Second edition

From Markov Chains to Non-equilibrium Particle Systems

Mu-Fa Chen

World Scientific

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Beijing Normal University, China

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FROM MARKOV CHAINS TO NON-EQUILIBRIUM PARTICLE SYSTEMS (2nd Edition)

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Preface to the First Edition

The main purpose of the book is to introduce some progress on probability theory and its applications to physics, made by Chinese probabilists, especially by a group at Beijing Normal University in the past 15 years. Up to now, most of the work is only available for the Chinese-speaking people. In order to make the book as self-contained as possible and suitable for a wider range of readers, a fundamental part of the subject, contributed by many mathematicians from different countries, is also included. The book starts with some new contributions to the classical subject—Markov chains, then goes to the general jump processes and symmetrizable jump processes, equilibrium particle systems and non-equilibrium particle systems. Accordingly the book is divided into four parts. An elementary overlook of the book is presented in Chapter 0. Some notes on the bibliographies and open problems are collected in the last section of each chapter. It is hoped that the book could be useful for both experts and newcomers, not only for mathematicians but also for the researchers in related areas such as mathematical physics, chemistry and biology.

The present book is based on the book "Jump Processes and Particle Systems" by the author, published five years ago by the Press of Beijing Normal University. About 1/3 of the material is newly added. Even for the materials in the Chinese edition, they are either reorganized or simplified. Some of them are removed. A part of the Chinese book was used several times for graduate students, the materials in Chapter 0 was even used twice for undergraduate students in a course on Stochastic Processes. Moreover, the galley proof of the present book has been used for graduate students in their second and third semesters.

The author would like to express his warmest gratitude to Professor Z. T. Hou, Professor D. W. Stroock and Professor S. J. Yan for their teachings and advices. Their influences are contained almost everywhere in the book. In the past 15 years, the author has been benefited from a large number of colleagues, friends and students, it is too many to list individually here. However, most of their names appear in the "Notes" sections, as well as in the Bibliography and in the Index of the book. Their contributions and cooperations are greatly appreciated. The author is indebted to Professor X. F. Liu, Y. B. Li, B. M. Wang, X. L. Wang, J. Wu, S. Y. Zhang and Y. H. Zhang for reading the galley proof, correcting errors and improving the quality of the presentations. It is a nice chance to acknowledge the financial support during the past years by Fok Ying-Tung Educational Foundation, Foundation of Institution of Higher Education for Doctoral Program, Foundation of State Education Commission for Outstanding Young Teachers and the

National Natural Science Foundation of China. Thanks are also expressed to the World Scientific for their efforts on publishing the book.

M. F. Chen
Beijing
November 18, 1991

Preface to the Second Edition

The main change of this second edition is Chapter 5 on "Probability Metrics and Coupling Methods" and Chapter 9 on "Spectral Gap" (or equivalently, "the first non-trivial eigenvalue"). Actually, these two chapters have been rewritten, within the original text. In the former chapter, the topic of "optimal Markovian couplings" is added and the "stochastic comparability" for jump processes is completed. In the latter chapter, two general results on estimating spectral gap by couplings and two dual variational formulas for spectral gap of birth-death processes are added. Moreover, a generalized Cheeger's approach is renewed for unbounded jump processes. Next, Section 4.5 on "Single Birth Processes" and Section 14.2 on "Ergodicity of Reaction-diffusion Processes" are updated. But the original technical Section 14.3 is removed. Besides, a large number of recent publications are included. Numerous modifications, improvements or corrections are made in almost every page. It is hoped that the serious effort could improve the quality of the book and bring the reader to enjoy some of the recent developments.

