On Coagulation-Fragmentation Processes with Diffusion

Dong Han

(Shanghai Jiaotong University
This talk is based on the work joined with Chunha Hu.)

Outline

- **Background and Models**
- **Main Results**
  1. **Existence and Uniqueness**
  2. **Stationary Distribution**
  3. **Critical line and Phase Transition**
  4. **Hydrodynamic Limit**
- **Some Problems**

Background and Models

- Coagulation-Fragmentation Models with Diffusion

  The Coagulation-fragmentation models with diffusion is to describe the random aggregation, split and diffusion of clusters of particles on $d-$dimensional integer lattices which can model aerosols, blood coagulation, chemical polymerization and so on.

  For example, consider chemical polymerization on plane ($d = 2$).

  Let $a(x, k)$:denote the number of k-clusters (molecules) in site x (integer on plane).

  C(k,j) (coagulation rate) : $a(x, k) \rightarrow\leftarrow a(x, j) \quad \rightharpoonup \quad a_t(x, k + j)$

  F(k, j) (fragmentation rate) : $a(x, k + j) \quad \rightharpoonup \quad a(x, k) \leftrightarrow a(x, j)$

  D(.)p(x,y) (diffusion rate) : $a(x, k) \quad \rightharpoonup \quad a(x, k) - 1; a(y, k) + 1$

- $C_{ij} > 0, F_{ij} = 0, D(.) = 0$ or $F_{ij} > 0, C_{ij} = 0, D(.) = 0$.

  Marcus (1968, *Technometrics*)

  Kingman (1982, *Stoch. Proc. Appli.*)

  Aldous (1999, *Bernoulli*)

  Bertoin (2006, *Cambridge Univ. Press*)

- $F_{ij} > 0, C_{ij} > 0, D(.) = 0$.

  Han (1995, *J. Stat. Phys.*)

  Jeon (1998, *Commun. Math. Phys.*)

  Durrett, Granovsky and Gueron (1999, *J. Theor. Probab.*)

  Kolokoltsov (2004, *J. of Stat. Phys.*)

- $F_{ij} > 0, C_{ij} > 0, D(.) > 0$.

– Generators for the Infinite Dimensional Coagulation-Fragmentation Models with Diffusion

$$Lf(A) = L^D f(A) + L^C f(A) + L^F f(A), \qquad f \in \mathcal{L}_l, A \in \mathbb{X}^l,$$

where $A = (a(x,k) : a(x,k) \in \mathbb{N}, x \in \mathbb{Z}^d, k \in \mathbb{N}_+)$, and

$$L^D f(A) = \sum_{y,x:|x-y|=1} \sum_k \frac{1}{2^d} D(a(x,k))[f(A^k_{x,y}) - f(A)],$$

$$L^C f(A) = \sum_x \sum_{i,j} C_{ij} D(a(x,i)) D((a(x,j)) - \delta_{ij})[f(A^+_{x,ij}) - f(A)],$$

$$L^F f(A) = \sum_x \sum_{2 \le i+j} F_{ij} D(a(x,i+j))[f(A^-_{x,ij}) - f(A)],$$

$$\mathbb{X} = \{A = (a_t(x,k)) : A \in \mathbb{N}^{\mathbb{Z}^d \times \mathbb{N}_+}\}$$

$$\mathbb{X}^l = \{A : A \in \mathbb{X}, ||A||_l < \infty\}.$$

$$||A||_l = \sum_{x \in \mathbb{Z}^d} \sum_k a(x,k) l_{x,k} < \infty,$$

where $l_{x,k}$ is a positive function on $\mathbb{Z}^d \times \mathbb{N}_+$ such that there exists a constant c satisfying $\sum\limits_{y:} \sum_k a(y,k) l_{y,k} \leq c l_x$ for every x .

$\mathcal{L}_l$: the set of Lipschiz functions for the norm $||.||_l$

$$\begin{aligned}
A^k_{x,y} &:= A + I_{y,k} - I_{x,k}, \text{ if } |x-y| = 1 \\
A^+_{x,ij} &:= A + I_{x,i+j} - I_{x,i} - I_{x,j} \\
A^-_{x,ij} &:= A - I_{x,i+j} + I_{x,i} + I_{x,j}.
\end{aligned}$$

- Four Questions

  (a) Existence and uniqueness of Feller process

  (b) A closed form of stationary distribution in finite domain.

