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Exactly solvable model of a coalescing random graph

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An initially empty (no edges) graph of order M evolves by randomly adding one edge at a time. This edge connects either two linked components and forms a new component of larger order (coalescence of graphs) or increases (by one) the number of edges in a given linked component (cycling). Assuming that the vertices of the graph have a finite valence (the number of edges connected with a given vertex is limited) the kinetic equation for the distribution of linked components of the graph over their orders and valences is formulated and solved by applying the generating function method. The evolution process is shown to reveal a phase transition: the emergence of a giant linked component whose order is comparable to the total order of the graph. The kinetics of growth of this component is studied for arbitrary initial conditions. Found are the time dependences of the average order and the valence of the giant component. The distribution over orders and valences of the linked components of the graph is derived for an initially empty graph comprising M bare polyvalent vertices.

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I. INTRODUCTION

The systems wherein collisions and subsequent coalescence of the system components lead to the changes in their number and sizes are highly widespread in nature [1–3]. It is thus not surprising that a huge effort was directed to the study of the coagulation processes in diverse concrete coagulating systems, such as clouds, aerosols, hydrosols, etc. An impressive list of the coagulation processes can be found in the review articles [3–6]. The main problem that faces the theory of coagulation is how to find the particle mass spectrum, the number of particles of given mass at time t.

In studying the coagulation processes one starts from the kinetic equation, which governs the time evolution of the concentrations $c(g,t)$ of the particle with mass g at time t. This equation is (the Smoluchowski equation),

$$\frac{dc(g,t)}{dt} = \frac{1}{2}\sum_{l=1}^{g-1} K(g-l,l)c(g-l,t)c(l,t) - c(g,t)\sum_{l=1}^{\infty} K(g,l)c(l,t). \quad (1)$$

Here g and l are the particle masses in units of a monomeric mass. This equation is derived from a simple balance principle: the increase in the g-particle concentration $c_g(t)$ comes from the coalescence of g-l and l particles [the first term on the right-hand side (RHS) of this equation]. The second term describes the consumption of g particles by all other participants of the coagulation process and thus enters with the negative sign. The coagulation kernel $K(g,l)$ is the rate of coalescence of the particles containing g and l monomers. This equation has been used countless times to study very diverse phenomena ranging from the coagulation of aerosols and suspensions and ending with the formation of planets.

A random graph is a collection of points (vertices) randomly connected by lines (edges). The random graph can be considered as a collection of linked clusters. (The linked cluster is a graph in which each vertex is connected by one or several edges with any other vertex belonging to it). The interest to the structure of the random graphs comes from their close resemblance to many dynamical processes such as polymerization [7–16], evolution of social networks [17], percolation [18–20], and phase transitions [21].

Most studies of random graphs rely upon the combinatorial analysis [22–25]. Another method applies the kinetic approach where one edge is randomly added to the graph. In this case the graph evolution is analogous to the coagulation process in a system of particles that move, collide, and coalesce on colliding, forming a larger daughter particle.

The efficiency of the Smoluchowski equation for studying the evolution of random graphs had been clearly demonstrated in Refs. [9,12–15,26,27], where the analogy between the particle coalescence and the graph transformation by randomly adding edges to the evolving graph is shown. Indeed, if we consider a graph comprising $N_1, N_2, \ldots, N_g, \ldots$ linked components then any additional edge either converts a couple of components to one or produces an additional cycle if it connects two vertices in one component.

The above consideration assumes the infinite valence of the vertices, i.e., the number of outgoing edges is not limited. It is clear that if the valence of each vertex in the evolving graph is finite then the resulting structures will occur more loosely. The attempts to consider such structures appeared more than half a century ago [7,8], even earlier than the paper of Erdös and Rényi [22], in connection with the theory of polymerization. Indeed, the polymerization process has many common features with the evolution of random graphs: newly appearing chemical bonds connect the active functional centers and form the polymer structure.

This paper aims at the consideration of the evolution of a random graph with the vertices of finite valence. The idea of my approach is close to that of Refs. [9,12–14] where the Smoluchowski equation applies for studying initially monodisperse and monovalent random graphs. The evolution process in this case produces only treelike linked components whose total valence is fully determined by their order. In the case of cycles or more complex initial conditions the Smoluchowski equation is not applicable and should be replaced by another one. This step is done in this paper.

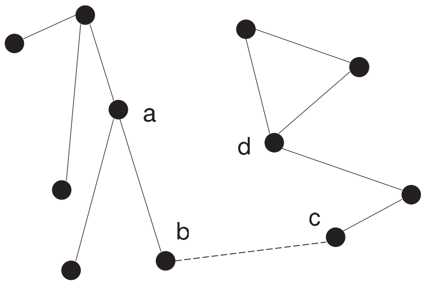

FIG. 1. Evolution of a random graph. Shown is a fragment of the random graph comprising two linked component of orders 6 and 5. Each vertex has the valence 3. Extra edge *cd* (dash line) appearing in the the graph can thus connect the vertices *b* and *c*, but it cannot connect the vertices *a* and *d*, because they have not free valences. Neither extra edges *bd* or *ac* are possible.