Roughly speaking, this book deals with two subjects: Markov Jump Processes (Parts I and II) and Interacting Particle Systems (Parts III and IV). If one is interested only in the second subject, it is not necessary to read all of the first nine chapters, but instead, may have a look at Chapters 4, 5, 7, 9 plus §2.3 or so. A quick way to read the book is glancing at the elementary Chapter 0, to get some impression about what studied in the book, to have some test of the results, and to choose what for the further reading. Sometimes, I feel crazy to write such a thick book, this is due to the wider range of topics. Even though it can be shorten easily by moving some details but the resulting book would be much less readable. Anyhow, I believe that the reader can make the book thin and thin.

A concrete model throughout the whole book is Schlögl's (second) model, which is introduced at the beginning (Example 0.3) to show the power of our first main result and discussed right after the last theorem (Theorem 16.3) of the book about its unsolved problems. This model, completely different from Ising model, is typical from non-equilibrium statistical physics. Its generalization is the polynomial model or more generally, the class of reaction-diffusion processes. Locally, these models are Markov chains. But even in this case, the uniqueness problem of the process was opened for several years, though everyone working in this field believes so. From physical point of view, the Markov chains should be ergodic and this is finally proved in Chapter 4. Thus, to study the phase transitions, we have to go to the infinite dimensional setting. The first hard stone is the construction of the corresponding Markov processes. For which, the mathematical tool is prepared in Chapter 5 and the construction is done in Chapter 13. The model is essentially irreversible, it can be reversible (equilibrium) only in a special case. The proof of a criterion for the reversibility is prepared in Chapter 7 and completed in Chapter 14. The topics studied in almost every chapter are either led by or related to Schlögl's model, even though sometimes it is not explicitly mentioned. Actually, the last four chapters are all devoted to the reaction-diffusion processes.

The Schlögl model possesses the main characters of the current mathematics: infinite dimensional, non-linear, complex systems and so on. It provides us a chance to re-examine the well developed finite dimensional mathematics, to create new mathematical tools or new research topics. It is not surprising that many ideas and results from different branches of mathematics, as well as physics, are used in the book. However, it is surprising that the methods developed in this book turn out to have a deep application to Riemannian geometry and spectral theory. This is clearly a different story. Since there are so much progress made in the past ten years or more, a large part of the new materials are out of the scope of this book, the author has decided to write a separate book under the title "Eigenvalues, Inequalities and Ergodic Theory".

It is a pleasure to recall the fruitful cooperation with my previous students and colleagues: Y. H. Mao, F. Y. Wang, Y. Z. Wang, S. Y. Zhang, Y. H. Zhang et al. Their contributions heighten remarkably the quality of the book.

The author acknowledges the financial support during the past years by the Research Fund for Doctoral Program of Higher Education, the National Natural Science Foundation of China, the Qiu Shi Science and Technology Foundation and the 973 Project. Thanks are also expressed to the World Scientific for their efforts on publishing this new edition of the book.

M. F. Chen
Beijing
August 29, 2003

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Chapter 0

An Overview of the Book: Starting from Markov Chains

In this chapter, we introduce some background of the topics, as well as some results and ideas, studied in this book. We emphasize Markov chains, and discuss our problems by using the language as elementary and concrete as possible. Besides, in order to save the space of this section, we omit most of the references which will be pointed out in the related "Notes" sections.

0.1 Three Classical Problems for Markov Chains

For a given transition rate (i.e., a Q-matrix $Q = (q_{ij})$ on a countable state space), the uniqueness of the Q-semigroup $P(t) = (P_{ij}(t))$, the recurrence and the positive recurrence of the corresponding Markov chain are three fundamental and classical problems, treated in many textbooks. As an addition, this section introduces some practical results motivated from the study of a type of interacting particle systems, reaction-diffusion processes.

Definition 0.1. Let E be a countable set. Suppose that $(P_{ij}(t))$ is a sub-Markov transition probability matrix having the following properties.

