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The Duality of Heterogeneous Coagulation-Fragmentation Processes *

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Abstract

This paper study the duality of heterogeneous coagulation-fragmentation process (HCFP) which models the coagulation, fragmentation and diffusion of clusters of particles on lattice. The closed form of stationary distribution for HCFP is obtained, and then the integrated form of BBGKY hierarchy of HCFP is given.

Keywords: Heterogeneous coagulation-fragmentation, stationary distribution, duality.

AMS Subject Classification: 60K35.

§1. Introduction

The model of homogeneous coagulation process is proposed by Smoluckowski (1916), who derived an infinite system ordinary differential equations for describing the coagulation of collision moving according to Brownian motion. Since then the model has been widely generalized and studied (see refs. [5], [6], [7], [8], [9], [11], [12], [13], [14]). For readers who are interested in mathematical aspects of the coagulation-fragmentation models, we recommend two survey papers of Aldous (1999) and Collet (2004).

Most of the related works on coagulation-fragmentation models focus mainly on the problem that whether the distribution of the density of the cluster particles as a function of time and space is a solution to the coagulation-fragmentation equations. However, in the theory of stochastic interacting particle systems one of fundamental problem is to seek all stationary distributions. As far as we know, there are only a few models such as symmetric simple exclusion processes, basic contact processes, zero-range processes and voter models for which one can completely characterize all stationary distributions, see [Liggett, 1985]. For coagulation-fragmentation models, Han (1995) and

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Durrett (1999) gave an explicit form of the stationary distribution to the homogeneous coagulation-fragmentation model. Berestyki (2004) gave the equilibrium measures to the exchangeable coagulation-fragmentation model. When we consider the diffusion effect in the coagulation-fragmentation model, can we give the closed form of the stationary distribution of it (HCFP)? Moreover, what is the duality of it? In this paper, we mainly solve above two problems. We find the jumping rate function such that the stationary distribution of heterogeneous coagulation-fragmentation can be given out explicitly, and also give the integrated form of BBGKY hierarcky of the heterogeneous coagulation-fragmentation process.

§2. The Heterogeneous Coagulation-Fragmentation Processes

In this section, some notations and preliminaries are given. Consider the following interacting particles system: In each site $x \in \mathbb{Z}^d$ of d-dimensional integer lattice, particles can coagulate to form a cluster, and two clusters can coagulate to form a larger one, and larger cluster can fragmentate into two smaller ones, and all of them can also move to their neighbor sites y.

Let Σ be a finite subset of $\mathbb{Z}^d$, $\mathbb{N} = \{0, 1, 2, \cdots\}$, $\mathbb{N}_+ = \{1, 2, \cdots\}$ and $\mathbb{X}(\Sigma) = \{A : A \in \mathbb{N}^{\Sigma\times\mathbb{N}_+}\}$, where $A = (a(x, k) : a(x, k) \in \mathbb{N}, x \in \Sigma, k \in \mathbb{N}_+)$. Here we assume that the number, $|\Sigma|$, of set Σ is at least great than 2. Thus, A can be regarded as a matrix with indexes in $\Sigma \times \mathbb{N}_+$. For each $x \in \Sigma$, denote by $a(x, k)$ the number of k-clusters in site x. Let $I_{x,i} = (a(y, j) : y \in \Sigma, j \in \mathbb{N}_+) \in \mathbb{X}(\Sigma)$ be a matrix such that $a(y, j) = 0$ for $(y, j) \neq (x, i)$ and $a(y, j) = 1$ for $(y, j) = (x, i)$. For $A \in \mathbb{X}(\Sigma)$, let

$$\begin{aligned}
&A^k_{x,y} := A + I_{y,k} - I_{x,k}, && \text{if } \ a(x, k) > 0 \ \text{ and } \ \|x - y\| = 1,\\
&A^+_{x,ij} := A + I_{x,i+j} - I_{x,i} - I_{x,j}, && \text{if } \ a(x, i) > 0 \ \text{ and } \ a(x, j) > 0,\\
&A^-_{x,ij} := A - I_{x,i+j} + I_{x,i} + I_{x,j}, && \text{if } \ a(x, i + j) > 0,\\
&A_x := (a(x, 1), a(x, 2), \cdots),
\end{aligned}$$

