^{N} j^{-\mu}} \approx \frac{1-\mu}{N^{1-\mu}} i^{-\mu} \tag{2}$$

where μ, the Zipf exponent is in the range $0 < \mu < 1$. Note that $P_i \ll 1$ for all i.

2. In each unit time duration, two vertices i and j are selected with probabilities P_i and P_j.
3. If $i = j$ or an edge connecting i and j already exists, do nothing (fermionic constraint); otherwise, an edge is added between the vertices i and j.
4. Steps 2 and 3 are repeated for NK times.

Then the probability that a given pair of vertices i and j ($i \neq j$) is not connected by an edge is given by $(1-2P_iP_j)^{NK} \simeq e^{-2NKP_iP_j} \equiv 1 - f_{ij}$, while that it does is $f_{ij} = 1 - e^{-2NKP_iP_j}$. Since each edge b_{ij} is produced independently, this process generates a graph G with probability

$$\begin{aligned} P(G) &= \prod_{b_{ij}\in G}(1-e^{-2NKP_iP_j})\prod_{b_{ij}\notin G}e^{-2NKP_iP_j} \\ &= e^{-2NK\sum_{i>j}P_iP_j}\prod_{b_{ij}\in G}(e^{2NKP_iP_j}-1) \\ &= e^{-NK(1-M_2)}\prod_{b_{ij}\in G}(e^{2NKP_iP_j}-1), \end{aligned} \tag{3}$$

where we used the notation $M_n \equiv \sum_{i=1}^N P_i^n$. By a graph G, we mean a configuration of undirected edges connecting a subset of $N(N-1)/2$ pairs of labeled vertices $i = 1, 2, \ldots, N$.

We then evaluate the ensemble average of any graph theoretical quantity A by

$$\langle A\rangle = \sum_G P(G)A(G). \tag{4}$$

The generating function of k_i, $g_i(\omega) \equiv \langle \omega^{k_i}\rangle$, is first expressed as

$$g_i(\omega) = \exp\left\{\sum_{j(\neq i)}\ln[1-(1-\omega)f_{ij}]\right\}. \tag{5}$$

For the static model, the sum is evaluated as [19],

$$g_i(\omega) = e^{-(1-\omega)2NKP_i}. \tag{6}$$

From this, one has, when $K_\ell \ll K \ll K_u$ with $K_\ell \sim N^{-\mu}$ and $K_u \sim N^{1-\mu}$,

$$\langle k_i\rangle = \omega\frac{d}{d\omega}g_i(\omega)\bigg|_{\omega=1} = \sum_{j(\neq i)}(1-e^{-2NKP_iP_j}) = 2KNP_i \propto i^{-\mu}, \tag{7}$$

and the average degree $\langle k\rangle$ is

$$\langle k\rangle = \frac{2\langle L\rangle}{N} = \frac{1}{N}\sum_i\langle k_i\rangle = 2K. \tag{8}$$

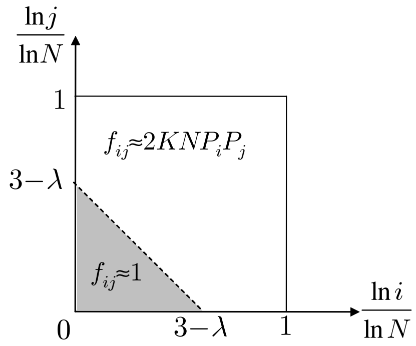

Figure 1. The occupation probability of a bond for finite K has two distinct regions due to the fermionic constraint when $2 < \lambda < 3$.

From Eq. (7) one immediately sees that the degree exponent λ is related to the Zipf exponent μ by

$$\lambda = 1 + 1/\mu. \tag{9}$$

Note that since $2KNP_iP_j \sim N^{2\mu-1}/(ij)^{\mu}$ for finite K,

$$f_{ij} \approx 2KNP_iP_j \tag{10}$$

when $0 < \mu < 1/2$ ($\lambda > 3$). This is the bosonic limit. However, when $1/2 < \mu < 1$ ($2 < \lambda < 3$), which most interesting real-world networks satisfy, f_{ij} does not necessarily take the form of Eq. (10). In fact,

$$f_{ij} \approx \begin{cases} 1 & \text{when} \quad ij \ll N^{2-1/\mu}, \\ 2KNP_iP_j & \text{when} \quad ij \gg N^{2-1/\mu}. \end{cases} \tag{11}$$

This is due to the fermionic constraint. Thus, for $2 < \lambda < 3$, one has two distinct regions in the i-j plane as shown in Fig. (1).