(1) **Normal condition.**

$$P_{ij}(t) \geqslant 0, \quad \sum_j P_{ij}(t) \leqslant 1, \qquad i, j \in E, \ t \geqslant 0.$$

(2) **Chapman-Kolmogorov equation.**

$$P_{ij}(t+s) = \sum_k P_{ik}(t) P_{kj}(s), \qquad i, j \in E, \ t, s \geqslant 0.$$

(3) **Jump condition.** $\lim_{t\to 0} P_{ij}(t) = \delta_{ij}$ for all $i, j \in E$. It is well-known that for such a $(P_{ij}(t))$, we have a Q**-matrix** $Q = (q_{ij})$ deduced by

(4) Q**-condition.**

$$\lim_{t\to 0} \left(P_{ij}(t) - \delta_{ij}\right)/t = q_{ij} \qquad \text{for all } i, j \in E,$$

where

$$0 \leqslant q_{ij} < \infty, \ \ i \neq j, \quad 0 \leqslant q_i := -q_{ii} \leqslant \infty, \quad \sum_{j\neq i} q_{ij} \leqslant q_i.$$

Because of the Q-condition, we often call $P(t) = (P_{ij}(t))$ a **Q-process**.

Unless otherwise stated, throughout this chapter, we suppose that the Q-matrix $Q = (q_{ij})$ is **totally stable and conservative**. That is

$$q_i < \infty, \quad \sum_{j\neq i} q_{ij} = q_i, \qquad i \in E. \tag{0.1}$$

The first problem of our study is when there is only one Q-process $P(t) = (P_{ij}(t))$ for a given Q-matrix $Q = (q_{ij})$ (Then, the matrix Q is often called **regular**). This problem was solved by Feller (1957) and Reuter (1957).

Theorem 0.2 (Uniqueness criterion). For a given Q-matrix $Q = (q_{ij})$, the Q-process $(P_{ij}(t))$ is unique if and only if (abbrev. iff) the equation

$$(\lambda + q_i)u_i = \sum_{j\neq i} q_{ij}u_j, \quad 0 \leqslant u_i \leqslant 1, \qquad i \in E \tag{0.2}$$

has only the trivial solution $u_i \equiv 0$ for some (equivalently, for all) $\lambda > 0$.

Certainly, this criterion has many applications. For instance, it gives us a complete answer to the birth-death processes (cf. Corollary 0.8 below). However, it seems hard to apply the above criterion directly to the following examples.

Example 0.3 (Schlögl's model). Let S be a finite set and $E = \mathbb{Z}_+^S$, where $\mathbb{Z}_+ = \{0, 1, \cdots\}$. The model is defined by the following Q-matrix $Q = (q(x, y) : x, y \in E)$:

$$q(x,y) = \begin{cases} \lambda_1 \binom{x(u)}{2} + \lambda_4 & \text{if } y = x + e_u \\ \lambda_2 \binom{x(u)}{3} + \lambda_3 x(u) & \text{if } y = x - e_u \\ x(u)\, p(u,v) & \text{if } y = x - e_u + e_v \\ 0 & \text{for other } \ y \neq x, \end{cases}$$

$$q(x) = -q(x,x) = \sum_{y\neq x} q(x,y),$$

where $x = (x(u) : \ u \in S)$, $\binom{n}{k}$ is the usual combination, $\lambda_1, \cdots, \lambda_4$ are positive constants, $(p(u,v) : \ u, v \in S)$ is a transition probability matrix on S and e_u is the element in E having value 1 at u and 0 elsewhere.

The Schlögl model is a model of chemical reaction with diffusion in a container. Suppose that the container consists of small vessels. In each vessel $u \in S$, there is a reaction described by a birth-death process. The birth and death rates are given, respectively, by the above first two lines in the definition of $(q(x, y))$. Moreover, suppose that between any two vessels u and v, there is a diffusion, with rate given by the third line of the definition. This model was introduced by F. Schlögl (1972) as a typical model of non-equilibrium systems. See Haken (1983) for related references.