The remainder of the paper is divided as follows. In the next section the basic equation and the initial conditions are formulated. Assuming that the coalescence rate is proportional to the product of the valences of coalescing components the equation for the bivariate generating function and the moments of the order-valence distribution is derived in Sec. III. The exact expression for the bivariate generating function for the order-valence spectrum is derived in Sec. IV. In Sec. V it is shown that after a critical time a giant cluster emerges and evolves by attaching smaller linked components. The average order of the giant component and its total valence as the functions of times are analyzed in this section. The distribution of the linked components of the evolving graph is found in Sec. VI for an initially empty graph with polyvalent vertices. Sections VII and VIII summarize and discuss the results of this paper.

II. BASIC EQUATIONS

The time evolution of a random graph can be considered as a chain of coalescences of couples of linked components of the graph by randomly appearing edges connecting their vertices (see Fig. 1). In contrast to commonly known coagulation any extra edge diminishes the valence of each component by one. This process is represented by the scheme,

$$(g_1,\sigma_1+1)+(g_2,\sigma_2+1)\to(g_1+g_2,\sigma_1+\sigma_2). \tag{2}$$

The probability of coalescence is proportional to the product of total valences of two coalescing graphs. The maximal valence of a vertex is denoted as s. In the process of coalescence the valence of each linked component changes. Our model assumes that the probability to join an edge to a given vertex is independent of its free valence, which permits us not to count the numbers of vertices with given free valence. The respective equation looks as follows:

$$\frac{dc_{g,\sigma}(t)}{dt}=\frac{1}{2}\sum_{l,\eta}(\sigma-\eta+1)(\eta+1)c_{g-l,\sigma-\eta+1}(t)c_{l,\eta+1}(t)$$
$$-\sigma c_{g,\sigma}(t)\sum_{l,\eta}\eta c_{l,\eta}(t). \tag{3}$$

Here $c_{g,\sigma}=N_{g,\sigma}/M$ are the concentrations of the linked components, $N_{g,\sigma}$ is the total number of the graph components having the order g (g is the number of vertices in the component and σ its valence), and M is the total number of vertices in the graph.

Equation (3) should be supplemented with the initial conditions,

$$c_{g,\sigma}(0)=c^0_{g,\sigma}. \tag{4}$$

In what follows we consider initially monodisperse graphs with

$$c^0_{g,\sigma}=\delta_{g,1}w_\sigma. \tag{5}$$

Here $\delta_{i,k}$ is the Kroneker δ and w_σ is the probability to find the vertex with given valence σ. Of course, $\sum_\sigma w_\sigma=1$.

The process of cycle formation diminishes the valence of the component by two,

$$(g,\sigma)\to(g,\sigma-2). \tag{6}$$

The rate of this process is,

$$\frac{1}{2M}[(\sigma+2)(\sigma+1)c_{g,\sigma+2}(t)-\sigma(\sigma-1)c_{g,\sigma}(t)]. \tag{7}$$

In the thermodynamic limit $[M\to\infty, N(g,\sigma)\to\infty, N(g,\sigma)/M=c_{g,\sigma}(t)<\infty]$ the cycling does not contribute unless the concentration of the graph components with the valence of order M be finite.

III. GENERATING FUNCTION

In this section the method of generating functions applies for the solution of the kinetic Eq. (3). The exact expressions for the lower moments of the generating function are then derived for arbitrary initial conditions.

A. Basic equations and initial conditions

Let us introduce the bivariate generating function

$$\mathcal{F}(z,\xi;t)=\sum_{g,\sigma}c_{g,\sigma}(t)z^g\xi^\sigma. \tag{8}$$

It is not difficult to derive the equation for $\mathcal{F}$. On multiplying both sides of Eq. (3) by $z^g\xi^\sigma$ and summing over all g and σ give the equation for $\mathcal{F}$,

$$\frac{\partial\mathcal{F}}{\partial t}=\frac{1}{2}\left(\frac{\partial\mathcal{F}}{\partial\xi}\right)^2-\xi\frac{\partial\mathcal{F}}{\partial\xi}S. \tag{9}$$

Here

$$S=S(t)=\sum_{g,\sigma}\sigma c_{g,\sigma}(t)=\xi\left.\frac{\partial\mathcal{F}}{\partial\xi}\right|_{\xi=1} \tag{10}$$

is the average valence of the whole system.

The concentration $c_{g,\sigma}(t)$ is expressed through the generating function as follows:

$$c_{g,\sigma}(t)=\frac{1}{2\pi i}\oint\frac{d\xi}{\xi^{\sigma+1}}\mathcal{R}_g(\xi;t), \tag{11}$$

where

$$\mathcal{R}_g(\xi;t)=\frac{1}{2\pi i}\oint\frac{\mathcal{F}(z,\xi;t)dz}{z^{g+1}}. \tag{12}$$

Equation (10) should be supplemented with the initial condition

$$\mathcal{F}(z,\xi;0)=\mathcal{F}_0(z,\xi), \tag{13}$$

where the function $\mathcal{F}_0(z,\xi)$ is assumed to be known. In what follows we consider only monodisperse polyvalent initial conditions,

$$\mathcal{F}_0(z,\xi)=zw(\xi), \tag{14}$$

i.e., the initial graph is a collection of bare vertices with distributed valences, described by the function $w(\xi)$ normalized by the condition $w(1)=1$. Then $w(\xi)$ generates the probabilities w_σ for a given vertex to have the valence σ: $w(\xi)=\sum_\sigma w_\sigma \xi^\sigma$. For example, for monovalent graphs

$$w(\xi)=\xi^s, \tag{15}$$

where s is the vertex valence. If the initial graph consists of the vertices of two valence s_1 and s_2 then