3. Potts model formulation

It is well known that the q-state Potts model provides a useful connection between the geometric bond percolation problem and the thermal systems through the Kasteleyn construction [20]. The $q \to 1$ limit of the Potts model corresponds to the bond percolation problem. The same approach can be used for the random graph problem. From the viewpoint of the thermal spin system, this is basically the infinite range model since all pairs of spins interact with each other albeit with inhomogeneous interaction strength.

Consider the q-state Potts Hamiltonian given by

$$-H = 2NK \sum_{i>j} P_iP_j[\delta(\sigma_i, \sigma_j) - 1] + h_0 \sum_{i=1}^{N} [q\delta(\sigma_i, 1) - 1], \tag{12}$$

where K is the interaction, h_0 is a symmetry-breaking field, $\delta(x, y)$ the Kronecker delta function, and σ_i the Potts spins taking integer values $1, 2, \ldots, q \equiv r + 1$. The partition function $Z_N(q, h_0)$ is

$$Z_N(q,h_0) = \mathrm{Tr}\, e^{-H} = \mathrm{Tr} \prod_{i>j} \left[e^{-2NKP_iP_j} + (1 - e^{-2NKP_iP_j}) \delta(\sigma_i, \sigma_j) \right] \times \prod_i e^{h_0(q\delta(\sigma_i,1)-1)}, \tag{13}$$

where Tr denotes the sum over q^N spin states. Expanding the first product and taking the Tr operation, one has

$$Z_N(q,h_0) = \sum_G P(G) \prod_{s\geq 1} (e^{srh_0} + re^{-sh_0})^{n_G(s)}. \tag{14}$$

where $n_G(s)$ is the number of s-clusters, a cluster with s vertices in a given graph G. In particular, $Z_N(q, 0) = \langle q^C \rangle$, where $C = \sum_s n_G(s)$ is the total number of clusters in graph G. Thus $Z_N(q, 0)$ is the generating function of C.

The magnetization of the Potts model at $q = 1$ is

$$m(1,h_0) = \lim_{q\to 1} \frac{1}{rN} \frac{\partial}{\partial h_0} \ln Z_N(q,h_0) = \sum_{s\geq 1} P(s)(1 - e^{-sh_0}) = 1 - \mathcal{P}(e^{-h_0}), \tag{15}$$

where we have introduced the cluster size distribution $P(s) \equiv n(s)(s/N)$ with $n(s) = \langle n_G(s) \rangle$ and the generating function $\mathcal{P}(z) = \sum_{s\geq 1} P(s) z^s$.

When $h_0 = 0$, the magnetization vanishes for finite N. However, when we take the limit $h_0 \to 0$ after the thermodynamic limit $N \to \infty$, the contribution from the giant cluster whose size is S can survive to give

$$m(1, h_0 \to 0) = \left\langle \frac{S}{N} \right\rangle. \tag{16}$$

The susceptibility defined as $\chi(q, h_0) \equiv (1/q)(\partial/\partial h_0) m(q, h_0)$ on the other hand is related to the mean cluster size:

$$\bar{s} = \chi(1, h_0 \to 0) = \lim_{h_0\to 0} \lim_{N\to\infty} \sum_s P(s) s e^{-sh_0} = \sum_{s\neq\langle S\rangle} sP(s), \tag{17}$$

while the number of loops per vertex $\langle N_{\rm loop} \rangle / N$ is given as

$$\ell \equiv \frac{\langle N_{\rm loop} \rangle}{N} = \frac{\langle L \rangle}{N} - 1 + \frac{1}{N} \frac{\partial}{\partial q} \left[\ln Z_N(q,0) \right]_{q=1}. \tag{18}$$

