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The Equilibrium Behavior of Reversible Coagulation-Fragmentation Processes

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The coagulation-fragmentation process models the stochastic evolution of a population of N particles distributed into groups of different sizes that coagulate and fragment at given rates. The process arises in a variety of contexts and has been intensively studied for a long time. As a result, different approximations to the model were suggested. Our paper deals with the exact model which is viewed as a time-homogeneous interacting particle system on the state space Ω_N, the set of all partitions of N. We obtain the stationary distribution (invariant measure) on Ω_N for the whole class of reversible coagulation-fragmentation processes, and derive explicit expressions for important functionals of this measure, in particular, the expected numbers of groups of all sizes at the steady state. We also establish a characterization of the transition rates that guarantee the reversibility of the process. Finally, we make a comparative study of our exact solution and the approximation given by the steady-state solution of the coagulation-fragmentation integral equation,which is known in the literature. We show that in some cases the latter approximation can considerably deviate from the exact solution.

KEY WORDS: Coagulation-fragmentation processes; interacting particle systems; reversibility; equilibrium.

1. INTRODUCTION

The coagulation-fragmentation process (CFP) models the stochastic evolution in time of a population of N particles, distributed into groups that coagulate and fragment at different rates. The model arises in different contexts of application. Some examples are polymer kinetics, astrophysics, aerosols, and biological phenomena such as animal grouping and blood

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cell aggregation [see e.g., Barrow,[6] Hidy and Brock (eds.),[17] and Okubo[23]]. Our paper focuses on the study of the steady state of the process, and is organized as follows.

Section 2 describes the history of the problem, mainly the following two approximations to the model: (i) the dynamical system of Smoluchowski differential equations and (ii) the coagulation-fragmentation integral equation derived from (i) by passing to the continuum state space.

In Section 3, we present the definition of the exact model viewed as a time-homogeneous interacting particle system on the state space of all partitions of the total number N of particles, the approach that was suggested in a recent paper by Gueron.[14]

Section 4, which is divided into three subsections, contains the main results of our study of the steady state distributions of the whole class of reversible CFPs. We establish a characterization of transition rates providing the reversibility, and find explicitly the invariant measure of the processes considered. Further, we construct the generating function for the sequence of values of the partition function of the reversible invariant measure for different N, and derive explicit formulas for a variety of important quantities associated with the steady state.

In Section 5, we compare the known steady state solution $f(x)$, $x \geqslant 0$ of the coagulation-fragmentation integral equation with the corresponding exact solution given by the functional $f(N; k)$ ($=$the expected number of groups of size $k \leqslant N$ at equilibrium). We prove that for a fixed $x = k$, $f(N; k) \sim f(x)$, as $N \to \infty$. However, we also discover the possibility of a considerable deviation of the approximation $f(x)$ from the exact solution in the case when k is large, i.e., $k = k(N) \sim N$, as $N \to \infty$.

Finally, Section 6 discusses three particular CFPs. Implementing the results of our previous study we obtain for these processes the explicit expressions for partition functions and other quantities of interest. The CFPs considered provide examples where the previously mentioned deviation indeed occurs.

2. THE HISTORY OF THE PROBLEM

There is a huge literature on CFP dispersed in a variety of journals in different fields of science. We describe here briefly only the lines of research immediately related to the subject of our paper.

2.1. The Smoluchowski System of Coagulation-Fragmentation Differential Equations

To the best of our knowledge, the systematical study of the deterministic version of CFP started at the beginning of the century by Smoluchowski [see Drake,[9] Ernst,[12] and Jeon,[18] for reference], who derived a system of differential equations approximating the time evolution of the density (per unit volume) $c_j = c_j(t)$, $t \geqslant 0$ of clusters (groups) of particles A_j of size j, $j = 1, 2,...$, in a population of infinite size. This system, generalized to CFP (Smoluchowski considered only pure coagulation), can be written as

$$\dot{c}_j = \frac{1}{2} \sum_{k=1}^{j-1} K_{j-k,k} c_{j-k} c_k - \sum_{k=1}^{\infty} K_{jk} c_j c_k - \frac{1}{2} \sum_{k=1}^{j-1} F_{j-k,k} c_j + \sum_{k=1}^{\infty} F_{jk} c_{j+k}, \qquad j = 1, 2,... \tag{2.1}$$

Here, the reaction coefficients $K_{jk} = K_{kj}$ and $F_{jk} = F_{kj}$ represent the rates of the reactions $A_k + A_j \to A_{k+j}$ and $A_{j+k} \to A_j + A_k$, respectively. The Becker-Döring equation, derived in 1935, is a particular case of (2.1) when only reactions of the type $A_k + A_1 \to A_{k+1}$ and $A_j \to A_{j-1} + A_1$ are possible [Ball *et al.*,[5] and Penrose[24, 25]].

Note that the dynamical system (2.1) can be viewed as an approximation of the Kolmogorov backward equations for the expected density $c_j(t)$, $t \geqslant 0$, obtained by neglecting dependence between clusters.

Questions concerning the existence and uniqueness of solutions to (2.1), exact solutions for special reaction rates, the phenomenon of gelation (the appearance of an infinitely large cluster), and total mass conservation, pose difficult mathematical problems, some of which have been solved [e.g., Drake,[9] Hendriks *et al.*,[16] McLeod,[20] Spouge,[27] van Dongen and Ernest,[34, 35] White,[36] Ziff and McGrady,[38] and Jeon[18]].

Gueron[14] raised the question of the validity of the system (2.1) for the description of time dynamics of CFPs. The CFP as defined by Gueron[14] is a continuous-time homogeneous Markov chain on the state space Ω_N of all partitions of N. Based on this approach, the exact version of (2.1) was derived, and for small values of N a numerical procedure for computing the stationary distribution of group sizes was proposed.

Comprehensive expository papers by Aldous[2, 3] focus on Smoluchowski equations for pure coagulation, viewed as a deterministic model. The main emphasis in these papers is given to construction of abstract coalescing stochastic models, seemingly unrelated to the coagulation context, and such that the expected density of clusters at any time $t \geqslant 0$ satisfies the equations (2.1) under $F = 0$. Aldous[2] describes a number of open problems related to (2.1) and their continuous analogue represented in the next section.

2.2. The Coagulation-Fragmentation Integral Equation

Difficulties in treatment of the Smoluchowski equations lead to formulation of a continuous (in state space) model of the CFP. Assuming that the size of groups x ranges in $[0, +\infty)$, the following integro-differential equation describing the evolution of $c(x, t)$, $t \geqslant 0$, the expected number of groups of size x at time t, was derived:

$$\begin{aligned}\frac{\partial}{\partial t} c(x, t) = {} & \frac{1}{2} \int_0^x K(x-y, y)\, c(x-y, t)\, c(y, t)\, dy \\ & - \int_0^\infty K(x, y)\, c(x, t)\, c(y, t)\, dy \\ & - \frac{1}{2} \int_0^x F(x-y, y)\, c(x, t)\, dy \\ & + \int_0^\infty F(x, y)\, c(x+y, t)\, dy \end{aligned} \tag{2.2}$$

Here, the symmetric (in $x \geqslant 0$ and $y \geqslant 0$) kernels $F(x, y) \geqslant 0$, $K(x, y) \geqslant 0$ represent, correspondingly, the rate of fragmentation of a group of size $x+y$ into two groups of sizes x and y, and the rate of coagulation of two groups of sizes x and y into one group of size $x+y$. Equation (2.2), formulated in 1945 by Blatz and Tobolsky (for the case $F=0$) [for references see Aizenman and Bak[1]], has been subsequently studied by many authors. A crucial contribution was made by Aizenman and Bak[1] that proved the existence and uniqueness of solutions, and convergence to the equilibrium (stationary solution) as $t \to \infty$, in the case where the kernels K and F are constant and equal to each other. They also proved the exponential decay (in time) of the free energy of the system. The latter result, viewed as an analogue of the Bolzmann's H-theorem, provided the thermodynamic justification of (2.2). Stewart and Dubovskii[32] generalized most of the results[1] to constant kernels that are not necessarily equal. Problems concerning the uniqueness and existence of solutions of (2.2) for bounded and unbounded kernels, in particular for the special cases of pure coagulation ($F \equiv 0$) or pure fragmentation ($K \equiv 0$), have been addressed in a number of papers. Some of this work can be found in Stewart,[29–31] and Dubovskii and Stewart,[10] and the references therein.