$$w(\xi)=a\xi^{s_1}+b\xi^{s_2}, \tag{16}$$

with $a+b=1$. The coefficients a and b can be expressed through the average initial valence $\bar{s}=as_1+bs_2$. Assuming $s_2>s_1$ we find,

$$a=\frac{\bar{s}-s_1}{s_2-s_1},\quad b=\frac{s_2-\bar{s}}{s_2-s_1}. \tag{17}$$

For the modified Poisson distribution of the initial valences we have

$$w(\xi)=\xi^r e^{-\bar{\Delta}(1-\xi)}, \tag{18}$$

where $\Delta=\overline{s^2}-\bar{s}^2$ and $\bar{s}=\Delta$. At $r=0$ this distribution contains neutral vertices that do not participate in the coalescence process. The vertices with $s=1$ inhibit the graph growth.

B. Moments

We begin by formulating the closed equation for $\bar{S}(t)=\partial_\xi\mathcal{F}(1,1;t)$. On differentiating Eq. (9) over ξ and putting then $\xi=1$ one gets $\dot{S}=-S^2$. From here we immediately find,

$$S(t)=\frac{\bar{s}}{\bar{s}t+1}. \tag{19}$$

It is also possible to write down the equations for other moments. For the number concentration $N(t)=\sum_{g,\sigma}c_{g,\sigma}(t)=\mathcal{F}(1,1;t)$ one has

$$\dot{N}=-\tfrac{1}{2}S^2. \tag{20}$$

The solution to this equation is

$$N(t)=N_0-\frac{\bar{s}^2t}{2(\bar{s}t+1)}. \tag{21}$$

The initial concentration N_0 includes the total number of neutral components.

The total mass concentration $M=\sum_{g,\sigma}gc_{g,\sigma}(t)=\partial_z\mathcal{F}(1,1;t)$ is conserved,

$$\dot{M}=0. \tag{22}$$

It is not difficult to derive the equation for $Q=\mathcal{F}''_{\xi,\xi}(1,1;t)-S$. The result is

$$\frac{dQ}{dt}=Q^2. \tag{23}$$

The solution to this equation is well known

$$Q(t)=\frac{1}{t_c-t}, \tag{24}$$

where

$$t_c=\frac{1}{Q(0)}=\frac{1}{\overline{s^2}-2\bar{s}}. \tag{25}$$

In this equation $\overline{s^2}=\sum_\sigma\sigma^2w_\sigma$. This result evidences on the emergence of a giant linked component at $t=t_c$ whose order is comparable to the total mass of the graph.

This remarkable effect (referred to as gelation in colloid and polymer chemistry) had been discovered in the salient paper of Erdös and Rényi [22] and then widely discussed in the coagulation community (see review article [3]).

Of interest is to find the second moment of the mass distribution $\phi_2=\sum_{g,\sigma}g^2c_{g,\sigma}(t)=\partial_z z\partial_z\mathcal{F}(1,1;t)$. On differentiating twice Eq. (9) over z and using Eqs. (19), (20), and (23) leads to a simple result,

$$\dot{\phi}_2=U^2, \tag{26}$$

where the mixed moment

$$U=\sum_{g,\sigma}g\sigma c_{g,\sigma}(t)=\mathcal{F}''_{z,\xi}(1,1;t) \tag{27}$$

meets the following equation,

$$\dot{U}=UQ. \tag{28}$$

From here we find,

$$U=\bar{s}\frac{t_c}{t_c-t}. \tag{29}$$

Hence,

$$\phi_2(t)=\phi_2(0)+(\bar{s})^2\frac{t}{t_c-t}. \tag{30}$$

It is important to emphasize that all above equations are valid below the gelation time. The postgel period demands a special consideration (see below).

IV. SOLVING THE KINETIC EQUATION

Let us denote

$$P(t)=\exp\left[-\int_0^t S(t')dt'\right]. \tag{31}$$

On substituting

$$c_{g,\sigma}(t)=P^\sigma(t)b_{g,\sigma}(t) \tag{32}$$

into Eq. (3) and replacing the time variable

$$\tau=\int_0^t P^2(u)du \tag{33}$$

removing the loss term from the kinetic equation Eq. (3) and converting it to the recurrences for $b(g,\sigma;t)$,

$$\frac{db_{g,\sigma}(\tau)}{d\tau} = \frac{1}{2}\sum_{l,\eta}(\sigma-\eta+1)(\eta+1)b_{g-l,\sigma-\eta+1}(\tau)b_{l,\eta+1}(\tau). \tag{34}$$

The dependence of τ and P on t is readily found from Eqs. (19) and (33)

$$\tau(t) = \frac{t}{\bar{s}t+1} \quad \text{and} \quad P(t) = 1-\bar{s}\tau = \frac{1}{\bar{s}t+1}. \tag{35}$$

Let us now introduce the bivariate generating function,

$$F(z,\xi;\tau) = \sum_{g,\sigma} b_{g,\sigma}(\tau)z^g\xi^\sigma \tag{36}$$

From Eq. (34) one finds,

$$\frac{\partial F}{\partial \tau} = \frac{1}{2}\left(\frac{\partial F}{\partial \xi}\right)^2. \tag{37}$$

The initial condition to this equation is

$$F(z,\xi;0) = F_0(z,\xi), \tag{38}$$

where F_0 is a known function.