3.1 Partition function and free energy

A convenient way to evaluate the partition function is to resort to the vector-spin representation where one associates an r-dimensional vector $\vec{S}(\sigma_i)$ of unit length to each spin value σ_i, where $\vec{S}(1) = (1, 0, \ldots, 0)$ and $\vec{S}(\sigma_i)$ with $\sigma_i = 2, 3, \ldots, q$ point to the remaining r corners of the r-dimensional tetrahedron. The interaction term in the hamiltonian then takes the form of a perfect square, $\left[\sum_i P_i \vec{s}(\sigma_i)\right]^2$, and the standard saddle point analysis can be applied [19]. As a result, the free energy can be evaluated for general q. In the $q \to 1$ limits, it becomes

$$F(y, h_0) = \frac{1}{4K} y^2 - \frac{1}{N} \sum_{i=1}^{N} (e^{-h_i} - 1 + h_i), \tag{19}$$

where $h_i = h_0 + NP_i y$ and y is the solution of

$$\frac{y}{2K} = \sum_{i=1}^{N} P_i (1 - e^{-h_i}). \tag{20}$$

When $h_0 \to 0$, a non-trivial solution of Eq. (20) begins to appear when $(2K)^{-1} < N \sum_{i=1}^{N} P_i^2$, which gives the following characteristic value K_c

$$K_c = \frac{1}{2N \sum_{i=1}^{N} P_i^2} \approx \begin{cases} \frac{1-2\mu}{2(1-\mu)^2} & 0 < \mu < 1/2 \\ \frac{1}{2(1-\mu)^2 \zeta(2\mu)} N^{-(2\mu-1)} & 1/2 < \mu < 1. \end{cases} \tag{21}$$

Since $\langle k \rangle = 2K$ and $\langle k^2 \rangle = (1/N) \sum_{i=1}^{N} \langle k_i^2 \rangle = \langle k \rangle + N^{-1} \sum_{i=1}^{N} \langle k_i \rangle^2 = 2K + 4NK^2 \sum_{i=1}^{N} P_i^2$, the condition $K = K_c$ is equivalent to the well-known condition $\langle k^2 \rangle / \langle k \rangle = 2$ [11]. The thermodynamic quantities, m, $\bar{s}$, and ℓ evaluated from Eqs. (19) and (20) are shown in Fig. 2.

4. Cluster size distribution and largest cluster size

Beyond the largest cluster size or the mean cluster size, the whole distribution of cluster size $P(s)$ for the static model can be derived from Eqs. (19) and (20). The result is the same as that obtained from the branching process approach [12,19]. In the branching process approach, one neglects the presence of loops. For $K > K_c$, we do have a macroscopic number of loops but they mostly belong to the giant cluster, leaving the finite clusters effectively tree. Thus one can neglect the loops as long as the properties of finite clusters are concerned.

The cluster size distribution $P(s)$ near $K_c(N)$ takes the form

$$P(s) \sim s^{1-\tau} e^{-s/s_c} \tag{22}$$

with $s_c \sim (K - K_c)^{-1/\sigma}$. The critical exponents τ and σ are evaluated as shown in Table 1. These values are the same as those derived by Cohen *et al.* [21] for the site percolation problem except $\tau = \lambda$ for $2 < \lambda < 3$. The giant cluster size $\langle S \rangle = mN$ can

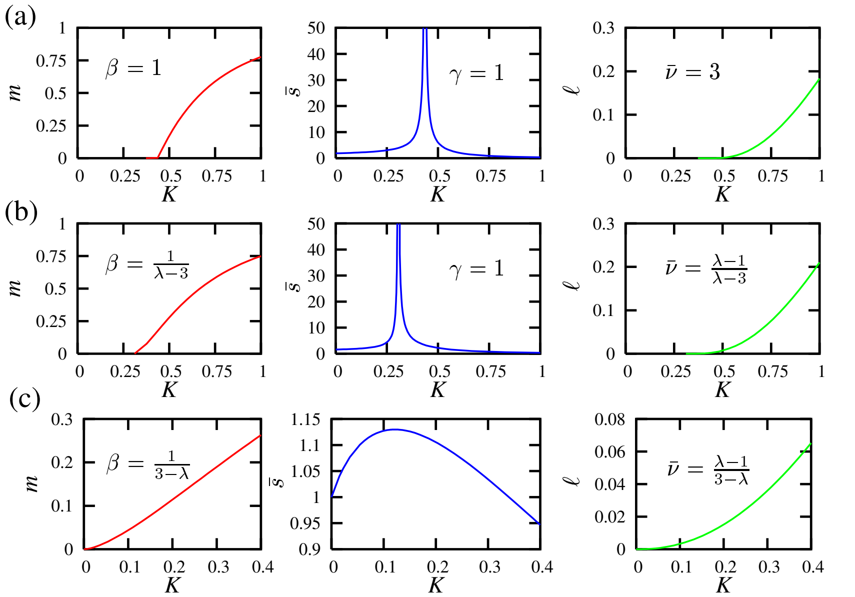

Figure 2. Giant cluster size m, mean cluster size $\bar{s}$, and number of loops $\ell = \langle N_{\rm loop}\rangle/N$ vs. K for $\mu = 5/19$ ($\lambda = 4.8$) (a), $\mu = 5/13$ ($\lambda = 3.6$) (b), and $\mu = 5/7$ ($\lambda = 2.4$) (c). Also shown in the panel are the critical exponents associated with the percolation transition, defined by $m \sim (K-K_c)^{\beta}$, $\bar{s} \sim (K-K_c)^{-\gamma}$, and $\ell \sim (K-K_c)^{\bar{\nu}}$.