Gueron and Levin[15] investigated (2.2) in the context of animal grouping, studying the solution in the case when the kernels are of the form

$$K(x, y) = b(x)\, b(y), \qquad F(x, y) = b(x+y), \qquad x, y \geqslant 0 \tag{2.3}$$

They showed that, for a given population size $M > 0$, the unique stationary solution $f(x) := \lim_{t \to \infty} c(x, t)$, $x \geqslant 0$ in this case is given by the function

$$f(x) = \frac{e^{-\lambda x}}{b(x)} \tag{2.4}$$

where the coefficient λ is subject to the condition

$$\int_0^\infty z f(z)\, dz = M \tag{2.5}$$

As we now explain, the form (2.3) is a particular case of kernels satisfying the detailed balance condition for $f(x)$. In fact, for $f(x)$ to be the equilibrium solution of (2.2), it is sufficient that it satisfy

$$\begin{gathered}\int_0^x K(x-y, y)\, f(x-y)\, f(y)\, dy = \int_0^x F(x-y, y)\, f(x)\, dy, \qquad x \geqslant 0\\ \int_0^\infty K(x, y)\, f(x)\, f(y)\, dy = \int_0^\infty F(x, y)\, f(x+y)\, dy, \qquad x \geqslant 0\end{gathered} \tag{2.6}$$

These two conditions are satisfied simultaneously if we require the "deterministic detailed balance" (see the next section) with respect to $f(x)$:

$$K(x, y)\, f(x)\, f(y) = F(x, y)\, f(x+y), \qquad x, y \geqslant 0 \tag{2.7}$$

It is easy to see that the kernels in (2.3) indeed satisfy (2.7).

3. DEFINITION OF THE MODEL

We follow the formulation of the model suggested by Gueron.[14] Consider a population of N particles distributed into groups of various sizes that undergo stochastic evolutions (in time) of coagulation (merging) and fragmentation (splitting). The possible events are merging of two groups into one, and splitting of one group into two groups (fragments). The stochastic process is a time-homogenous interacting particle system (IPS) φ_t, $t \geqslant 0$ defined as follows.

For a given N, denote by η a partition of the whole population N into n_i groups of size i, $i = 1, 2,..., N$, namely, $\eta = (n_1,..., n_N)$, where the numbers of groups $n_i \geqslant 0$ are subject to the condition:

$$\sum_{i=1}^N i n_i = N \tag{3.1}$$

The finite set $\Omega = \Omega_N = \{\eta\}$ of all partitions (configurations) of N is the state space of the process φ_t, $t \geqslant 0$. The rates of the infinitesimal (in time) transitions are assumed to depend only on the sizes of the interacting groups, and are given by:

1. For i and j such that $2 \leqslant i + j \leqslant N$ we denote by $\psi(i, j)$ the rate of merging $(i, j) \to (i + j)$ of two groups of sizes i and j into one group of size $i + j$;
2. The rate of splitting, $(i + j) \to (i, j)$, of a group of size $i + j$ into two fragments of sizes i and j, is denoted by $\phi(i, j)$.

Hereafter, we refer to the coagulation and fragmentation rates $\psi(i, j)$, and $\phi(i, j)$ as intensities. The intensities are required to satisfy $\psi(i, j) = \psi(j, i) \geqslant 0$ and $\phi(i, j) = \phi(j, i) \geqslant 0$. We also assume that the total intensities of merging $\Psi(i, j; \eta)$ and splitting $\Phi(i, j; \eta)$ at a configuration $\eta = (n_1,..., n_N) \in \Omega_N$ are given by:

$$\Psi(i, j; \eta) := \Psi(i, j; n_i, n_j) = \psi(i, j)(n_i n_j)^\gamma, \qquad i \neq j, \qquad 2 \leqslant i + j \leqslant N$$

$$\Psi(i, i; \eta) := \Psi(i, i; n_i, n_i) = \psi(i, i)(n_i(n_i - 1))^\gamma, \qquad 2 \leqslant 2i \leqslant N$$

$$\Phi(i, j; \eta) := \Phi(i, j; n_{i+j}) = \phi(i, j)(n_{i+j})^\gamma, \qquad 2 \leqslant i + j \leqslant N \tag{3.2}$$

where $\gamma > 0$. Note that the case $\gamma = 1$ corresponds to the mass action kinetics which is a physically motivated assumption. Finally, observe that if the intensities $\psi(i, j)$, $\phi(i, j)$ are such that the CFP is an irreducible Markov chain on Ω_N, then the process has a unique stationary distribution.

4. REVERSIBLE CFP

4.1. Reversible Measures

Reversibility is known to be an effective tool in the study of the equilibrium of Markov processes. We can recommend Liggett,[21] Kelly,[19] and Whittle[37] as excellent references for the subject.

Recall that the physical interpretation of the reversibility of a Markov process φ_t, $t \geqslant 0$ with respect to a probability measure μ on the state space of the process is that for all $t \geqslant 0$ the two processes φ^μ_s, $0 \leqslant s \leqslant t$ and φ^μ_{t-s}, $0 \leqslant s \leqslant t$ starting from the same initial distribution μ have the same finite-dimensional distributions. The importance of reversible measures is based on the following two facts:

1. Reversible measures form a subset of steady-state distributions of a Markov process. This implies that if a reversible process is ergodic its unique stationary distribution is the reversible measure;
2. The detailed balance equation (see (4.10) later) provides, in the cases to which it applies, an efficient way for explicit derivation of reversible measures of a process.

We first characterize the class of intensities ϕ and ψ providing the reversibility of the CFPs. This characterization is given in terms of the ratios of intensities, rather then intensities themselves, as one can expect from the detailed balance condition. To that end, we need some more notation.

For some given i, j and a fixed N, let $\eta = (n_1, \dots, n_N) \in \Omega_N$ be a configuration such that $n_i, n_j > 0$. The configuration obtained from η via the transition $(i, j) \to (i+j)$ is denoted by $\eta^{(i, j)}$.

Similarly, if η is a configuration such that $n_{i+j} > 0$, we denote by $\eta_{(i, j)}$ the configuration obtained from η via the transition $(i+j) \to (i, j)$.

We agree to write $\eta^{(i, j)} = \eta$ and $\eta_{(i, j)} = \eta$ if η is not of the form required before.

For $\eta \neq \zeta \in \Omega_N$, we denote the total intensity of infinitesimal transition from η to ζ by $V(\eta, \zeta)$. It follows from the definion of CFP that $V(\eta, \zeta)$ is equal to either $\Psi(i, j; \eta)$, or $\Phi(i, j; \eta)$ or 0. By (3.2), the total intensities are of the form $V(\eta, \zeta) = v(\eta, \zeta)\, h(\eta, \zeta)$, where v and h denote, respectively, the intensity and the weight function corresponding to the transition $\eta \to \zeta$.