It is more convenient to deal with the function $Y(z,\xi;\tau) = F'_\xi(z,\xi,\tau)$. We differentiate Eq. (37) over ξ and obtain,

$$\frac{\partial Y}{\partial \tau} = Y\frac{\partial Y}{\partial \xi}. \tag{39}$$

Two characteristics of this equation $\tau Y + \xi = C$ and $Y = D$ (C and D are the integration constants) allow one to write down the solution to this equation in the form:

$$Y(z,\xi;\tau) = Y_0(z,\theta), \tag{40}$$

where $Y_0(z,\xi) = \partial_\xi F_0(z,\xi)$ and $\theta = \theta(z,\xi;\tau)$ is the solution to the transcendent equation,

$$\theta = \xi + \tau Y_0(z,\theta). \tag{41}$$

At $s=3$ and initially empty graph this equation is readily solved. The result is

$$\theta = \frac{2\xi}{1+\sqrt{1-12\tau z\xi}}. \tag{42}$$

The generating function $Y(z,\xi;t)$ is thus,

$$Y(z,\xi;\tau) = \frac{\theta-\xi}{\tau} = \frac{\xi(1-\sqrt{1-12\tau z\xi})}{\tau(1+\sqrt{1-12\tau z\xi})}. \tag{43}$$

V. POSTCRITICAL BEHAVIOR

This section focuses on the postcritical behavior of the moments $S(t)$, $M(t)$, and $Q(t)$.

A. General analysis

All these moments are expressed in terms of $\hat{\theta} = \theta^{(1)}$, where $\theta^{(\xi)} = \theta(1,\xi P,t)$ meets the equation,

$$\theta^{(\xi)} = P\xi + \tau Y_0(1,\theta^{(\xi)}). \tag{44}$$

Indeed,

$$\begin{aligned}\bar{S}(t) &= \left.\frac{\partial \mathcal{F}(z,\xi;t)}{\partial \xi}\right|_{z=\xi=1} = \left.\frac{\partial F(z,P\xi;t)}{\partial \xi}\right|_{z=\xi=1} \\ &= PY(1,P;t) = P\frac{(\hat{\theta}-P)}{\tau}.\end{aligned} \tag{45}$$

Similarly, we find

$$\mathcal{F}''_{\xi\xi}(1,\xi;t) = P\partial_\xi Y(1,\xi P;t) = \frac{P}{\tau}\partial_\xi(\theta^{(\xi)} - P\xi). \tag{46}$$

The derivative $\partial_\xi\theta^{(\xi)}$ is readily found from Eq. (44)

$$\partial_\xi\theta^{(\xi)} = \frac{P}{1-\tau Y'_0(1,\theta^{(\xi)})}. \tag{47}$$

Then we find,

$$\mathcal{F}''_{\xi\xi}(1,\xi;t)|_{\xi=1} = P^2\frac{Y'_0(\hat{\theta})}{1-\tau Y'_0(\hat{\theta})}. \tag{48}$$

The combination $Q = \mathcal{F}''_{\xi\xi} - S(t)$ as the function of $\hat{\theta}$ is [see Eqs. (45) and (48)],

$$Q = P^2\frac{Y'_0(\hat{\theta})}{1-\tau Y'_0(\hat{\theta})} - P\frac{(\hat{\theta}-P)}{\tau}. \tag{49}$$

At $\hat{\theta} = 1$ (the precritical period) Eqs. (45) and (48) reproduce the results of Eqs. (19) and (24)

Now we find the expression for the total mass of the graph in the postcritical period. We note that

$$\begin{aligned}\mathcal{F}(z,1;t) &= F(z,P;t) = P\int_0^1 Y(z,P\eta;\tau)d\eta \\ &= P\int_0^1 Y_0(z,\theta^{(\eta)})d\eta,\end{aligned} \tag{50}$$

and replace the variables $\eta \to \theta^{(\eta)}$. On substituting $d\eta = P^{-1}(1-\tau\partial_{\theta^{(\eta)}}Y_0)d\theta^{(\eta)}$ into Eq. (50) gives,

$$\mathcal{F}(z,1;t) = \int_0^{\tilde{\theta}} Y_0(z,\zeta)d\zeta - \frac{\tau}{2}Y_0^2(z,\tilde{\theta}), \tag{51}$$

where

$$\tilde{\theta}(z,\tau) = \theta(z,P;\tau). \tag{52}$$

From this equation we have,

$$\begin{aligned}\partial_z\mathcal{F}(z,1,t) &= Y_0\partial_z\tilde{\theta} + \int_0^{\tilde{\theta}}\partial_z Y_0(z,\zeta)d\zeta \\ &\quad - \tau Y_0\partial_z Y_0 - \tau\partial_{\tilde{\theta}}Y_0\partial_z\tilde{\theta}.\end{aligned} \tag{53}$$

Taking $\tilde{\theta}$ from Eq. (52), gives,

$$\partial_z\tilde{\theta} = \frac{\tau\partial_z Y_0}{1-\tau\partial_{\tilde{\theta}}Y_0}. \tag{54}$$

We thus have,

$$\partial_z\mathcal{F}(z,1,t) = \int_0^{\tilde{\theta}(z,\tau)}\partial_z Y_0(z,\theta)d\theta. \tag{55}$$