Example 0.4 (Dual chain of spin system). Let S be a countable set, and X be the set of all finite subsets of S. For $A \in X$, let $|A|$ denote the number of elements in A. For various concrete models, their Q-matrices $(q(A,B) : A, B \in X)$ usually satisfy the following condition:

$$\sum_{B\in X} q(A,B)\,(|B|-|A|) \leqslant C + c\,|A|, \qquad A \in X \tag{0.3}$$

for some constant $C, c \in \mathbb{R} := (-\infty, \infty)$. A particular case is that

$$q(A,B) = \sum_{u\in A} c(u) \sum_{F:\, F\triangle(A\setminus u)=B} p(u,F),$$

where

$$c(u) \geqslant 0, \quad \sup_u c(u) < \infty, \quad p(u,A) \geqslant 0, \quad \sum_A p(u,A) = 1$$

and $\sup_u c(u) \sum_A p(u,A)\,|A| < \infty$. Then (0.3) holds with $C = 0$ and $c = \sup_u c(u) \sum_F p(u,F)\,[|F|-1]$.

Intuitively, we can interpret the last Markov chain as follows. Let A be the set of sites occupied by particles (finite!). At each site there is at most one particle. Then the process evolves in the following way: each $u \in A$ is removed from A at rate $c(u)$ and is replaced by a set F with probability $p(u,F)$; when an attempt is made to put a point at site u which is already occupied, the two points annihilate one another. The dual chain of a spin system is often used as a dual process of an infinite particle system. This dual approach is one of the main powerful tools in the study of infinite particle systems (cf. Liggett (1985), Chapter 3, Section 4).

Now, we state our first main result.

Theorem 0.5. Let $Q = (q_{ij})$ be a Q-matrix on E. Suppose that there exist a sequence $\{E_n\}_1^\infty$ and a non-negative function φ such that

$$E_n \uparrow E, \qquad \sup_{i\in E_n} q_i < \infty, \qquad \lim_{n\to\infty} \inf_{i\notin E_n} \varphi_i = \infty.$$

If in addition

$$\sum_j q_{ij}(\varphi_j - \varphi_i) \leqslant c\,\varphi_i, \qquad i \in E \tag{0.4}$$

holds for some $c \in \mathbb{R}$, then the Q-process is unique.

To compare this theorem with Criterion 0.2, we reformulate Criterion 0.2 as follows.

Theorem 0.6 (Alternative uniqueness criterion). Given a Q-matrix $Q = (q_{ij})$, for the uniqueness of the Q-process, it is sufficient that the inequality

$$\sum_j q_{ij}(\varphi_j - \varphi_i) \geqslant \lambda\varphi_i, \quad i \in E$$

has no bounded solution $(\varphi_i : i \in E)$ with $\sup_i \varphi_i > 0$ for some (equivalently, for all) $\lambda > 0$. Conversely, these conditions plus $\varphi \geqslant 0$ are also necessary.

Take $E_n = \{i \in E : q_i \leqslant n\}$. By Theorem 0.5, we have the following result.

Corollary 0.7. If there exist a function φ: $\varphi_i \geqslant q_i$, $i \in E$, and a constant $c \in \mathbb{R}$ such that (0.4) holds, then the Q-process is unique.

To see these results are practical, for Schlögl's model (Example 0.3), we can either take $\varphi(x) = c[1 + (\sum_{u\in S} x(u))^3]$ and apply Corollary 0.7, or take $\varphi(x) = c[1 + \sum_u x(u)]$ and apply Theorem 0.5 with $E_n = \{i : i \leqslant n\}$, where c is a constant chosen by a simple computation. For Example 0.4, simply take $\varphi(A) = c[1 + |A|]$ for a suitable c and apply Theorem 0.5 with $E_n = \{A : |A| \leqslant n\}$. For instance, for Schlögl's model, when $\sum_u x(u)$ is large, then (0.4) should hold because the order of the death rate is higher than the one of the birth rate. On the other hand, for bounded $\sum_u x(u)$, we can choose c large enough so that (0.4) also holds.