In this paper, we study only the case where for each pair i, j: $2 \leqslant i + j \leqslant N$, we have either $\phi(i, j)\, \psi(i, j) > 0$ or $\phi(i, j) = \psi(i, j) = 0$. Consequently, we define the ratios of intensities

$$q(i, j) = \begin{cases} \dfrac{\psi(i, j)}{\phi(i, j)}, & \text{if} \quad \phi(i, j)\, \psi(i, j) > 0 \\ 0 & \text{otherwise} \end{cases} \tag{4.1}$$

Theorem 1. Suppose that

$$q(i, j) > 0, \qquad 2 \leqslant i + j \leqslant N \tag{4.2}$$

Then the CFP φ_t, $t \geqslant 0$ is reversible iff the ratios of the intensities are of the form

$$q(i, j) = \frac{a(i+j)}{a(i)\, a(j)}, \qquad 2 \leqslant i+j \leqslant N \tag{4.3}$$

for some function $a = a(i) > 0$, $i = 1,..., N$.

Proof. The proof is obtained by using the Kolmogorov cycle condition [for references see Anderson[4]]. For given partitions $\zeta, \eta \in \Omega$ denote by

$$L = L_{(\zeta, \eta)} = (\zeta = \eta_0, \eta_1, ..., \eta_{k-1}, \eta_k = \eta), \qquad \eta_0, ..., \eta_k \in \Omega \tag{4.4}$$

a path of length k in Ω, from ζ to η, and define the following three quantities associated with the path $L_{(\zeta, \eta)}$:

$$\begin{aligned} \mathscr{A} &= \mathscr{A}(L_{(\zeta, \eta)}) = \prod_{l=0}^{k-1} V(\eta_l, \eta_{l+1}) \\ \mathscr{B} &= \mathscr{B}(L_{(\zeta, \eta)}) = \prod_{l=0}^{k-1} v(\eta_l, \eta_{l+1}) \\ \mathscr{H} &= \mathscr{H}(L_{(\zeta, \eta)}) = \prod_{l=0}^{k-1} h(\eta_l, \eta_{l+1}) \end{aligned} \tag{4.5}$$

We have $\mathscr{A} = \mathscr{B}\mathscr{H}$, for any path L in Ω. Next, for any closed path (cycle) $L_{(\zeta, \zeta)} = (\eta_0 = \zeta, \eta_1, ..., \eta_{k-1}, \eta_k = \zeta)$ we define the cycle $L'_{(\zeta, \zeta)}$ in the reverse direction, i.e., $L'_{(\zeta, \zeta)} = (\eta_k = \zeta, \eta_{k-1}, ..., \eta_1, \eta_0 = \zeta)$.

The Kolmogorov cycle criterion states that a CFP is reversible iff

(i) $V(\zeta, \eta) = 0$ implies $V(\eta, \zeta) = 0$, $\zeta, \eta \in \Omega$;

(ii) $\mathscr{A}(L_{(\zeta, \zeta)}) = \mathscr{A}(L'_{(\zeta, \zeta)})$, $\zeta \in \Omega$, for all closed non-self-intersecting paths L in Ω.

If $q(i, j) = 1$ for all i, j such that $2 \leqslant i+j \leqslant N$, one can verify directly that (i) and (ii) are satisfied. Therefore, from condition (ii) and the fact that the weight function h is the same for all intensities, we have $\mathscr{H}(L_{(\zeta, \zeta)}) = \mathscr{H}(L'_{(\zeta, \zeta)})$, $\zeta \in \Omega$ and, consequently,

$$\mathscr{B}(L_{(\zeta, \zeta)}) = \mathscr{B}(L'_{(\zeta, \zeta)}), \qquad \zeta \in \Omega \tag{4.6}$$

for all reversible CFPs. In view of (i) and the assumption (4.2), we further assume that the considered paths L are such that $\mathscr{B} > 0$, i.e., $v(\eta_l, \eta_{l+1}) > 0$,

$l=0, 1,..., k-1$. It is straightforward to see that the condition (4.6) is satisfied under (4.3), which proves the sufficiency part of the theorem.

The proof that (4.6) implies (4.3) is obtained by induction on N. The case $N=2$ is obvious. Assuming that the claim is true for $N-1$, we define the mapping $U: \Omega_{N-1} \to \Omega_N$ given by

$$U(\eta)=\tilde{\eta}, \qquad \eta=(n_1,..., n_{N-1}) \in \Omega_{N-1}, \qquad \tilde{\eta}=(n_1+1, n_2,..., n_{N-1}, 0) \in \Omega_N$$

Denote $U(\Omega_{N-1})=\tilde{\Omega}_N \subset \Omega_N$. By the assumption $q(i, j)>0$, the mapping U induces a one-to-one mapping of the set of all paths in Ω_{N-1} into the set of paths in $\tilde{\Omega}_N$. The latter implies that the intensities $\phi(i, j)$, $\psi(i, j)$, $2 \leqslant i+j \leqslant N-1$ of a reversible CFP on Ω_N should satisfy the condition (4.6) and, by the induction hypothesis, the ratios $q(i, j)$, $2 \leqslant i+j \leqslant N-1$ should be of the required form (4.3), defined by the values $a(i)>0$, $i=1,..., N-1$.

Now it is left to show that the same is true for the rest of the ratios $q(i, N-i)$, $1 \leqslant i \leqslant N-1$. First, given $a(N-1)$, $a(1)$, $q(1, N-1)>0$, define $a(N)=a(N-1)\, a(1)\, q(1, N-1)$. By the assumption $q(i, j)>0$, $2 \leqslant i+j \leqslant N$, there exists a path $L_1(\zeta, \eta)$ in Ω_N from $\zeta=(1, 0,..., 0, 1, 0)$ to $\eta=(0, 1,..., 0, 1, 0, 0)$ that does not pass through the state $\eta_1=(0,..., 0, 1) \in \Omega_N$. Define the path $L_2(\eta, \zeta)=(\eta, \eta_1, \zeta)$ of length 3 in Ω_N. Finally, applying (4.6) to the cycle $L_1(\zeta, \eta) \cup L_2(\eta, \zeta)$ shows that, by virtue of the cycle condition, the only unknown ratio, $q(2, N-2)$, is uniquely determined by the rest of the ratios associated with the cycle. Hence, $q(2, N-2)$ must be of the required form. The same argument proves the assertion for the values $q(i, N-i)$, $i=3,..., N-1$. □

Remark 1.

(i) Our inspiration for the form (4.3) of the ratios of reversible intensities came from the celebrated paper by Spitzer, 1977, in which he introduced nearest-particle systems [see Liggett,[21] Chap. 7].

(ii) The form (4.3) of the nonzero ratios of the intensities together with our assumption (4.1) are equivalent to what is known in a variety of applied sciences as the deterministic detailed balance condition on intensities [see for references Kelly[19] and Whittle[37]]. In our setting, the above condition on the intensities ψ and ϕ reads

$$a(i)\, a(j)\, \psi(i, j)=a(i+j)\, \phi(i, j), \qquad i, j\colon 2 \leqslant i+j \leqslant N \tag{4.7}$$

for some $a(i)>0$, $i=1,..., N$.

For the case $\gamma = 1$, Morgan[22] proved Kendall's conjecture that, under a technical condition similar to (4.2), deterministic reversibilty (4.7) is equivalent to stochastic reversibility (= stochastic detailed balance), as defined by (4.10) later. Our Theorem 1 provides a quite different and shorter proof of this fact, under the condition (4.2), for all $\gamma > 0$.

(iii) In applications, there is also some interest in irreducible CFPs that do not satisfy the condition (4.2). In this case one can verify, using the cycle condition, that the process is still reversible if the representation (4.3) holds for all nonzero ratios $q(i, j)$. An important example of such CFPs is

$$q(i, j) = \begin{cases} 0, & \text{if} \quad i > 1, \quad j > 1 \\ > 0, & \text{otherwise} \end{cases} \tag{4.8}$$

It is easy to see that $N - 1$ arbitrary quantities $q(1, j) > 0$, $j = 1, ..., N - 1$ conform with the representation (4.3), which implies that all the CFP of the type considered are reversible. As we already mentioned in Section 2.1, the approximation to the time dynamics of these processes is given by the Becker-Döring equation that has been extensively studied by many authors.

