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

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Stellingen

Propositions belonging to the thesis

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

by Alessio Troiani

In the thesis we investigate a model of a low-temperature and low-density lattice gas with particles of two different types in a finite volume Λ surrounded by a gas reservoir in which the two types of particles have density $e^{-\beta\Delta_1}$, $e^{-\beta\Delta_2}$ respectively, where β is the inverse temperature and $\Delta_2 > \Delta_1 > 0$ are the “activation energies” of the two species of particles. We consider a “binding energy” $U > 0$ between particles of different types. A Hamiltonian energy function is defined on the space of configurations and particles move according to Kawasaki dynamics. We study how the system nucleates, i.e., how the transition from the configuration where Λ is empty (denoted by $\square$) to a configuration where Λ is filled with a large checkerboard cluster (denoted by $\boxplus$) happens. We need dual coordinates to study the geometry of configurations.

1. Configuration $\square$ is not a global minimizer of the Hamiltonian if and only if $\Delta_1 + \Delta_2 < 4U$.
2. For fixed number of particles of type 2 and for $\Delta_1 < U$, the value of the Hamiltonian is minimized by those configurations where all particles of type 2 are surrounded by particles of type 1 and whose support, in dual coordinates, is a polyomino of minimal perimeter. Configuration $\boxplus$ is a global minimizer of the Hamiltonian.
3. Let Γ^* be the energy barrier separating $\square$ from $\boxplus$. If $\Delta_1 < U$ and $4U - \Delta_1 - \Delta_2 > 0$ is small, then the energy barrier separating any configuration from the set $\{\square, \boxplus\}$ is smaller than Γ^* .
4. If $\Delta_1 < U$ and $4U - \Delta_1 - \Delta_2 > 0$ is small, then in the limit as $\beta \rightarrow \infty$, the expected value of the nucleation time is asymptotic to $Ke^{\beta\Gamma^*}$. If $\Lambda \rightarrow \mathbb{Z}^2$, then the asymptotics of the prefactor K can be identified and exhibits different behavior in at least three different parameter regimes.
5. When $\Delta_1 < U$ and $4U - \Delta_1 - \Delta_2 > 0$ is small, the cardinality of the entrance set of the set of critical configurations increases with Δ_2 .
6. Consider the totally asymmetric simple exclusion process on $\mathbb{Z}$ with jump rate at site i given by $r_i = 1$ for $i \neq 0$ and $r_0 = r$. The maximal stationary current $j(r)$ is non-decreasing in r , with $j(r) = \frac{1}{4}$ for $r \geq 1$. It is conjectured that $j(r) < \frac{1}{4}$ for $r < 1$.
7. Before starting my PhD program in Leiden, I have been a swimmer competing in national and international sports events for almost twenty years. There, as for academic research, what counts is a combination of talent, passion and hard work.
8. In many of the academic courses I took when I was studying engineering, emphasis was given to project management. I was taught how to deal with endeavors that had clearly defined goals and objectives. Moving to the world of research, where often not even the relevant questions are obvious beforehand, I felt a bit of a shock. Now, after four years, I realize that this uncertainty was both the challenge and the enjoyment.