$|A_x| = \sum\limits_k ka(x, k)$ and $|A| = \sum\limits_{x\in\Sigma} |A_x|$. Here, $A^k_{x,y}$ means that the state of the process obtained from a state A after a jump of a cluster of size k from site x to the site y, and $A^+_{x,ij}$ denotes that the state obtained from a state A after a cluster of size i coagulates with a cluster of size j to form a cluster of size $i + j$ in the site x, i.e.,

$$(i) + (j) \to (i + j).$$

$A^-_{x,ij}$ means that the state obtained from a state A after a cluster of size $i+j$ breaks into a cluster of size i and a cluster of size j in site x, i.e.,

$$(i+j) \to (i) + (j)$$

and A_x denotes the distribution of the numbers of the different clusters in site x.

Let N denote the total number of particles in the system, then $N = \sum\limits_{x\in\Sigma} |A_x|$. Let $\mathbb{X}_N(\Sigma) = \{A : A \in \mathbb{X}(\Sigma), |A| = N\}$, and $\mathbb{X}$ be the limit of $\mathbb{X}_N(\Sigma)$ as $(N \to \infty, B \nearrow \mathbb{Z}^d)$. Now we define the heterogeneous random coagulation-fragmentation process (HCFP) considered in the paper as follows: the process, denoted by $\{A_N(t), t \geq 0\}$, is a continuous-time irreducible Markov chain on the finite state space $\mathbb{X}_N(\Sigma)$ with state transition rates

$$Q_{AA'} := \begin{cases} \dfrac{1}{2^d} g(a(x,k)), & \text{if } A' = A^k_{x,y}, \\ K_{ij} g(a(x,i)) g(a(x,j) - \delta_{ij}), & \text{if } A' = A^+_{x,ij}, \\ F_{ij} g(a(x,i+j)), & \text{if } A' = A^-_{x,ij}, \\ 0, & \text{if } A' \neq A^k_{x,y}, A^+_{x,ij}, A^-_{x,ij} \end{cases}$$

and

$$Q_{AA} = - \sum_{A'\in\mathbb{X}_N(\Sigma), A'\neq A} Q_{AA'},$$

where $A, A' \in \mathbb{X}_N(\Sigma)$, $g(\cdot)$ denotes the diffusion rate which is a positive function except $g(0) = 0$, K_{ij} and F_{ij} are coagulation and fragmentation kernels respectively, and $\delta_{ij} = 1$ for $i = j$ and 0 for $i \neq j$. Here the choice of rates of coagulation, fragmentation and diffusion reflect the case like in a polymer system that, reaction occurs with a probability proportional to both the number of reactants, and inversely proportional to the volume; here the density is taken to be equal to one, so that the volume coincides with the total number of units N. Though there are many ways of action of the diffusion on the coagulation and fragmentation, the main reason for us to take the special forms, $g(a(x,i))g(a(x,j) - \delta_{ij})$ and $g(a(x,i+j))$, is that we can easily obtain the stationary distribution of the process by the forms. Note that the coagulation and fragmentation do not depend directly on the diffusion rate when $g(k) = k$.

The HCFP which evolves on the d-dimension integer lattice $\mathbb{Z}^d$ with the dynamics split into two parts: diffusion and reaction. The diffusion represents the migrations of individual clusters between different sites. It consists in independent symmetric random walks with nearest neighbor jumps, we denote the associated generator by L_d. The reaction part describes the coagulation between two cluster and the fragmentation of k-cluster $(k \geq 2)$ at site x, and this part of the generator is denoted by L_r.