Example 1 demonstrates that without the assumption (4.2), the representation (4.3) for positive ratios $q(i, j)$ is not a necessary condition for the reversibility of an irreducible CFP, i.e., in this case stochastic reversibility does not imply (4.7).

Example 1. Let $N = 7$. Then the state space Ω_7 consists of 15 states η. Consider the CFP on Ω_7 having the following 12 ratios of intensities: $q(2, 1) = q(2, 3) = q(3, 1) = q(1, 5) = q(2, 5) = 0$, $q(1, 6) = 2$ and $q(1, 1) = q(1, 4) = q(2, 2) = q(3, 3) = q(2, 4) = q(3, 4) = 1$. Now, assume that the representation (4.3) holds for the last 6 ratios and denote $a(1) = b > 0$. Then, $q(1, 1) = 1$ implies $a(2) = b^2$, and consequently, $q(2, 2) = 1$ implies $a(4) = b^4$, $q(2, 4) = 1$ implies $a(6) = b^6$, $q(3, 3) = 1$ implies $a(3) = b^3$, $q(1, 4) = 1$ implies $a(5) = b^5$. Finally, $q(3, 4) = 1$ implies $a(7) = b^7$. This says that $q(1, 6) = 2$ is not of the required form under any choice of $b > 0$.

For the convenience of the reader, we give in Fig. 1, (as explained in the Appendix), a scheme of the state space of the above CFP. This helps verifying the irreducibility and the reversibilty of the process.

Hereafter, we restrict our study to reversible CFPs, denoting their unique invariant measure on Ω_N by $\mu = \mu_N$. Our next result provides the explicit expression for μ_N.

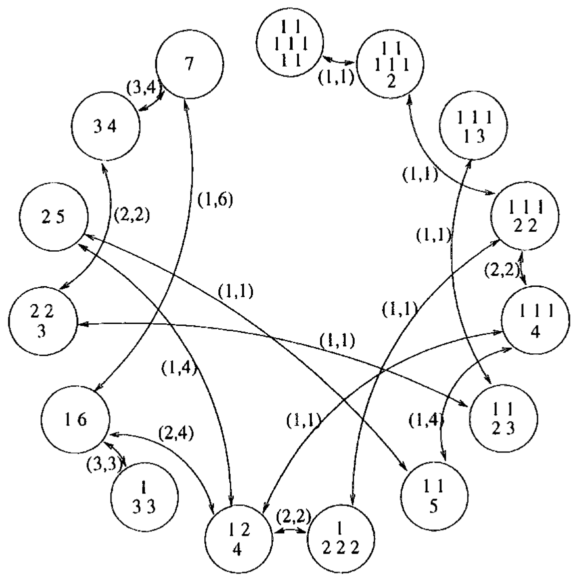

Fig. 1. A graphic illustration of the example given in Section 4. See detailed explanation in the Appendix.

Theorem 2. Suppose that all nonzero ratios of intensities $q(i, j)$ are of the form (4.3), being generated by r, $2 \leqslant r \leqslant N$ values $a(i_1),..., a(i_r)$, $1 \leqslant i_1,..., i_r \leqslant N$ of a function $a = a(i) > 0$, $i = 1, 2,..., N$. Then the corresponding CFP φ_t, $t \geqslant 0$ on Ω_N is reversible with respect to the invariant measure $\mu = \mu_N$ given by

$$\mu_N(\eta) = C_N \frac{a(i_1)^{n_{i1}}\, a(i_2)^{n_{i2}} \cdots a(i_r)^{n_{ir}}}{(n_{i_1}!)^\gamma\, (n_{i_2}!)^\gamma \cdots (n_{i_r}!)^\gamma}, \qquad \eta = (n_1,..., n_N) \in \Omega_N \quad (4.9)$$

where $C_N = C_N(a)$ is the partition function that depends only on the function a.

Proof. The proof follows from verifying that μ_N, given by (4.9), satisfies the condition of detailed balance:

$$V(\eta, \zeta)\, \mu(\eta) = V(\zeta, \eta)\, \mu(\zeta), \qquad \eta, \zeta \in \Omega_N \quad (4.10)$$

for $q(i, j)$ and μ as in the statement of the theorem. In fact, it follows from the preceding definitions, that it is enough to check (4.10) for those pairs of configurations $\eta, \eta^{(i,j)} \in \Omega_N$, for which $q(i, j) \neq 0$. In this case we have from (4.9), (3.2) and (4.3)

$$\frac{\mu(\eta^{(i,j)})}{\mu(\eta)} = q(i, j)\left(\frac{n_i n_j}{n_{i+j}+1}\right)^{\gamma} = \frac{\Psi(i, j; \eta)}{\Phi(i, j; \eta^{(i,j)})}, \qquad i \neq j \tag{4.11}$$

The same argument can be used in the case $i = j$. □

Remark 2.

(i) For the case $\gamma = 1$ the equilibrium distribution (4.9) is known in the context of clustering and chemical kinetics processes obeying the deterministic detailed balance condition, see Kelly,[19] and Whittle.[37]

(ii) Let, for a moment, Z_i, $i = 1,..., N$ be independent Poisson random variables with respective means $a(i) > 0$, $i = 1,..., N$. Then it is easy to see that the distribution μ_N has the following meaning: $\eta = (n_1,..., n_N) \in \Omega_N$

$$\mu_N(\eta) = \text{Prob.}\left\{Z_1 = n_1,..., Z_N = n_N \,\middle|\, \sum_{i=1}^{N} iZ_i = N\right\} \tag{4.12}$$

In the case when nonzero ratios of the intensities of a reversible CFP are not of the form (4.3), the expression for μ_N is different from (4.9).

Example 1′. Figure 1 indicates that the state space Ω_7 of the CFP considered can be represented as the union of the following two connected and disjoint sets of states η (numbered as explained in the Appendix): $A_1 = \{1, 2, 4, 5, 7, 8, 9, 10, 11, 13\}$ and $A_2 = \{3, 6, 12, 14, 15\}$. The only "bridge" between the sets A_1 and A_2 is the arrow (1, 6). Now with the help of (4.11), we arrive at the following expression for μ_7:

$$\mu_7(\eta) = \begin{cases} 1/2C_7 u_7(\eta), & \text{if } \eta \in A_1 \\ C_7 u_7(\eta), & \text{if } \eta \in A_2 \end{cases} \tag{4.13}$$

where C_7 is the normalizing constant and $u_7(\eta) = (n_1!)^{-\gamma} \cdots (n_7!)^{-\gamma}$, $\eta = (n_1,..., n_7) \in \Omega_7$.

4.2. Functionals of the Invariant Measure

We deal hereafter only with the case $\gamma = 1$, and $q(i, j) > 0$ for all $2 \leqslant i + j \leqslant N$. Our objective now is to derive explicit expressions for some important functionals of the invariant measure μ_N, given by (4.9) in the case $r = N$.