be obtained from the relation $\sum_{s\neq\langle S\rangle} P(s) = 1 - \frac{\langle S\rangle}{N}$. In particular, at $K = K_c(N)$, it scales as

$$\langle S\rangle \sim \begin{cases} N^{1/(\tau-1)} & (\lambda > 3), \\ K_c(N)N^{1/(\tau-1)} \sim N^{1-\mu} & (2 < \lambda < 3). \end{cases} \tag{23}$$

Similarly, $\bar{s}$ at $K_c(N)$ for finite N can be obtained from $\bar{s} \sim \int_{s<\langle S\rangle} s^{2-\tau} ds$. We find

$$\bar{s} - 1 \sim \begin{cases} N^{1/\bar{\nu}} & (\lambda > 3), \\ K_c(N)^2 N^{1/\bar{\nu}} \sim N^{-1/\bar{\nu}} & (2 < \lambda < 3). \end{cases} \tag{24}$$

Table 1. The critical exponents τ and σ describing the cluster size distribution.

	τ	σ
$\lambda > 4$	$\frac{5}{2}$	$\frac{1}{2}$
$3 < \lambda < 4$	$\frac{2\lambda-3}{\lambda-2}$	$\frac{\lambda-3}{\lambda-2}$
$2 < \lambda < 3$	λ	$\frac{3-\lambda}{\lambda-2}$

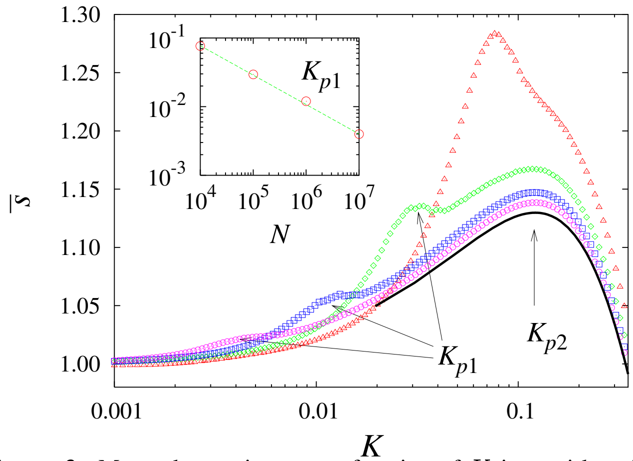

Figure 3. Mean cluster size $\bar{s}$ as a function of K in semi-logarithmic scales with $\mu = 5/7$ for $N = 10^4(\triangle)$, $10^5(\diamond)$, $10^6(\square)$, and $10^7(\bigcirc)$. In addition to the peak at K_{p1}, another peak is shown at $K_{p2} \simeq 0.1\,N$ for $N = 10^5$, 10^6, and 10^7, respectively. The solid line represents the exact solution. The measured values of K_{p1} ($\bigcirc$) as a function of N are plotted in the inset together with the guide line whose slope is $1 - 2\mu$ for comparison.

5. Evolution of the scale-free random graphs

As K, the mean number of links per node, increases, nodes join to form small clusters and the clusters join to form bigger clusters. Thus the mean cluster size increases. For $\lambda > 3$, there exists a sharp percolation transition at which the giant cluster appears suddenly. Also cycles of all order (*i.e.*, loops of arbitrary size) appear near the transition. Since there are many large but finite clusters, the mean cluster size $\bar{s}$ diverges. Soon after $K > K_c$, however, the giant cluster begins to swallow up those big finite clusters and $\bar{s}$ becomes smaller.