Now we give the generator for a cylinder function f by

$$L f(A) = L_d f(A) + L_r f(A), \tag{2.1}$$
$$L_r = L_k + L_f,$$

where L_d, L_k, L_f are diffusion operator, coagulate operator and fragment operator respectively defined as follows:.

$$L_d f(A) = \sum_{y,x:|x-y|=1} \sum_k \frac{1}{2^d} g(a(x,k))[f(A^k_{x,y}) - f(A)];$$
$$L_k f(A) = \sum_x \sum_{i,j} K_{ij} g(a(x,i)) g((a(x,j) - \delta_{ij}))[f(A^+_{x,ij}) - f(A)];$$
$$L_f f(A) = \sum_x \sum_{2\le i+j} F_{ij} g(a(x,i+j))[f(A^-_{x,ij}) - f(A)], \tag{2.2}$$

§3. The Stationary Distribution

The stationary distributions for the homogeneous random coagulation-fragmentation processes have been given by Han (1995) and Durrett, Granovsky and Gueron (1999). Here we shall present the stationary distribution for the HCFP. Assume that

$$H_1: \ \text{The diffusion rate } g(\cdot) \text{ satisfies } \sup_m |g(m+1) - g(m)| < \infty.$$
$$H_2: \ K_{ij} = K_{ji}, \quad F_{ij} = F_{ji}, \quad K_{ij} h(i) h(j) = F_{ij} h(i+j), \qquad i,j \ge 0, \tag{3.1}$$

where $h(\cdot)$ is a positive function. As Van Dongen and Ernst (1984) stated, when the process describes the system of polymers in which intramolecular reactions do not occur, and therefore only branched-chain (non-cyclic) polymers are formed and all un-reacted functional groups are equally reactive, $k!h(k)$ may denote the number of distinct ways of forming a k-mers from k distinguishable units and the equation (3.1) states that the number of distinct ways for $(i+j)$-mers to break up into i-mer and j-mers $(F(i,j)h(i+j))$ equals the number of bonds between (i) and (j) polymers in $(i+j)$-mer configurations $(K(i,j)h(i)h(j))$. In fact, the total fragmentation rate of a k-mer is taken to be proportional to the number of bonds in Van Dongen and Ernst (1984), i.e.,

$$\frac{1}{2} \sum_{i+j=k} F_{ij} = \frac{1}{\lambda}(k-1).$$

$1/\lambda$ $(\lambda > 0)$ represents the fragmentation strength. The equation (3.1) is usually called detailed balance condition.

Note that the condition H_1 is not necessary for obtaining the stationary distribution in the following, but it can guarantee that the limit process ($N \to \infty$ and $B \nearrow \mathbb{Z}^d$) of $\{A_N(t), t \ge 0\}$ is a unique Feller process (see [8]).

Theorem 3.1 Suppose the two conditions H_1 and H_2 hold. Then $\{A_N(t), t \geq 0\}$ has a unique stationary distribution μ_N given by

$$\mu_N(A) = \frac{1}{Z_N} \prod_{x\in\Sigma} \prod_{k=1}^{N} \frac{[h(k)]^{a(x,k)}}{g(a(x,k))!}, \qquad A \in \mathbb{X}_N(\Sigma) \tag{3.2}$$

and the process is reversible with this stationary distribution, where Z_N is the normalization factor, i.e.,

$$Z_N = \sum_{A\in\mathbb{X}_N(\Sigma)} \prod_{x\in\Sigma} \prod_{k=1}^{N} \frac{[h(k)]^{a(x,k)}}{g(a(x,k))!}, \tag{3.3}$$

where $g(m)! = g(1)g(2)\cdots g(m)$ with $g(0)! := 1$. Usually, Z_N is called the partition function of the process.