For a given reversible CFP with an invariant measure μ_N on Ω_N, define the random varibles $n_k(\eta)$, $k = 1, 2,..., N$ as the number of groups of size k in a configuration $\eta \in \Omega_N$. We also define the following associated quantities:

$$f(N; k) = E(n_k(\eta)), \qquad k = 1, 2,..., N$$

$$h(N; k, l) = cov(n_k(\eta), n_l(\eta)), \qquad k \neq l = 1, 2,..., N$$

$$\sigma^2(N; k) = Var(n_k(\eta)), \qquad k = 1, 2,..., N$$

Letting $r = N$ in (4.9), we denote through the rest of the paper

$$c_N = \frac{1}{C_N} = \sum_{\eta \in \Omega_N} \frac{a(1)^{n_1} a(2)^{n_2} \cdots a(N)^{n_N}}{(n_1!)^\gamma (n_2!)^\gamma \cdots (n_N!)^\gamma}, \qquad \eta = (n_1,..., n_N) \in \Omega_N \tag{4.14}$$

Theorem 3. Let μ_N be given by (4.9) for $r = N$. Then

$$f(N; k) = a(k) \frac{c_{N-k}}{c_N}, \qquad k = 1,..., N \tag{4.15}$$

$$h(N; k, l) = a(k)\, a(l) \left(\frac{c_{N-k-l}}{c_N} - \frac{c_{N-k} c_{N-l}}{(c_N)^2} \right), \qquad k \neq l = 1, 2,..., N \tag{4.16}$$

$$\sigma^2(N; k) = a^2(k) \left(\frac{c_{N-2k}}{c_N} - \left(\frac{c_{N-k}}{c_N} \right)^2 \right) + a(k) \frac{c_{N-k}}{c_N},$$
$$k = 1, 2,..., N; \qquad c_{-m} = 0, \qquad m = 1, 2,... \tag{4.17}$$

Proof. The relationship (4.15) follows from the identity

$$\frac{\partial}{\partial a(k)} c_N = c_{N-k} = \frac{c_N}{a(k)} f(N; k) \tag{4.18}$$

which is easy to obtain from (4.14). The relationship (4.16) can be derived by differentiating (4.18) with respect to $a(l)$, $l \neq k$. Finally, the relationship (4.17) is obtained by differentiating the first two terms of (4.18) with respect to $a(k)$. □

To implement Theorem 3 we need the expression for c_N. Usually, the calculation of partition functions is a difficult mathematical problem treated in statistical physics [see Thompson[33]]. Our treatment of the problem is based on the following approach. We assume that the ratios $q(i, j) = a(i+j)/a(i)\, a(j)$, $i, j = 1, 2,...,$ of the intensities are generated by the coefficients $a_n = a(n) > 0$, $n = 1, 2,...$ of the Taylor series expansion of the function $S(x)$ defined by

$$S(x) = \sum_{n=1}^{\infty} a_n x^n, \qquad x \in D_S \subseteq R^1$$

We further assume that the radius of convergence R_S of the series is given by

$$R_S = \lim_{n \to \infty} \frac{a_n}{a_{n+1}} > 0 \tag{4.19}$$

The key result for our subsequent study is contained in the following lemma:

Lemma 1. Under these assumptions, we have

1. The values c_n, $n = 1, 2,...$ are the coefficients of the Taylor series expansion of the function $g(x)$ defined by

$$g(x) = e^{S(x)} = \sum_{n=0}^{\infty} c_n x^n, \qquad x \in D_g \subseteq R^1 \tag{4.20}$$

   where $D_g = D_S$.

2. The coefficients c_n, $n = 0, 1,...$ are determined by the difference equation $c_0 = 1$, $c_1 = a(1)$,

$$(n+1)\, c_{n+1} = \sum_{k=0}^{n} (k+1)\, a(k+1)\, c_{n-k}, \quad n = 1, 2,... \tag{4.21}$$

Proof. By the definition of the function $S(x)$, we write

$$e^{a(1)\,x} \times e^{a(2)\,x^2} \times e^{a(3)\,x^3} \times \cdots e^{a(N)\,x^N} \times \cdots = e^{S(x)}, \qquad x \in D_S$$

We expand now each term of the infinite product in the left-hand side of this identity into the Taylor series

$$e^{a(k)\,x^k} = \sum_{j=0}^{\infty} \frac{(a(k))^j\, x^{kj}}{j!}, \qquad k = 1, 2,...$$

and collect terms of these expansions. The coefficient c_N of the power x^N in the product is the sum of all contributions of factors of the type

$x^{n_1}x^{2n_2}x^{3n_4}\cdots x^{Nn_N}$, such that $n_1 + 2n_2 + \cdots + Nn_N = N$. Since the coefficient of each term of this type is equal to

$$\frac{a(1)^{n_1}\, a(2)^{n_2} \cdots a(N)^{n_N}}{n_1!\, n_2! \cdots n_N!}$$

our first assertion follows from (4.14).

Finally, the two relationships $g(x) = e^{S(x)}$ and $g'(x) = g(x)\, S'(x)$ imply $D_g = D_S$, while the difference equation (4.21) follows from the second of the above relationships. □

Remark 3.

(i) The exponential generating function (4.20) for the sequence c_n, $n = 1, 2,\ldots$, is known in physical chemistry and queuing theory in the context of CFPs satisfying the deterministic detailed balance condition [see e.g., Kelly,(19) Chap. 8].

(ii) The relationship between the two sequences $\{c_n\}$ and $\{a_n\}$ is a known topic in the theory of univalent functions in the complex domain [see Pommerenke,(26) and references therein]. The topic is related to the Bieberbach conjecture which is now a theorem. Note also that identities analogous to (4.20) are common in enumerative combinatorics literature [see e.g., Stanley(28)].

(iii) The recurrence formula (4.21) can be obtained straightforward from (4.15) and the total mass conservation law (3.1).

In view of the first assertion of the Lemma 1, we denote hereafter $R = R_S = R_g$. The following theorem describes the limiting behavior, as $N \to \infty$ of the quantities considered in Theorem 3.

Theorem 4. Suppose that

$$R = \lim_{n \to \infty} \frac{c_n}{c_{n+1}} \tag{4.22}$$

Then, for a fixed k, we have

$$\lim_{N \to \infty} f(N; k) = a(k)\, R^k, \qquad k = 1, 2,\ldots \tag{4.23}$$

$$\lim_{N \to \infty} h(N; k, l) = 0, \qquad k \neq l = 1, 2,\ldots \tag{4.24}$$

$$\lim_{N \to \infty} \sigma^2(k; N) = a(k)\, R^k, \qquad k = 1, 2,\ldots \tag{4.25}$$

Proof. From (4.22), we have

$$\lim_{N \to \infty} \frac{c_{N-k}}{c_N} = R^k, \qquad k = 1, 2,... \tag{4.26}$$

Consequently, all three assertions follow from Theorem 3. □

Remark 4. As we pointed in Section 2.1, the Smoluchowski approximation is based on the assumption of independence (zero interactions) between the densities of different groups (clusters) during the time evolution of CFP. Our result (4.24) provides a partial justification of this assumption for large N at the steady state of reversible CFPs. It should be noted that a phenomenon of independence of sites in a system of interacting particles at the steady state, is widely known in statistical physics for mean-field models [see Durrett,[11] and Beguin *et al.*[7] for explanation and references]. It is not difficult to understand that a CFP approaches a mean-field, as $N \to \infty$, which explains (4.24).

Refering to our assumption (4.22), the following natural conjecture related to the relationship between the two sequences $\{a_n\}$ and $\{c_n\}$ turns out to be a challenging analytical problem:

Conjecture. The existence of the limit in (4.19) implies the existence of the limit in (4.22).

In the conclusion of this section, we address the following question which is common in statistical mechanics: What is the the probability, say p_∞, of a cluster of infinite size at the steady state, as $N \to \infty$? First, we easily obtain the following general statement for the CFP considered:

Corollary 1. For CFPs obeying the conditions of Theorem 4, $p_\infty < 1$.