This is the generating function for the mass distribution. The average mass is then

$$M=\int_0^{\hat{\theta}}\partial_z Y_0(1,\theta)d\theta. \tag{56}$$

For an initially polyvalent empty graph

$$\partial_z\mathcal{F}(z,1,t)=w[\tilde{\theta}(z,\tau)] \tag{57}$$

and

$$M(t)=w(\hat{\theta}). \tag{58}$$

For an initially monovalent empty graph the result of Ref. [14] is readily reproduced,

$$M(t)=\hat{\theta}^s. \tag{59}$$

Similar consideration gives the expression for the second moment of the order spectrum $c_g(t)=\sum_\sigma c_{g,\sigma}(t)$,

$$\begin{aligned}\phi_2(t)&=\frac{d}{dz}zw(\tilde{\theta})\bigg|_{z=1}\\&=w(\hat{\theta})+\bar{s}f(\hat{\theta})\frac{\bar{s}tf(\hat{\theta})}{1+\bar{s}t[1-f'(\hat{\theta})]}.\end{aligned} \tag{60}$$

At the precritical period this equation reproduces the general result Eq. (30).

B. Emergence of giant component

From Eq. (44) we obtain,

$$\hat{\theta}=P+\tau w'(\hat{\theta}). \tag{61}$$

Noting that $P+\bar{s}\tau=1$ [Eq. (35)] we find that $\hat{\theta}=1$ is the solution to Eq. (61). However, at $t>t_c=\bar{s}^2-2\bar{s}$ there is another solution $\hat{\theta}<1$ that corresponds to the emergence of the giant component. Indeed, the sol mass given by Eq. (56) diminishes as the upper limit of integration $\hat{\theta}$ drops down.

In order to demonstrate what is going on, let us consider the monovalent initial condition $w(\xi)=\xi^s$ and solve Eq. (61) with respect to st. The result looks as follows:

$$st=\frac{1}{\hat{\theta}(1+\hat{\theta}\dots+\hat{\theta}^{s-3})}. \tag{62}$$

The limit $\hat{\theta}\to 1$ in this equation reproduces the expression Eq. (15) for the critical time.

Equation (62) is analytically solvable at $s=3$ and $s=4$. At $s=3$ and $t>1/3$ we have,

$$\hat{\theta}=\frac{1}{3t}. \tag{63}$$

It is easy to check that Eq. (42) gives $\hat{\theta}=1$ at $t<t_c=1/3$ and $\hat{\theta}=1/3t$ at $t>t_c=1/3$.

At $s=4$ the result is a bit more complex. At $t\geqslant 1/8$

$$\hat{\theta}=\frac{1}{2(t+\sqrt{t^2+t})}. \tag{64}$$

VI. SPECTRUM

The spectrum of the linked components is expressed in terms of the generating function $\mathcal{F}$ as follows:

$$\begin{aligned}c_{g,\sigma}(t)&=\frac{1}{2\pi i}\oint\frac{dz}{z^{g+1}}\frac{1}{2\pi i}\oint\frac{\mathcal{F}(z,\xi;t)d\xi}{\xi^{\sigma+1}}\\&=\frac{P^\sigma}{2\pi i}\oint\frac{dz}{z^{g+1}}\frac{1}{2\pi i}\oint\frac{F(z,\xi;t)d\xi}{\xi^{\sigma+1}}.\end{aligned} \tag{65}$$

Let us integrate by parts in the last integral,

$$\begin{aligned}\frac{1}{2\pi i}\oint\frac{F(z,\xi;t)d\xi}{\xi^{\sigma+1}}&=\frac{1}{2\pi i\sigma}\oint\frac{\partial_\xi F(z,\xi;t)d\xi}{\xi^\sigma}\\&=\frac{1}{2\pi i\sigma}\oint\frac{Y(z,\xi;t)d\xi}{\xi^\sigma}.\end{aligned} \tag{66}$$

The last integral is expressed through the initial generating function Y_0

$$\frac{1}{2\pi i\sigma}\oint\frac{Y(z,\xi;t)d\xi}{\xi^\sigma}=\frac{1}{2\pi i\sigma}\oint\frac{Y_0[z,\theta(z,\xi;t)]d\xi}{\xi^\sigma}. \tag{67}$$

Finally we have,

$$c_{g,\sigma}(t)=\frac{P^\sigma}{2\pi i\sigma}\oint\frac{d\xi}{\xi^\sigma}\frac{1}{2\pi i}\oint\frac{Y_0[z,\theta(z,\xi;t)]dz}{z^{g+1}}. \tag{68}$$

A. Evolution of empty graph

For the initially empty polyvalent graph

$$Y(z,\xi;0)=Y_0(z,\xi)=\bar{s}zf(\xi). \tag{69}$$

Here $f(\xi)=\bar{s}^{-1}w'(\xi)$. Hence (in what follows we omit hat over θ),

$$\theta=\xi+\bar{s}z\tau f(\theta). \tag{70}$$

Now we calculate the integral

$$R_g(\xi,\tau)=\frac{1}{2\pi i}\oint\frac{Y(z,\xi;\tau)dz}{z^{g+1}}. \tag{71}$$

Let us replace the integration variable $z\to\theta$. To this end we solve Eq. (70) with respect to z

$$z=\frac{\theta-\xi}{\bar{s}z\tau f(\theta)}, \tag{72}$$

and differentiate it. The result is,

$$dz=\frac{d\theta}{\tau\bar{s}f(\theta)}-\frac{(\theta-\xi)df}{\bar{s}\tau f^2}. \tag{73}$$

