Metastability for low-temperature Kawasaki dynamics with two types of particles

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Summary

Metastability is a phenomenon that may occur in a system subject to a noisy dynamics. It is characterized by the existence of different times scales on which the system evolves. On a short time scale the system is in an apparent equilibrium and explores a limited region of its state space, whereas on a long time scale it undergoes rapid transitions between different regions of the state space. In thermodynamics metastability is related to first-order phase transitions. The classical example of metastable behavior is the freezing of a supercooled liquid: the system stays for a long time in the (metastable) liquid phase before reaching the (stable) solid phase and the crossover is triggered by the appearance of a critical droplet of the solid phase inside the liquid phase. However, metastable phenomena do not only occur in physics: they appear in many fields such as biology, chemistry, economics and computer science.

A behavior of the above type can be modeled by defining an energy function H on the state space $\mathcal{X}$ of the system and by considering a dynamics on $\mathcal{X}$ that allows transitions towards states with higher energy with low probability. In this framework, the metastable and the stable state correspond, respectively, to a local and a global minimizer of the energy. The crossover time towards the stable state is determined by the depth of the deepest valley separating the stable and the metastable state.

In the context of metastability, typical questions that are addressed concern the probability distribution of the time it takes to observe the transition from the metastable to the stable state, the shape of the critical configurations that trigger the transition, and the typical trajectories the dynamics follows in order to realize the transition. Over the years, different approaches have been developed to tackle these questions. However, a unified theory is still lacking, and a detailed analysis of specific models and of model-dependent properties is required to deal with the key questions of interest.

In this thesis we consider a model of a low-temperature and low-density two-dimensional lattice gas with particles of two different types subject to Kawasaki dynamics in a large finite box Λ with an open boundary. Each pair of particles occupying neighboring sites has a negative binding energy provided their types

are different, while each particle has a positive activation energy that depends on its type. There is no binding energy between particles of the same type. At the boundary of Λ particles are created and annihilated in a way that represents the presence of an infinite gas reservoir. We start the dynamics from the configuration where Λ is empty (denoted by $\square$) and are interested in the transition time to configuration where Λ is full (denoted by $\boxplus$). This transition is triggered by a critical droplet appearing somewhere in Λ.

The structure of the thesis is as follows. In Chapter 1 we introduce the main approaches developed in the literature to deal with metastability, and we present the most relevant results obtained for models related to ours. In Chapter 2 we introduce our model and identify the values of the parameters for which the transition from $\square$ to $\boxplus$ exhibits metastable behavior in the limit of low temperature. Under *three hypotheses*, we determine the distribution and the expectation of the transition time, and identified the so-called critical configurations that satisfy a certain "gate property". The first hypothesis assumes that configuration $\boxplus$, corresponding to the liquid phase, is a minimizer of H. The second hypothesis requires that the valleys of the energy landscape are not too deep. The third hypothesis requires that the critical configurations have an appropriate geometry. Subject to these three hypotheses, several theorems are derived, for which *three model-dependent quantities* need to be identified as well: (1) the energy barrier $\Gamma^\star$ separating $\square$ from $\boxplus$; (2) the set $\mathcal{C}^\star$ of critical configurations; (3) the cardinality $N^\star$ of the set of protocritical configurations, which can be thought of as the "entrance" set of $\mathcal{C}^\star$. In Chapter 3 the first two hypotheses are verified and the value $\Gamma^\star$ of the energy barrier separating $\square$ and $\boxplus$ is identified. These results are sufficient to establish the exponential probability distribution of the nucleation time divided by its mean, and to determine the mean nucleation time up to a multiplicative factor $1 + o(1)$ in the limit of low temperature. In Chapter 4 we show that the model satisfies the third hypothesis, and we identify the set of critical configurations. We give a geometric characterization of the configurations in $\mathcal{C}^\star$ and compute the value of $N^\star$.