Proof. It follows from (4.23) that, for $N = \infty$, the probability to have a cluster of a given finite size k is greater than zero, if $a(k) > 0$, which proves our claim. □

To study the existence $(= p_\infty > 0)$ of a cluster of infinite size at the steady state, a more subtle analysis is required. Clearly, for $p_\infty > 0$ it is sufficient that

$$f_{\alpha N}(\infty) := \lim_{N \to \infty} \sum_{k=\alpha N}^{N} f(N; \alpha N) > 0, \qquad \text{for some} \quad 0 < \alpha \leqslant 1 \tag{4.27}$$

By (4.15), this is equivalent to the following condition:

$$f_{\alpha N}(\infty) = \lim_{N \to \infty} c_N^{-1} \sum_{k=\alpha N}^{N} a(k)\, c_{N-k} > 0 \tag{4.28}$$

for some α, as before. We will show in Section 6 that $p_\infty > 0$ for all three models considered there. Our study will be based on the asymptotics of c_N, as $N \to \infty$, and the following argument:

$$f_{\alpha N}(\infty) \geqslant \lim_{N \to \infty} \delta_N \sum_{k=\alpha N}^{\alpha_1 N} a(k) \tag{4.29}$$

where $\delta_N := \min_{\alpha N \leqslant k \leqslant \alpha_1 N} c_N^{-1} c_{N-k}$, $0 < \alpha < \alpha_1 < 1$.

Finally, note that the formation of a giant cluster is related to the violation of the total mass conservation law as $N \to \infty$. This phenomenon is known in a variety of applied sciences. A rigorous explanation of the physical meaning of the phenomenon in the context of chemical kinetics of clusters is given by Penrose.[25]

5. COMPARISON WITH THE STEADY STATE SOLUTION OF THE INTEGRAL EQUATION (2.2)

As explained in Section 2.2 (see (2.4)), the steady state solution of (2.2) for the ratios of intensities (= kernels of the integral equation) of the form (4.3), is given by

$$f(x) = a(x)\, e^{-\lambda x}, \qquad x \geqslant 0, \qquad \text{s.t.} \quad \int_0^\infty x f(x)\, dx = M \tag{5.1}$$

where the constant $\lambda = \lambda(M) > 0$, $M > 0$ is determined by the value of the total mass M. Recall that $f(x)$ denotes here the expected number of groups of size x, $x \geqslant 0$ at the steady state. Therefore, to study the validity of (2.2), we take $M = N$, $x = k$ and compare the values of $f(N; k)$ and $f(k)$ for large N and fixed k. From (4.23) we have

$$\lim_{N \to \infty} \frac{f(N; k)}{f(k)} = R^k \lim_{N \to \infty} e^{k\lambda(N)}, \qquad k = 1, 2, \ldots \tag{5.2}$$

First observe that the limit in the right-hand side of (5.2) exists. In fact, differentiating both sides of the mass conservation law in (5.1) with respect to N, and using the fact that $a(x) > 0$, $x > 0$, yields $\lambda'(N) < 0$, $N > 0$. Viewing the left-hand side of the conservation law as the Laplace transform of the function $a(x)$, $x > 0$, we make the standard assumption that

$$a(x) \sim x^{\alpha} e^{\gamma x}, \qquad x \to \infty \tag{5.3}$$

Now we can justify the steady state solution (5.1) of (2.2) as an approximation to $f(N; k)$ for large N and fixed k.

Assertion. For all functions $a(x)$, $x \geqslant 0$ satisfying (5.3) we have

$$\lim_{N \to \infty} \frac{f(N; k)}{f(k)} = 1, \qquad k = 1, 2,... \tag{5.4}$$

Proof. Under the assumptions (4.19) and (5.3),

$$R = \lim_{x \to \infty} \frac{a(x)}{a(x+1)} = e^{-\gamma}$$

Moreover, it is easy to see from the mass conservation law and the preceding discussion that

$$\lim_{N \to \infty} \lambda(N) = \gamma \tag{5.5}$$

Now (5.2) implies the assertion. □

However, a close look at the expressions for the two quantities indicates the possibility of a considerable difference in their asymptotic behavior when $N \geqslant k = k(N) \to \infty$, as $N \to \infty$. In the three models considered in the next section, we demonstrate that this phenomenon indeed occurs.

6. EXAMPLES

In this section we consider three particular reversible CFPs with positive coagulation and fragmentation intensities, generated by the functions (1) $a(i) = \beta/i$; (2) $a(i) = \beta$ and (3) $a(i) = \beta i$, where $\beta > 0$ and $i = 1, 2,...$.

The steady state solutions $f(x)$ of the integral equation (2.2) for these cases were derived by Aizenman and Bak,[1] (for $\beta = 1$) and Stewart and Dubovskii,[32] for case (2), and Gueron and Levin[15] for all three cases. The values of the constant λ for these models can be found explicitly from the mass conservation law: (1) $\lambda = \beta/N$; (2) $\lambda = \sqrt{\beta/N}$ and (3) $\lambda = \sqrt[3]{2\beta/N}$.

6.1. The Case $a(i) = \beta/i$, $i = 1, 2,..., \beta > 0$

Here we have

$$S(x) = -\beta \ln(1-x), \qquad |x| < 1 \tag{6.1}$$

with $R = 1$. Consequently,

$$\begin{aligned} g(x) &= \frac{1}{(1-x)^\beta} \\ &= 1 + \beta x + \beta(\beta+1)\frac{x^2}{2} + \cdots + \frac{\beta(\beta+1)\cdots(\beta+n-1)}{n!}x^n + \cdots \end{aligned} \tag{6.2}$$

As a result,

$$c_n = \frac{\Gamma(\beta+n)}{\Gamma(\beta)\,\Gamma(n+1)}, \qquad n = 1, 2,... \tag{6.3}$$

Note that the corresponding distribution μ_N is the widely known Ewens sampling formula [for references see Ewens[13]] originated in population genetics.

Further, from (6.3) we have

$$c_n \sim \Gamma^{-1}(\beta)\, n^{\beta-1}, \qquad \text{as} \quad n \to \infty \tag{6.4}$$

which gives the following limiting behavior of the partition function:

$$\begin{cases} \lim_{n\to\infty} c_n = \infty, & \text{if} \quad \beta > 1 \\ c_n = 1, \qquad n = 1, 2,..., & \text{if} \quad \beta = 1 \\ \lim_{n\to\infty} c_n = 0, & \text{if} \quad 0 < \beta < 1 \end{cases} \tag{6.5}$$

This implies that 1 is a critical value of the parameter β for the CFP considered. Also, observe that by (4.15) and (6.3) we have

$$Nf(N; N) \sim \beta N^{1-\beta}, \qquad \text{as} \quad N \to \infty$$

which explains the physical meaning of the critical value. Here, $f(N; N)$ is interpreted as the probability of coagulation into one cluster (total consensus). Now we are able to identify the crucial difference in the asymptotic behavior of $f(N; k(N))$ and $f(k(N))$, in the case when $k(N) \to \infty$, as $N \to \infty$. Namely, we have:

$$\frac{f(N; N)}{f(N)} \sim e^{\beta} N^{1-\beta}, \qquad \text{as} \quad N \to \infty$$

and for all $0 \leqslant \alpha < 1$,

$$\frac{f(N; \alpha N)}{f(\alpha N)} \sim (1-\alpha)^{\beta-1} e^{\alpha\beta}, \qquad \text{as} \quad N \to \infty$$

Next, it follows from Theorem 4 that

$$\lim_{N \to \infty} f(N; k) = \frac{\beta}{k}$$

for any fixed $k = 1, 2,...$. Particularly, in the case $\beta = 1$, the expected number of groups of size k does not depend on N and is equal to

$$f(N; k) = \frac{1}{k}, \qquad k = 1, 2,..., N$$

Figure 2 plots $f(x)$ and $f(N; k)$ for the values $\beta = 1/2, 1, 5$ and $N = 100$. Note the difference between these two quantities for $\beta = 1/2$.