Next, we consider a typical case. Let $E = \{0, 1, 2, \cdots\} = \mathbb{Z}_+$. Suppose that the solution (u_i) to the equation

$$(\lambda + q_i)u_i = \sum_{j\neq i} q_{ij}u_j, \quad u_0 = 1, \qquad i \in E \tag{0.5}$$

is non-decreasing: $u_i \uparrow$ as $i \uparrow$, then, from Criterion 0.2, it is easy to see that the process is unique iff $\lim_{i\to\infty} u_i = \infty$. On the other hand, if we take $E_n = \{i \in \mathbb{Z}_+ : i \leqslant n\}, c = \lambda$ and $\varphi_i = u_i, i \in E$, then the hypotheses of Theorem 0.5 are reduced to the condition: $\lim_{i\to\infty} \varphi_i = \lim_{i\to\infty} u_i = \infty$, which is the same as above. Thus, the conditions of Theorem 0.5 are not only sufficient but also necessary for this particular case. This remark plus the next result gives us another view of justifying the power of Theorem 0.5.

Corollary 0.8. For the **single birth Q-matrix** on $E = \mathbb{Z}_+$:

$$q_{i,i+1} > 0, \quad q_{i,i+k} = 0, \quad k \geqslant 2,\ i \in E$$

(but there is no restriction to the death rates), the Q-process is unique iff $\sum_{k=0}^{\infty} m_k = \infty$, where

$$m_0 = \frac{1}{q_{01}}, \quad m_n = \frac{1}{q_{n,n+1}}\left[1 + \sum_{k=0}^{n-1}\left(\sum_{j=0}^{k} q_{nj}\right)m_k\right], \qquad n \geqslant 1.$$

The key to prove this corollary is the non-decreasing property mentioned above, of the solution to (0.5) (cf. Theorem 3.16).

Now, we go to the next topic: recurrence. It is well known that for a regular Q, the corresponding Markov chain is recurrence iff so is its embedding chain. See Chung (1967). Here, we would like to mention a more precise formula. Note that for a given Q-matrix $Q = (q_{ij})$, we always have the minimal Q-process $(P_{ij}^{\min}(t))$, which can be obtained by the following procedure. Let $P_{ij}^{(0)}(t) \equiv 0$ and

$$P_{ij}^{(n+1)}(t) = \int_0^t e^{-q_i(t-s)} \sum_{k\neq i} q_{ik} P_{kj}^{(n)}(s)ds + \delta_{ij} e^{-q_i t}, \qquad n \geqslant 0,$$

then for fixed $i, j \in E$ and $t \geqslant 0$, $P_{ij}^{(n)}(t) \uparrow P_{ij}^{\min}(t)$ as $n \uparrow \infty$ (Theorem 2.21).

Theorem 0.9. We have

$$\int_0^\infty P_{ij}^{\min}(t)dt = \sum_{n=0}^\infty \Pi_{ij}^{(n)}/q_j \qquad \text{for all } i, j \in E,$$

where $\Pi_{ij}^{(0)} = \delta_{ij}$ and $(\Pi_{ij}^{(n)})$ is the n-th power of the matrix (Π_{ij}):

$$\Pi_{ij} = \begin{cases} \delta_{ij} & \text{if } q_i = 0 \\ (1-\delta_{ij})q_{ij}/q_i & \text{if } q_i \neq 0 \end{cases}$$

and we use the usual convention: $c/\infty = 0$ for $c \neq 0$; $c/0 = \infty$ for $c > 0$; $c + \infty = \infty$; $c \times \infty = \infty$ for $c > 0$; $0 \times \infty = 0$ and $0/0 = 0$.

