

Summary of thesis: Pattern Formation in Stochastic Reaction-Diffusion Systems with Microscopic Singularity

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Pattern formation phenomena are widely observed in a variety of macroscopic systems. To uncover universal pattern formation mechanisms that are independent of the specific constituents of individual systems, a number of theories have been proposed. Most of these studies have been conducted within macroscopic phenomenological frameworks based on partial differential equations (PDEs).

One of the most successful theoretical frameworks is the description of patterns based on reaction-diffusion equations. Reaction-diffusion equations are PDEs that describe the time evolution of the concentrations of chemical species, in which chemical reaction processes at each point in space and the diffusion of the chemical species are considered. These processes give rise to rich spatial structures. Examples include phase coexistence and Turing patterns. Phase coexistence refers to a phenomenon in which regions with different concentrations coexist, separated by interfaces. Turing patterns are spatial structures that spontaneously emerge when a homogeneous concentration field is destabilized by diffusion. Experimental studies have shown that these theoretically studied phenomena successfully account for the spatial structures observed in macroscopic reaction-diffusion systems.

More recently, however, pattern formation phenomena have also been observed at mesoscopic and microscopic scales. In such small systems, two aspects are expected to play important roles. The first is the effect of fluctuations. While fluctuations can be neglected in macroscopic systems, it is anticipated to have a non-negligible influence on pattern formation in such systems. The second is the effect of the spatial discreteness of a pattern. Here, the spatial discreteness of a pattern refers to situations in which the characteristic length of the pattern becomes comparable to the microscopic cutoff length of the model. This is in sharp contrast to the framework of PDEs, where patterns are described in terms of spatially continuous concentration fields. Consequently, patterns observed in small systems may exhibit behaviors that cannot be understood by PDEs.

Against this background, this thesis investigates how fluctuations and spatial discreteness affect phase coexistence and Turing patterns. We employ a stochastic reaction-diffusion model in which reaction vessels of volume Ω are arranged on a lattice. Both chemical reactions within each vessel and hopping of chemical species between neighboring vessels are taken into account, and all of them are described as Markov jump processes. Based on this model, we analyze phase coexistence and Turing patterns to clarify how the spatial structures that arise under fluctuations and spatial discreteness differ from their counterparts in macroscopic systems.

In Chapter 2, we examine the phase coexistence condition in the stochastic reaction-diffusion model. We focus on two regimes, one in which the hopping rate is large compared with the chemical reaction rates and another in which it is small, and we derive the phase coexistence conditions in each regime. As a result, we find that the phase coexistence condition depends on the hopping rate. Furthermore, the phase coexistence conditions in each regime are determined by two different potentials. In large hopping rate regime, the phase coexistence condition is governed by a potential defined from the reaction-diffusion equation, whereas in small hopping rate regime, it is determined by a potential defined from the Markov jump process describing the well-mixed chemical reaction dynamics in a single vessel.

In Chapter 3, we analyze Turing patterns that arise in the stochastic reaction-diffusion model. We focus on the situation where the characteristic length of the pattern becomes comparable to the lattice spacing, so that spatial discreteness plays a crucial role. In our analysis, we consider two different orders of limits and obtain qualitatively different results in each case. When we first take the deterministic limit $\Omega \rightarrow \infty$ followed by the long-time limit $t \rightarrow \infty$, we find that the stationary solutions of the corresponding spatially discrete deterministic equations become spatially chaotic. In contrast, when we first take the limit $t \rightarrow \infty$ followed by $\Omega \rightarrow \infty$, the resulting patterns are spatially periodic.

Chapter 4 is devoted to concluding remarks.