Regarding the existence of an infinite cluster, (4.29) and (6.4) give

$$f_{\alpha N}(\infty) \geqslant \beta(1-\alpha_1)^{\beta-1} \lim_{N \to \infty} \sum_{k=\alpha N}^{\alpha_1 N} k^{-1}, \qquad 1 > \alpha_1 > \alpha \tag{6.6}$$

So,

$$f_{\alpha N}(\infty) \geqslant \beta(1-\alpha_1)^{\beta-1} \ln \frac{\alpha_1}{\alpha} > 0, \qquad 1 > \alpha_1 > \alpha \tag{6.7}$$

This shows the existense of a cluster of size of order αN, $0 < \alpha < 1$. In this connection, note that, by (4.15) and (6.4), the probability to have in the case considered a cluster of a given size $k(N)$, such that $k(N)$, $N - k(N) \to \infty$, as $N \to \infty$, goes to zero.

6.2. The Case $a(i) = \beta$, $i = 1, 2,...$

This is an important test case for the validity of (2.2) as an approximation to the exact solution, particularly since, for constant kernels, (2.2)

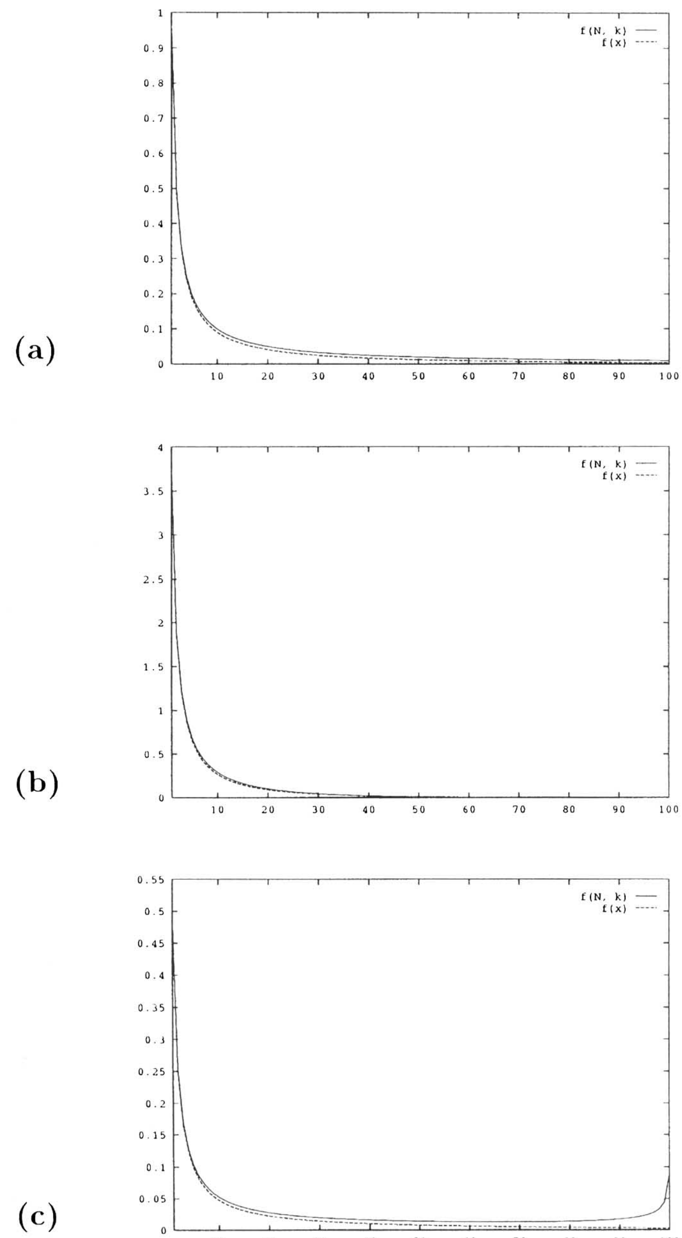

Fig. 2. $f(N, k)$ as a function of k and $f(x)$ as a function of x for the case $a(i) = \alpha_0/i$. The values used are $N = 100$ and $\alpha_0 = 1, 5, 1/2$ for panels (a), (b), and (c), respectively. The horizontal axis represents k for $f(N, k)$ and x for $f(x)$. See explanation in the text.

has a unique solution $c(x; t)$, $x, t \geqslant 0$, that approaches the equilibrium solution $f(x) = \beta e^{-\sqrt{\beta}\, x/\sqrt{N}}$, as $t \to \infty$ [Aizenman and Bak,[1] Stewart and Dubovskii[32]].

From Theorem 4 we have $\lim_{N \to \infty} f(N; k) = \beta$ for any fixed k. To find the asymptotic behavior of $f(N; k)$ as it approaches this limit, we derive another recurrence relation for c_n which is easier to analyze as $n \to \infty$ than (4.21).

Assertion 1. In the case $a(i) = \beta$, $i = 1, 2,...$, we have

1. $c_0 = 1$, $c_1 = \beta$, $(n+1)\, c_{n+1} = (2n + \beta)\, c_n - (n-1)\, c_{n-1}$, $n = 1, 2,...$.
2. The sequence c_n is monotonically increasing.
3. The function $f(N; k)$ is monotonically decreasing in k, $1 \leqslant k \leqslant N$.

Proof. In our case, $g(x) = e^{(\beta x/1-x)}$, $x \geqslant 0$. Consequently, $(1-x)^2\, g'(x) = \beta g(x)$, $x \geqslant 0$, which implies our first claim. Now the second claim can be proved by induction, while the last claim follows from the fact that in the case considered $f(N; k) = \beta c_{N-k}/c_N$, $k = 1,..., N$. □

We now get the rate of convergence of $f(N; k)$ to its limit, as $N \to \infty$ and k is fixed.

Assertion 2. In the considered case, for a fixed $k = 1, 2,...$, we have

$$f(N; k) = \beta \frac{c_{N-k}}{c_N} \sim \beta e^{-\sqrt{\beta}\, k/\sqrt{N}}, \qquad \text{as} \quad N \to \infty \tag{6.8}$$

Proof. We compute the leading term of the asymptotic expansion of c_n using the WKB method [Bender and Orszag[8]], assuming that the expansion exists. For any sequence of numbers, $\{t_n\}$, we define the forward difference $Dt_n = t_{n+1} - t_n$, $n = 0, 1, 2,...$.

We rewrite the recurrence equation in Assertion 1 as

$$(n+2)\, c_{n+2} = (2n + 2 + \beta)\, c_{n+1} - n c_n, \qquad n = 0, 1,... \tag{6.9}$$

We set now $c_n = e^{s_n}$, $n = 0, 1,...$ and assume the following two asymptotic inequalities for large n:

$$D^2 s_n \ll 1, \qquad D^2 s_n \ll (D s_n)^2 \tag{6.10}$$

This leads to

$$c_{n+1} = c_n e^{D s_n}, \qquad \text{and} \qquad c_{n+2} \sim c_n e^{2 D s_n}, \qquad \text{as} \quad n \to \infty \tag{6.11}$$

As a result, we obtain from (6.9)

$$(n+2)\, e^{2Ds_n} \sim (2n+2+\beta)\, e^{Ds_n} - n, \qquad \text{as} \quad n \to \infty \tag{6.12}$$

which, for large n, yields

$$e^{Ds_n} \sim 1 + \sqrt{\beta}\frac{1}{\sqrt{n}} \Rightarrow Ds_n \sim \sqrt{\beta}\frac{1}{\sqrt{n}} \tag{6.13}$$

Now we conclude that for large n,

$$c_n \sim e^{2\sqrt{\beta n}} \tag{6.14}$$

This verifies the validity of the assumptions (6.10). Finally, under the condition of the assertion, we have, by (6.14)

$$f(N; k) = \beta \frac{c_{N-k}}{c_N} \sim \beta e^{-\sqrt{\beta}\, k/\sqrt{N}}, \qquad \text{as} \quad N \to \infty$$

as required. □

To compare with the case 6.1, this assertion says that for a fixed k the asymptotic behavior of $f(N; k)$ is identical to that of $f(k)$, and the same is true for all $N \geqslant k = k(N)$: $N - k(N) \to \infty$, as $N \to \infty$. However, with the help of (6.14) one can again identify the disagreement between the two quantities when $N \geqslant k = k(N) \to \infty$, as $N \to \infty$. In particular, for $k = N - k_1$, $k_1 \leqslant N$ fixed, we obtain:

$$\frac{f(N; N-k_1)}{f(N-k_1)} \sim c_{k_1} e^{-\sqrt{\beta N}}, \qquad \text{as} \quad N \to \infty$$

To illustrate, we plotted $f(x)$ and $f(N; k)$ for the values $\beta = 1$ and $N = 100$ in Fig. 3a.