Such standard percolation transition picture is radically modified for $2 < \lambda < 3$ since $K_c(N) \sim N^{-1/\bar{\nu}}$. The mean cluster size as a function of K is of interest in particular. Fig. 3 shows $\bar{s}$ versus K for four values of N; 10^4, 10^5, 10^6, and 10^7. As N increases, the mean cluster size $\bar{s}$ approaches the exact solution represented by the solid line in Fig. 3. It does not diverge at any value of K, but instead its peak height decreases as N increases. We additionally find that the mean cluster size $\bar{s}$ has a small peak at K_{p1}, which scales as $N^{1-2\mu}$ as shown in the inset of Fig. 3. The value of K_{p1} is close to $K_c(N)$. The peak height scales as $\bar{s}$ at $K_c(N)$ derived in the previous section: $\sim N^{-1/\bar{\nu}} = N^{1-2\mu}$. The reason for the peak at K_{p1} is as follows. As K increases, the largest cluster size $\langle S \rangle$ and the mean cluster size $\bar{s} = \sum_{s \neq \langle S \rangle} sP(s)$ also increase. However, as K approaches $K_c(N)$, the cluster size distribution $P(s)$ begins to develop the exponential decaying part in its tail, i.e., for $s \gg s_c$. s_c decreases with increasing K after K passes K_c. At K_{p1}, $\langle S \rangle$ and s_c are equal. After K passing K_{p1}, the mean cluster size is dominated by s_c, which makes $\bar{s}$ decrease for $K > K_{p1}$. However, the mean cluster size increases again as soon as K becomes much larger than K_{p1} or $K_c(N)$ because of a prefactor $K^{1/\mu}$ of the cluster

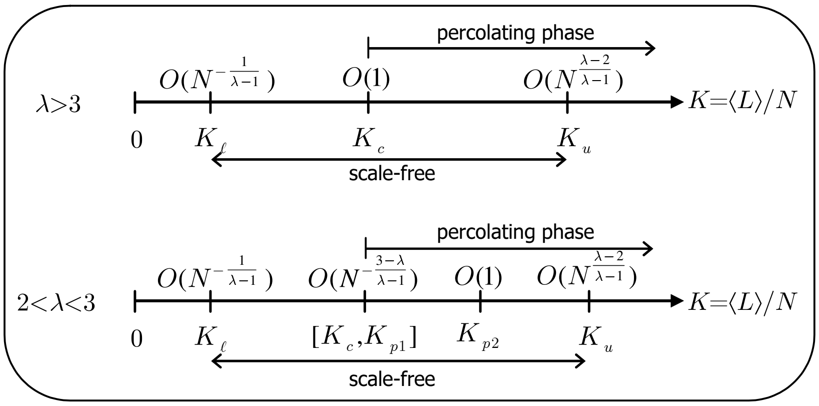

Figure 4. The "phase diagram" of the scale-free random graph as a function of the link density K.

size distribution $P(s)$ for $1 \ll s \ll s_c$ which increases with increasing K. The mean cluster size decreases only after the second peak at $K_{p2} = \mathcal{O}(1)$, where $s_c = \mathcal{O}(1)$, as shown in Fig. 3 as well as in the exact solution in Fig. 2. As in the case of $\lambda > 3$, cycles of all order begin to appear at $K \sim K^{1-2\mu} \sim K_c(N)$. Therefore, the system may be regarded as being in the percolating phase for $K > K_c(N)$.

In summary, the "phase diagram" of the scale-free random graph may be represented as in Fig. 4.

6. Conclusion

We have studied the percolation transition of the SF random graphs constructed by attaching edges with probability proportional to the products of two vertex weights. By utilizing the Potts model representation, the giant cluster size, the mean cluster size, and the numbers of loops and clusters are obtained from the Potts model free energy in the thermodynamic limit. Our general formulae for the giant cluster size and the mean cluster size are equivalent to those results obtained for a given degree sequence if the latter expressions are averaged over the grandcanonical ensemble. The Potts model formulation allows one to derive other quantities such as the number of loops easily. Using this approach, we then investigated the critical behaviors of the SF network realized by the static model in detail. Furthermore, to derive the finite size scaling properties of the phase transition, the cluster size distribution and the largest cluster size in finite size systems are also obtained and used. We found that there is a percolation transition for $\lambda = 1 + 1/\mu > 3$ so that a giant cluster appears abruptly when $K = \langle L\rangle/N$ is equal to K_c given by Eq. (21) while such a giant cluster is generated gradually without a transition for $2 < \lambda < 3$. Thus the process of formation of the giant cluster for the case of $2 < \lambda < 3$ is fundamentally different from that of $\lambda > 3$.

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