The first term thus contributes,

$$\begin{aligned}&\frac{1}{2\pi i}\oint\frac{Y(z,\xi;\tau)dz}{z^{g+1}}\\&\quad=\bar{s}(\tau\bar{s})^{g-1}\frac{1}{2\pi i}\oint\left[\frac{f^g(\theta)}{(\theta-\xi)^g}-\frac{f^{g-1}f'}{(\theta-\xi)^{g-1}}\right]d\theta.\end{aligned} \tag{74}$$

The second term in dz [Eq. (74)] allows for the integration by parts. After some algebra we obtain,

$$R_g(\xi,\tau)=\frac{1}{2\pi ig}\bar{s}(\bar{s}\tau)^{g-1}\oint\frac{f^g(\theta)}{(\theta-\xi)^g}d\theta. \tag{75}$$

On replacing $\zeta = \theta - \xi$ we come to the result,

$$R_g(\xi,\tau) = \frac{1}{2\pi i g}\bar{s}(\bar{s}\tau)^{g-1}\oint \frac{f^g(\zeta+\xi)}{\zeta^g}d\zeta. \tag{76}$$

Thus the spectrum is,

$$c_{g,\sigma}(t) = \frac{P^\sigma \bar{s}(\bar{s}\tau)^{g-1}}{2\pi i\sigma}\oint \frac{d\xi}{\xi^\sigma}\frac{1}{2\pi i g}\oint \frac{d\zeta}{\zeta^g}f^g(\zeta+\xi). \tag{77}$$

It is important to note that the spectrum is expressed as a product of two multipliers, the first of which depends on time while the second does not.

$$c_{g,\sigma}(t) = \frac{(\bar{s}t)^{g-1}}{(\bar{s}t+1)^{g+\sigma-1}}\mathcal{G}_{g,\sigma}, \tag{78}$$

where

$$\mathcal{G}_{g,\sigma} = \bar{s}\frac{1}{2\pi i\sigma}\oint \frac{d\xi}{\xi^\sigma}\frac{1}{2\pi i g}\oint \frac{d\zeta}{\zeta^g}f^g(\zeta+\xi). \tag{79}$$

In the case of monovalent vertices $f(\xi) = \xi^{s-1}$ and

$$\begin{aligned}\mathcal{G}_{g,\sigma} &= s\frac{1}{g\sigma}\begin{pmatrix} g-1 \\ g(s-1)\end{pmatrix}\delta_{\sigma,g(s-2)+2} \\ &= \bar{s}\frac{[g(s-1)]!}{g![g(s-2)+2]!}\delta_{\sigma,g(s-2)+2}.\end{aligned} \tag{80}$$

This result is known and cited elsewhere, e.g., in Ref. [14].

For the distributed valences with $f(\xi) = e^{\bar{s}(\xi-1)}$ Eq. (79) gives,

$$\begin{aligned}\mathcal{G}_{g,\sigma} &= \bar{s}\frac{1}{2\pi i\sigma}\oint \frac{d\xi}{\xi^\sigma}\frac{1}{2\pi i g}\oint \frac{d\zeta}{\zeta^g}e^{g\bar{s}(\zeta+\xi-1)} \\ &= \frac{\bar{s}}{g!\sigma!}e^{-g\bar{s}}(g\bar{s})^{g+\sigma-1}.\end{aligned} \tag{81}$$

In this case the order of the graph g no longer fixes the number of edges in linked components.

B. Spectrum of orders

Equation (57) can be used for deriving the spectrum of orders of the graph. Indeed, for an initially polyvalent empty graph [see Eq. (57)],

$$\partial_z\mathcal{F}(z,1,t) = w[\hat{\theta}(z,\tau)] = \sum_g g c_g(t)z^{g-1} \tag{82}$$

or

$$c_g(t) = \frac{1}{2\pi i g}\oint \frac{w[\hat{\theta}(z,\theta;t)]}{z^g}dz. \tag{83}$$

Let us replace the variables $z \to \theta$. To this end we use the equation for $\hat{\theta}$

$$z = \frac{\hat{\theta}-P}{\bar{s}\tau f}. \tag{84}$$

Differentiating this equation yields,

$$dz = \frac{d\hat{\theta}}{\bar{s}\tau f} - \frac{(\hat{\theta}-P)f'd\hat{\theta}}{\bar{s}\tau f^2}. \tag{85}$$

The first term in this equality contributes to $c_g(t)$ [Eq. (82)],

$$\oint \frac{(\bar{s}\tau f)^g w}{(\hat{\theta}-P)^g}\frac{d\hat{\theta}}{\bar{s}\tau f} = (\bar{s}\tau)^{g-1}\oint \frac{f^{g-1}wd\hat{\theta}}{(\hat{\theta}-P)^g}. \tag{86}$$

On integrating by parts in the second term gives,

$$\begin{aligned}&\oint \frac{(\bar{s}\tau f)^g w}{(\hat{\theta}-P)^g}\frac{(\hat{\theta}-P)f'd\hat{\theta}}{\bar{s}\tau f^2} \\ &\quad= (\bar{s}\tau)^{g-1}\oint \frac{f^{g-1}wd\hat{\theta}}{(\hat{\theta}-P)^g} - \bar{s}\frac{(\bar{s}\tau)^{g-1}}{g-1}\oint \frac{f^g d\theta}{(\theta-P)^{g-1}}.\end{aligned} \tag{87}$$