Proof We first check that

$$\mu_N(A')Q_{A'A} = \mu_N(A)Q_{AA'} \tag{3.4}$$

for all $A, A' \in \mathbb{X}_N(\Sigma)$. It is equivalent to check

$$\frac{Q(A,A')}{Q(A',A)} = \frac{\mu(A')}{\mu(A)}$$

for all $A, A' \in \mathbb{X}_N(\Sigma)$. In fact, we have

$$\frac{Q(A,A')}{Q(A',A)} = \frac{g(a(x,k))}{g(a(y,k)+1)} = \frac{g(a(x,k))}{h(k)} \frac{h(k)}{g(a(y,k)+1)} = \frac{\mu(A')}{\mu(A)}$$

for the case $A' = A^k_{x,y}$ and, by (2.1),

$$\begin{aligned}\frac{Q(A,A')}{Q(A',A)} &= \frac{K_{ij}}{F_{ij}} \frac{g(a(x,i))g(a(x,j))}{g(a(x,i+j)+1)} \\ &= \frac{h(i+j)}{Nh(i)h(j)} \frac{g(a(x,i))g(a(x,j))}{g(a(x,i+j)+1)} \\ &= \frac{h(i+j)}{g(a(x,i+j)+1)} \frac{g(a(x,i))}{h(i)} \frac{g(a(x,j))}{h(j)} = \frac{\mu(A')}{\mu(A)}\end{aligned}$$

for $A' = A^+_{x,ij}$, $i \neq j$. Similarly, we can check that (3.2) holds for $A' = A^+_{x,ij}$, $i = j$ and $A' = A^-_{x,ij}$. Thus, (3.2) holds for all $A, A' \in \mathbb{X}_N(\Sigma)$ and therefore

$$\sum_{A'\in\mathbb{X}_N(\Sigma)} \mu_N(A')Q_{A'A} = \mu_N(A) \sum_{A'\in\mathbb{X}_N(\Sigma)} Q_{AA'} = 0.$$

This means that μ_N is a reversible stationary distribution of the process. Since all states in $\mathbb{X}_N(\Sigma)$ connect mutually, that is, for $A, A' \in \mathbb{X}_N(\Sigma)$, there are $A_1, A_2, \cdots, A_k \in \mathbb{X}_N(\Sigma)$ $(k \geq 1)$ such that $Q(A, A_1)Q(A_1, A_2)\cdots Q(A_k, A') > 0$. This means that the process is an irreducible Markov chain on the finite state space, so the stationary distribution is unique.
□

§4. Duality

We define the Poisson polynomials by

$$k^{(N)}=\begin{cases}1, & k=0\\ N(N-1)(N-2)\cdots(N-k+1), & 0<k\le N\\ 0, & k>N\end{cases}$$

and Poisson polynomials for configurations $A\in\mathbb{X}$ and $B\in\mathbb{X}_N(\Sigma)$ by

$$D(A,B)=\prod_x\prod_k b(x,k)^{(a(x,k))}. \tag{4.1}$$

Theorem 4.1

$$L_dD(A,\cdot)(B)=L_d^*D(\cdot,B)(A), \tag{4.2}$$

$$\mathsf{E}[D(A,B_t)]=\mathsf{E}[D(A_t,B)], \tag{4.3}$$

where $L_dD(A,\cdot)(B)$ means that L_d acts on the second variable, L_d^* is the dual operator of L_d, and E is the expectation of independent product of the L_d-process starting from A and the L_d-process starting from B.

Proof By the definition of $D(\cdot,\cdot)$, we have

$$\begin{aligned}L_d^*D(\cdot,B)(A)) &= \sum_{x,y:|x-y|=1}\sum_k\Big[\frac{1}{2}a(y,k)D(A^k_{y,x},B)-D(A,B)\Big]\\ &= \sum_{x,y:|x-y|=1}\sum_k\Big\{\prod_{(z,j)\neq(x,k),(y,k)}b(z,j)^{(a(z,j))}\frac{1}{2}a(y,k)\\ &\quad\times[b(x,k)^{(a(x,k)+1)}b(y,k)^{(a(y,k)-1)}-b(x,k)^{(a(x,k))}b(y,k)^{(a(y,k))}]\Big\},\end{aligned} \tag{4.4}$$