Finally, by virtue of (4.28) and (6.14), we have

$$f_{\alpha N}(\infty) - f_{\alpha_1 N}(\infty) \leqslant \beta(\alpha_1 - \alpha) \lim_{N \to \infty} N e^{-\alpha\sqrt{\beta N}} = 0, \qquad 1 > \alpha_1 > \alpha > 0 \tag{6.15}$$

Since $f(N; N) \to 0$, as $N \to \infty$, the latter yields $f_{\alpha N}(\infty) = 0$, while (6.8) implies that

$$\lim_{N \to \infty} f(N; \alpha\sqrt{N}) = \beta e^{-\alpha\sqrt{\beta}}, \qquad 1 > \alpha > 0$$

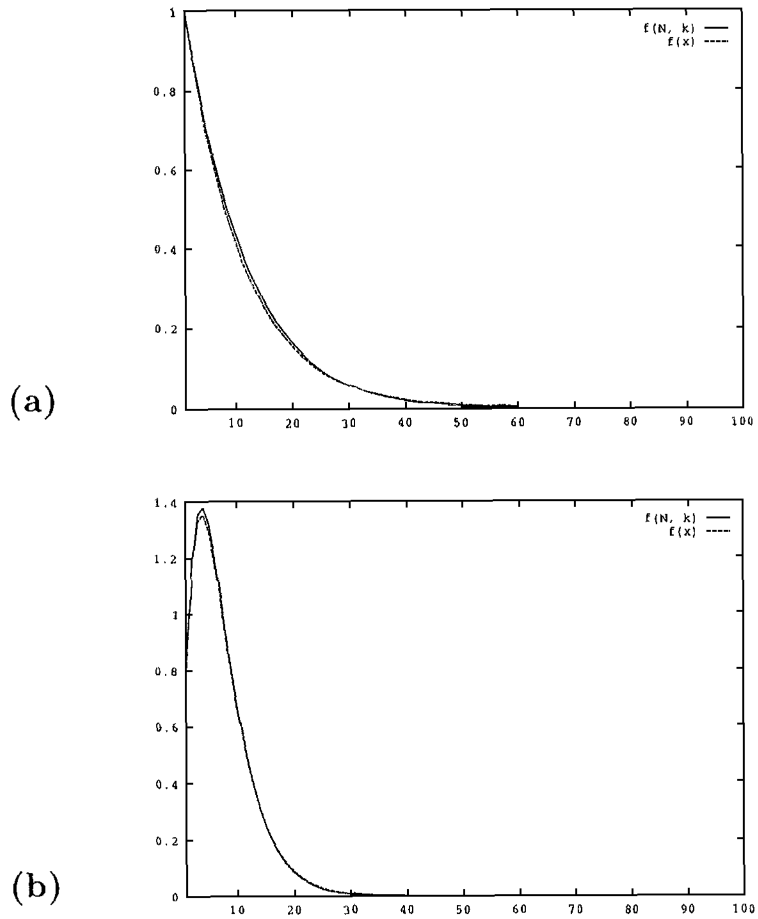

Fig. 3. $f(N, k)$ as a function of k and $f(x)$ as a function of x for the case (a) $a(i) = \alpha_0$ and (b) $a(i) = \alpha_0 i$ and for the values $\alpha_0 = 1$ and $N = 100$. The horizontal axis represents k for $f(N, k)$ and x for $f(x)$. See explanation in the text.

Hence, in our case, for a given $0 < \alpha < 1$ there is a probability to have a cluster of size of order $\alpha \sqrt{N}$, while the probability to have any cluster of size of order αN, $0 < \alpha < 1$, goes to zero, as $N \to \infty$.

6.3. The Case $a(i) = \beta i$, $i = 1, 2,\dots$, $\beta > 0$

Here we have

$$S(x) = \beta \sum_{k=1}^{\infty} k x^k = \beta \frac{x}{(1-x)^2}, \qquad |x| < 1 \tag{6.16}$$

Note that the above function $S(x)$, $|x| < 1$ is the real part of the well known Koebe function [Pommerenke[26]].

The following result is helpful in the analysis of the asymptotic behavior of the sequence c_n.

Assertion 1. In the case considered, $c_{-1} = 0$, $c_0 = 1$, $c_1 = \beta$,

$$(n+1)\, c_{n+1} = (3n+\beta)\, c_n - (3n-3-\beta)\, c_{n-1} + (n-2)\, c_{n-2}, \qquad (6.17)$$

for $n = 2, 3, \ldots$ and the sequence c_n is monotonically increasing.

Proof. Both claims follow from the relationship

$$(1-x)^3\, g'(x) = \beta(1+x)\, g(x), \qquad |x| < 1 \qquad \square$$

In a procedure similar to the one detailed in the proof of Assertion 2 in the previous example, we use the WKB method to obtain

$$c_n \sim e^{3/2 \sqrt[3]{2\beta n^2}}, \qquad \text{as} \quad n \to \infty \qquad (6.18)$$

Thus, (6.18) implies

$$f(N; k) = \beta k \frac{c_{N-k}}{c_N} \sim \beta k e^{-(\sqrt[3]{2\beta/N})\, k}, \qquad \text{as} \quad N \to \infty, \qquad k \text{ is fixed}$$

Thus, regarding the comparative asymptotic behavior of $f(N; k)$ and $f(k)$, we have here exactly the same situation as in the case 6.2. In particular, (6.18) implies:

$$\frac{f(N; N-k_1)}{f(N-k_1)} \sim c_{k_1} e^{-1/2 \sqrt[3]{2\beta N^2}}, \qquad \text{as} \quad N \to \infty, \qquad k_1 \text{ fixed} \qquad (6.19)$$

To illustrate, Fig. 3b plots $f(x)$ and $f(N, k)$ for the values $\beta = 1$ and $N = 100$.

Analysis identical to the one for the model 6.2 shows that, in our case, formation of infinite clusters has the same features.

APPENDIX

Figure 1 illustrates the example given in Section 4. We first explain how this figure should be read. The 15 states η of the CFP are the 15 partitions of $N = 7$. They are ordered lexicographically, and displayed clockwise as circles. The components of these states (i.e., the components of the partitions) are indicated in the circles. For example, the circle containing the numbers 1 1 2 3 corresponds to the partition $1+1+2+3=7$ of 7, that is, a state with two groups of size 1, one group of size 2 and one of size 3. The double headed arrows show the possible transitions between the states via coagulations or fragmentations of groups. The pairs of numbers near each arrow indicate the interacting groups in the related transition. For example, consider partitions number 5 and 7 (in the order, as defined earlier) that are connected by the arrow $(1, 4)$. This says that the coagulation of two groups of size 1 and 4 moves the system from the 5th state to the 7th, while the fragmentation of a group of size 5 into two groups of sizes 1 and 4 moves the system from the 7th state to the 5th state.

One can easily verify from the figure that this CFP is irreducible, and also that the interaction $(1, 6)$ is not a part of any cycle of the displayed graph. Therefore, for all cycles of the graph, we have $q(i, j) = 1$, which says that the process satisfies the Kolmogorov cycle condition for any choice of $q(1, 6)$.

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