  (c) Critical line and the phase transition

  (d) The hydrodynamic limits

Main Results

1. Existence and Uniqueness

H_1: $\quad \sup_{k \geq 0} |D(k+1) - D(k)| < \infty.$

H_2: $\quad \sup_{A \in \mathbb{X}^l} \sum_x \sum_{i,j} C_{ij} D(a(x,i)) D(a(x,j) - \delta_{ij}) l_{x,i} < \infty$

H_3: $\quad \sup_{A \in \mathbb{X}^l} \sum_x \sum_{i,j} F_{ij} D(a(x, i+j)) l_{x,i+j} < \infty.$

Theorem 1. There is a unique Feller process $\{P^A, A \in \mathbb{X}^l\}$ such that

$$\lim_{t \downarrow 0} \frac{E^A f(A(t)) - f(A)}{t} = Lf(A), \qquad A \in \mathbb{X}^l.$$

Back
Close

The sketch of proof.

(1) Prove that the martingale solutions $P_{N,M}$ corresponding to the operator $L_{N,M}$ and P_M to L_M are tight compact.

(2) Show that the weakly limit P of $\{P_M\}$ is a unique martingale solution corresponding to the operator L.

(3) Check that $\{P^A, A \in \mathbb{X}^l\}$ is a unique Feller process on $D([0,\infty), \mathbb{X}^l)$ with generator L.

$$L_{N,M}f(A) = L^D_{N,M}f(A) + L^K_{N,M}f(A) + L^F_{N,M}f(A)$$

$$
\begin{aligned}
L_{N,M}f(A) &= L^D_{N,M}f(A) + L^K_{N,M}f(A) + L^F_{N,M}f(A) \\
&= \sum_{y,x\in\mathbb{Z}^d_M:|x-y|=1} \sum_{k:k\le N} \frac{1}{2^d} g(a(x,k))[f(A^k_{x,y}) - f(A)] \\
&= \sum_{x\in\mathbb{Z}^d_M} \sum_{i,j\le N} K_{ij} g(a(x,i)) g((a(x,j)) - \delta_{ij})[f(A^+_{x,ij}) - f(A)] \\
&= \sum_{x\in\mathbb{Z}^d_M} \sum_{i,j:2\le i+j\le N} F_{ij} g(a(x,i+j))[f(A^-_{x,ij}) - f(A)].
\end{aligned}
$$

Back
Close

2. Stationary Distribution

H_1: $D(.)$ is a nondecreasing function on $\mathbb{N}_+$

H_2: There exists a non-negative function $h(.)$ and a positive constant λ such that

$$C_{ij}h(i)h(j) = \lambda F_{ij}h(i+j)$$

This equation is usually called the detailed balance condition and the number $1/\lambda$ is called fragmentation intensity.

In the chemical polymer model, $h(k)$ usually denotes the number of distinct ways of forming k-clusters from k particles.

Theorem 2 The process $\{L_N; A_t^N, t \geq 0\}$ in finite dimension has a unique reversible stationary distribution which is a product measure with the marginal distribution given by

$$\mu_N\{A : A_x = (a(x,1), \cdots, a(x,N))\} = \frac{1}{Z_N} \prod_{k=1}^{N} \frac{[\frac{N}{\lambda} h(k)]^{a(x,k)}}{D(a(x,k))!},$$

where Z_N is the normalization factor, $D(m)! = D(1)D(2)\cdots D(m)$. In particular,

$$\mu_N\{A : A_x = (a(x,1), \cdots, a(x,N))\} = \frac{1}{Z_N} \prod_{k=1}^{N} \frac{[\frac{N}{\lambda\gamma} h(k)]^{a(x,k)}}{a(x,k)!},$$

for $D(x) = \gamma k$.

3. Critical line and Phase Transition

Let $D(k) = \gamma k$, $(k \geq 0,\ \gamma > 0)$ and $\rho = \lambda\gamma$.

Assume that the detail balance condition holds and the generating function $F(x) = \sum_{k=1}^{\infty} h(k)x^k$ satisfies

$$F^{'}(r) = \lim_{x \to r-0} F^{'}(x) < +\infty;\ \ F^{''}(r) = \lim_{x \to r-0} F^{''}(x) = +\infty.$$

where r is positive radius of convergence of $F(x)$.

Critical line: (λ, γ): $\lambda\gamma = \rho_c =: rF^{'}(r)$.

Let

$$a_j^*(N) = [a_j - Na_j(\rho)]/\sqrt{Na_j(\rho)}, \quad a_j(\rho) = h(j)u^j/\rho$$

where $u \leq r$ satisfies $\rho = uF'(u)$ for $\rho < \rho_c$ and $u = r$ for $\rho \geq \rho_c$.

Theorem 3 (i) If $\rho < \rho_c$, then $\{a_j^*(N)\}$ converges to a mutually dependent Gaussian sequence $\{G_j\}$ as $N \to \infty$ with

$$E[G_j] = 0, \quad E[G_j G_l] = \delta_{jl} - g_j g_l$$

and

$$g_j = \frac{j\sqrt{h(j)r^j}}{\sqrt{rF'(r) + r^2 F''(r)}}$$

where $\delta_{jl} = 0$ for $j \neq l$ and $\delta_{jl} = 1$ for $j = l$.