note that

$$\begin{aligned}&a(y,k)b(y,k)^{(a(y,k)-1)}b(x,k)^{(a(x,k)+1)}\\ =\ &(b(y,k)-1)^{(a(y,k))}(a(x,k)+1)(b(x,k)+1)^{(a(x,k))}\\ =\ &(b(x,k)+1)^{(a(x,k))}[(a(x,k)-b(x,k)+1)(b(y,k)-1)^{(a(y,k))}\\ &+b(x,k)(b(y,k)-1)^{(a(y,k))}]\\ =\ &(b(y,k)+1)^{(a(y,k))}[b(x,k)^{(a(x,k))}+b(x,k)(b(x,k)-1)^{(a(x,k))}]\\ =\ &(b(y,k)+1)^{(a(y,k))}b(x,k)^{(a(x,k))}+b(x,k)(b(y,k)+1)^{(a(y,k))}(b(x,k)-1)^{(a(x,k))},\end{aligned} \tag{4.5}$$

and

$$(b(y,k)+1)^{(a(y,k))}=a(y,k)b(y,k)^{(a(y,k))}-b(y,k)b(y,k)^{(a(y,k)},\tag{4.6}$$

so we have

$$\begin{aligned} & a(y,k)b(x,k)^{(a(x,k)+1)}b(y,k)^{(a(y,k)-1)} \\ = \ & a(y,k)b(y,k)^{(a(y,k))}b(x,k)^{(a(x,k))} - b(y,k)b(y,k)^{(a(y,k))}b(x,k)^{(a(x,k))} \\ & + b(x,k)(b(y,k)+1)^{(a(y,k))}(b(x,k)-1)^{(a(x,k))}. \end{aligned} \tag{4.7}$$

Put (4.7) into (4.4), we have

$$\begin{aligned} L_d^* D(\cdot,B)(A) &= \sum_{x,y:|x-y|=1}\sum_k \left[\frac{1}{2}b(x,k)D(A,B^k_{x,y}) - \frac{1}{2}b(y,k)D(A,B)\right] \\ &= \sum_{x,y:|x-y|=1}\sum_k \frac{1}{2}b(x,k)[D(A,B^k_{x,y}) - D(A,B)] \\ &= L_d D(A,\cdot)(B). \end{aligned}$$

Thus (4.2) is proved. Furthermore, we also have

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathsf{E}[D(A_{t-s},B_s)] = 0, \qquad 0 \le s \le t, \tag{4.8}$$

then integrating over s, we get

$$\mathsf{E}[D(A,B_t)] = \mathsf{E}[D(A_t,B)]. \tag{4.9}$$

So Theorem 4.1 is proved. $\square$

Furthermore, if denote by A_t the process with generator L_d and starts from a given configuration $A \in \mathbb{X}_N(\Sigma)$, and by B_t the process with generator L and initial distribution μ. Write the correlation function of the process B_t by $u(A,t|\mu)$, that is

$$u(A,t|\mu) := \mathsf{E}_\mu[D(A,B_t)],$$

then we have

$$\begin{aligned} u(A,t|\mu) &= \sum_{A'} \mathsf{P}(t,A,A')u(A',0|\mu) \\ &\quad + \int_0^t \mathrm{d}s \sum_{A'} \mathsf{P}(t-s,A,A')\mathsf{E}_\mu[L_r D(A',B_s)], \end{aligned} \tag{4.10}$$

where $\mathsf{P}(t,A,A')$ is the transition probability go from A to A', in time t when the generator is L_d, and the equation (4.10) is called "BBGKY hierarchy" in physics.

Let ε be the expectation with respect to the product of the (A_t,B_t), by Theorem 4.1 we have

$$\frac{\mathrm{d}}{\mathrm{d}s}\varepsilon[D(A_{t-s},B_s)] = \varepsilon[L_r D(A_{t-s},B_s)], \tag{4.11}$$

where L_r acts on B_s. Then integrate (4.11) over s, we obtain (4.10).

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非齐次聚合分解过程的对偶性

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文章研究了格子点上带扩散的非齐次聚合分解过程(HCFP)的对偶性, 给出了HCFP的平稳分布和HCFP的积分形式的BBGKY hierarchy.

关键词: 非齐次聚合分解过程; 平稳分布; 对偶性.

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