The order spectrum of linked components in the graph is thus,,

$$\begin{aligned}c_g(t) &= \bar{s}\frac{(\bar{s}\tau)^{g-1}}{g(g-1)}\frac{1}{2\pi i}\oint \frac{f^g d\theta}{(\theta-P)^{g-1}} \\ &= \bar{s}\frac{(\bar{s}\tau)^{g-1}}{g(g-1)}\frac{1}{2\pi i}\oint \frac{f^g(\zeta+P)d\zeta}{\zeta^{g-1}}.\end{aligned} \tag{88}$$

C. Saddle-point estimations

Equation (88) is well adapted for the saddle-point estimations of the spectrum at large g. The condition

$$\frac{f'(\zeta_0+P)}{f(\zeta_0+P)} = \frac{1}{\zeta_0} \tag{89}$$

determines the position $\zeta_0 = \zeta_0(\tau)$ of the saddle point. The order spectrum in the limit of large g is thus,

$$\begin{aligned}c_g(t) &= \bar{s}\frac{(\bar{s}\tau)^{g-1}}{\sqrt{2\pi g f''(\zeta_0+P)}g(g-1)}\frac{f^g(\zeta_0+P)}{\zeta_0^{g-1}} \\ &\propto Ag^{-5/2}e^{g[\ln\bar{s}\tau+\ln f(\zeta_0+P)-\ln\zeta_0]}.\end{aligned} \tag{90}$$

The critical time is found from the condition

$$\ln\bar{s}\tau_c + \ln f(\zeta_{0,c}+P_c) - \ln\zeta_{0,c} = 0. \tag{91}$$

This condition removes the exponential factor from the critical spectrum [Eq. (90)]. The identities $\bar{s}\tau_c + P(\tau_c) = 1$ and $f(1) = 1$ allow one to find the solution to Eq. (91). It is

$$\zeta_{0,c} = \zeta_0(\tau_c) = \bar{s}\tau_c - \frac{\bar{s}}{\bar{s}^2-\bar{s}}. \tag{92}$$

The critical spectrum is thus,

$$\begin{aligned}c_g(t_c) &\approx \frac{\bar{s}}{\sqrt{2\pi f''(\zeta_0+P)g^5}} \\ &= \frac{\bar{s}^{3/2}}{\sqrt{2\pi\overline{s(s-1)(s-2)}g^5}} \propto g^{-5/2}.\end{aligned} \tag{93}$$

The identity $f''(1) = (\bar{s})^{-1}(w')''_{\zeta=1} = \overline{s(s-1)(s-2)}/\bar{s}$ is used in deriving the above equation.

In order to find the time dependence of the spectrum near the critical point we note that

$$\begin{aligned}&\frac{d}{d\tau}[\ln\bar{s}\tau + \ln f(\zeta_0+P) - \ln\zeta_0]|_{\tau=\tau_c} \\ &\quad= \frac{1}{\tau_c} + \frac{f'_c}{f_c}(\zeta'_{0,c}+P'_c) - \frac{\zeta'_{0,c}}{\zeta_{0,c}} = 0.\end{aligned} \tag{94}$$

Indeed, Eq. (89) provides the cancellation of the terms containing $\zeta'_{0.c}$. Next, applying the equalities $P'_c = -\bar{s}$ and $f'_c = (\overline{s^2 - s})/\bar{s}$ leads to Eq. (93).

Near the critical point Eq. (91) for the spectrum can be rewritten as

$$c_g(t) = c_g(t_c)e^{-Bg(t-t_c)^2}. \tag{95}$$

In principle, we can calculate the second derivative of the LHS of Eq. (94) and put $\tau = \tau_c$. However, it is much easier to use the expression for ϕ_2 [Eq. (30)]. At t close to t_c we have,

$$\phi_2(t) = \phi_2(0) + (\bar{s})^2\frac{t}{t_c - t} \approx (\bar{s})^2\frac{t_c}{t_c - t}. \tag{96}$$

On the other hand,

$$\phi_2(t) = \sum_g g^2 c_g(t) \approx \int_0^\infty c_g(t_c)e^{-Bg(t-t_c)^2} = A\sqrt{\frac{\pi}{B}}\frac{1}{t_c - t}. \tag{97}$$

Hence,

$$A\sqrt{\frac{\pi}{B}} = \bar{s}^2 t_c = \frac{\bar{s}}{\bar{s} - 2}. \tag{98}$$

Finally we have

$$c_g(t) = Ag^{-5/2}e^{-gB(t-t_c)^2} \tag{99}$$

with

$$A = \frac{\bar{s}^{3/2}}{\sqrt{2\pi\overline{s(s-1)(s-2)}}} \qquad B = \frac{\bar{s}(\bar{s}-2)^2}{2[\overline{s(s-1)(s-2)}]}. \tag{100}$$

VII. RESULTS AND DISCUSSION

The main results of this paper can be summarized as follows:

(i) The kinetic equation [Eq. (3)] describing the time evolution of the order-valence spectrum of linked components of a random graph with polyvalent vertices is formulated.

(ii) This equation is then reformulated in terms of the bivariate generating function for the spectrum and solved exactly for arbitrary initial conditions.

(iii) The time dependence of the lowest moments of the spectrum is found for arbitrary initial conditions. It is demonstrated that the present model successfully describes the emergence of the giant component after a critical time.

(iv) The spectrum of orders and valences is expressed through the contour integrals of initial distribution of the vertex valences [Eqs. (78) and (88)]. The asymptotic behavior of these integrals is studied by the saddle-point method. The asymptotic spectrum is shown to comprise two parts: the algebraic multiplier (standard $g^{-5/2}$ dependence) and an exponential factor [see Eq. (99)]. The coefficients in this expression contain the third moment of the valence distribution.