(ii) If $\rho \geq \rho_c$, then $\{a_j^*(N)\}$ converges to a mutually independent Gaussian sequence $\{G_j\}$ as $N \to \infty$ with

$$E[G_j] = 0, \quad E[G_j G_l] = \delta_{jl}$$

Back
Close

Example 1. RA_a model $(a \geq 3)$.

$$R(i,j) = [(a-2)i+2][(a-2)j+2].$$

$F(i,j)$ and $h(k)$ can be taken respectively by

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

and

$$h(k) = \frac{a^k[(a-1)k]!}{k![(a-2)k+2]!}.$$

Hence

$$2(k-1)h(k) = \sum_{i+j=k} R(i,j)h(i)h(j).$$

We can calculate that

$$r = \lim_{k\to\infty} \frac{h(k)}{h(k+1)} = \frac{(a-2)^{(a-2)}}{a(a-1)^{(a-1)}}$$

and $\rho_c = rF'(r) = (a-1)/[a(a-2)^2]$.

4. Hydrodynamic Limit

Under an appropriate scaling of the lattice space and time, we can derive the hydrodynamic limit for the evolution of the macroscopic cluster density. From microscopic to macroscopic consists in taking a limit when the distance between particles goes to zero. So we set that the distance between two neighboring sites is ϵ and ϵ goes to zero. Once this be done, we also scale time. The diffusion part of the generator needs acceleration by ϵ^{-2}, thus, we consider the generator

$$L_\epsilon = \epsilon^{-2} L^D + L^C + L^F.$$

Here we deal with the hydrodynamic Limit for the process by the method described in detail by Chen (2004, Second Edition).

Let $\Lambda_\ell \subset \mathbb{Z}$ be the finite volume with periodic boundary, $|\Lambda_\ell| = 2\ell + 1$ for some integer $\ell \in \mathbb{N}_+$, and

$$X = \{A : A \in N^{\mathbb{Z}\times\mathbb{N}_+}, ||A|| = \sum_x \sum_k a(k,x) < \infty\};$$

$$X^n(\ell) = \{A : A \in X, ||A|| = n, a(k,x) = 0, |x| > \epsilon^{-1}\ell\}.$$

Define the Poisson polynomials by

$$D_k^{(n)} = \begin{cases} 1, & k = 0 \\ n(n-1)(n-2)\cdots(n-k+1), & 0 < k \leq n \\ 0, & k > n. \end{cases}$$

and Poisson polynomials for configurations by

$$D : D(A,B) = \prod_x \prod_k D_{b(x,k)}^{(a(x,k))} \tag{1}$$

for $A \in X$ and $B \in X^n(\ell)$.

Lemma.

$$L_d D(A, .)(B) = L_d^* D(., B)(A),$$

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

where $L_d D(A, .)(B)$ means that L_d acts on the second variable, L_d^* is the adjoint operator of L_d, and $\mathbb{E}$ is the expectation of independent product of the L_d-process starting from A and the L_d-process starting from B.

Theorem 4. For any $n \in \mathbb{N}_+$ and $A \in X_\ell^{(n)}$ such that $|A_k| = n_k, k = 1, 2, \cdots, \sum_{k=1} n_k = n$, then the limit

$$\gamma(t, \bar{r}) := \lim_{\epsilon \to 0} u^\epsilon(A, t|\mu^\epsilon)$$

exists and satisfies the following integral equation

$$\begin{aligned} \gamma(t, \bar{r}) \; = \; & \prod_{i=1}^{S_1} (\int G(t, r_i - r)\rho(1, r)dr) \\ & \times \prod_{i=S_1+1}^{S_2} (\int G(t, r_i - r)\rho(2, r)dr) \cdots \prod_{i=S_{n-1}}^{S_n} (\int G(t, r_i - r)\rho(n, r)dr) \\ & + \int_0^t ds \int [\prod_{i=1}^{n} G(t - s, r_i - r_i^{'})dr^{'}] H(\gamma(s, \bar{r})) \end{aligned}$$

Some Problems

1. If the condition $\sup_{k\geq 0}|D(k+1)-D(k)|<\infty$ does not hold, for example, $D(k)=k^{\alpha}$ with $\alpha>1,$ whether or not the process is still unique corresponding to the generator L ?

2. We have the closed form of stationary distribution, μ_N, in finite domain. Under what conditions the limit distribution of μ_N as $N\to\infty$ exists and is still a stationary distribution ?

3. Is the process ergodic or non-ergodic when $\rho<\rho_c$ or $\rho>\rho_c$? Furthermore, if the process is non-ergodic (it is possible in the super-critical line), can one obtain more than one invariant probability measure ?

4. Is there large (moderate) deviation for the process in sub-critical line or super-critical line ?

Thank You !