To state a more practical criterion for the recurrence, we need an important concept. A function $h\colon E \to \mathbb{R}_+ = [0, \infty)$ is called **compact**, if for each $d \in \mathbb{R}_+$, the set $\{i \in E\colon h_i \leqslant d\}$ is finite.

Theorem 0.10. An irreducible Q-matrix $Q = (q_{ij})$ is regular with recurrent $P(t)$ iff the equation

$$\sum_{j\neq i} q_{ij} y_j \leqslant q_i y_i, \qquad i \notin H$$

has a compact solution (y_i) for some finite $H \neq \emptyset$.

The last topic is about the positive recurrence.

Theorem 0.11. Given an irreducible Q-matrix $Q = (q_{ij})$, suppose that there exist a compact function h and constants $K \geqslant 0$, $\eta > 0$ or $K = \eta = 0$ such that

$$\sum_j q_{ij}(h_j - h_i) \leqslant K - \eta h_i, \qquad i \in E. \tag{0.6}$$

Then the Markov chain is positive recurrent (exponentially ergodic) and hence has uniquely a stationary distribution.

To apply this theorem to Schlögl's model (Example 0.3), take $h(x) = \sum_{u \in S} x(u)$ and an arbitrary $\eta > 0$. Then one can find a $K < \infty$ such that the above inequality holds. Hence, Schlögl's model is always ergodic in finite dimensions. As for Example 0.4, since the empty set $\emptyset$ is an absorbing state, the answer is obvious. Finally, consider the linear growth model:

$$q_{i,i+1} = \lambda i + \delta, \quad q_{i,i-1} = \mu i, \quad \lambda, \mu, \delta > 0,$$
$$q_{i,j} = 0 \qquad \text{for other } j \neq i \pm 1, \ i, j \in \mathbb{Z}_+.$$

It is well known that this model is positive recurrent if and only if $\lambda < \mu$. Recall that this conclusion is usually obtained by studying three series, respectively, to show the regularity of Q, the recurrence and finally the positive recurrence of the chain (cf. Example 4.56 for details). However, it is obvious that Theorem 0.11 is applicable if and only if $\lambda < \mu$, for the natural choice that $h_i = i$ $(i \in \mathbb{Z}_+)$. Thus, Theorem 0.11 is sharp for this model and its advantage should be clear now.

Roughly speaking, the three problems discussed above consist of the subjects of the subsequent four chapters. Actually, we deal with the general case where the Q-matrix may not be conservative and furthermore the state space is allowed to be general too. Certainly, some results for the general state space are natural generalization of that for the discrete state space. However, it should be pointed out that the generalization is not trivial in many situations, for instance, the differentiability for the transition functions (see Section 1.3). Another case is the following. As we will see in Chapter 4, the ergodic theory for Markov chains are now quite complete but at the moment, our knowledge about the theory for general jump processes is still incomplete.

For general totally stable Q-matrix (i.e., $q_i < \infty$ for all i), the uniqueness problem had been open for a long period and was eventually solved by Hou (1974) for Markov chains and Chen and Zheng (1982) for the general setup. The general uniqueness criterion is given in Chapter 3.

0.2 Probability Metrics and Coupling Methods

The coupling technique has a long history and now has many applications. It is one of the basic tools used in the book. In this section, we discuss the relation between couplings and probability metrics, and introduce some coupling methods for Markov chains. Some preliminary applications are also introduced.

Definition 0.12. Let P_k be a probability measure on a measurable space $(E_k, \mathscr{E}_k)$, $k = 1, 2$. A probability measure $\widetilde{P}$ on $(E_1 \times E_2, \mathscr{E}_1 \times \mathscr{E}_2)$ is called a **coupling of P_1 and P_2** if $\widetilde{P}$ has the following **marginality**:

$$\widetilde{P}(B_1 \times E_2) = P_1(B_1), \quad \widetilde{P}(E_1 \times B_2) = P_2(B_2), \qquad B_k \in \mathscr{E}_k, \ k = 1, 2.$$