(v) An alternative derivation of all previously known results [7–14] for the initially empty monovalent graphs is given.

The structural properties of an evolving random graph change in adding extra edges one at a time. In particular, the distribution of the linked components in such graphs becomes broader with time. The distribution evolves to an algebraic one and a giant component emerges after a finite period of time (at $t > t_c$). This pattern is common for many types of random graphs.

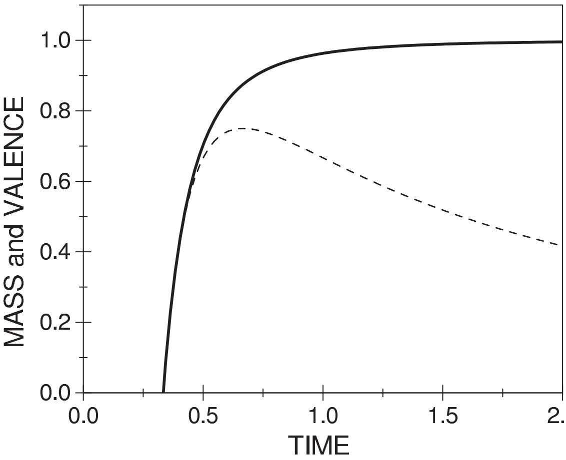

FIG. 2. The time dependence of total order (solid line) and total valence (dash line) of the giant component for $s = 3$.

The random graph with finite valence of the vertices is not an exclusion. In contrast to widely studied random graphs the time evolution of such graphs is described in terms of bivariate concentrations of linked components over their order g and valence σ. The coalescence rate depends on the total valences of the coalescing components. Each extra edge kills randomly a couple of free valences in the graph. Respectively, the graph jumps from the state with k free valences to the state with $k - 2$ valences. The analogy with the reaction of annihilation is clearly seen (see also Ref. [14]). The kinetic equation for the total valence has thus the form:

$$\dot{\bar{S}} = -\bar{S}^2.$$

The same result comes from the differentiation of the generating function [Eq. (6)]. At the postcritical period the part of the valent vertices belongs to the giant component. The valence and order of the gel have been found in Sec. V for the giant and small components. The results are displayed in Figs 2 and 3.

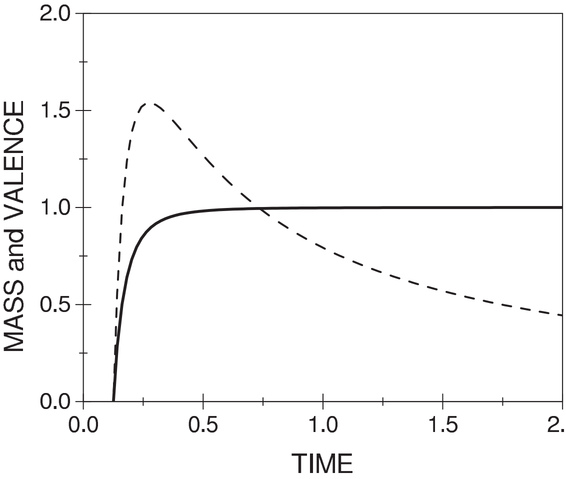

FIG. 3. Same as in Fig. 2 for $s = 4$.

As expected the critical time is shorter for the graphs with larger vertex valence s.

In the case of an initially empty graph the present model recalls the Flory model of polymerization. The point is that at large M when we can ignore cycling, the linking of bare vertices leads to the formation of trees, in which the valence and the mass of each component are connected. Indeed, the number of edges in the tree of mass g is $g-1$. Each edge reduces the valence of the component by 2. Hence, the valence of the component containing g vertices is $gs-2(g-1)=g(s-2)+2$. Of course, Eq. (80) reproduces this result. The ring formation was investigated numerically in Ref. [9]. Some analytical results on this issue had been reported in Refs. [10,11].

In principle, the present approach allows for consideration of cycling [see Eqs. (6) and (7)] but, in my opinion, it is better to do by applying the approach of Ref. [27].

VIII. CONCLUSIONS

In this paper the model describing the dynamics of the coalescing random graph has been proposed. In contrast to commonly accepted approaches relying upon the analogy between graph coalescence and the coagulating system with the product kernel [3] the present model considers the coalescence rate proportional to the product of the total valences of coalescing components. The dependence of the coalescence rate on the masses does not enter explicitly into the kinetic equation. This equation has been then formulated in terms of the bivariate generating function that has been found exactly for arbitrary initial conditions. In turn, this result allowed for finding the time dependences of the valence of the giant component and its mass.

The formal chemical kinetic approach Eq. (2) allows for consideration of thermodynamically large systems, where the total numbers of each linked component is of the total order of the graph M. This means that the giant component is indistinguishable in the thermodynamic limit, i.e., its concentration goes to zero as $M\to\infty$. Still we can distinguish this giant component from indirect evidences: its total order and valence contribute to the respective balances after the critical time.

There exists a more straightforward (but much more complex) approach to the time evolution of random graphs. I mean the approach of Ref. [27] that operates with the probability to find the graph in a given definite state. This probability obeys a master equation that had been solved by me for normal random graphs in Ref. [27]. It is likely that this approach can also be applied to the problem considered above.

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