Lecture 1: Exercises

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1 Exercise 1: Critical droplet Kawasaki dynamics

In this exercise you will compute the leading-order term for the mean metastable crossover time in the lattice-gas model with Kawasaki dynamics, found in den Hollander, Olivieri and Scoppola [2].

1.1 Notation and setting

We recall the Kawasaki dynamics you saw in Lecture 1 (and refer to Bovier and den Hollander [1, Section 18] for more deatils). Let $\Lambda \subset \mathbb{Z}^2$ be a large square box centered at the origin. Let

$$\partial^- \Lambda = \{x \in \Lambda \colon \; \exists\, y \notin \Lambda \colon \; \|y - x\| = 1\} \tag{1.1}$$

be the internal boundary of Λ, and put $\Lambda^- = \Lambda \backslash \partial^- \Lambda$. With each site $x \in \Lambda$ we associate an occupation variable $\eta(x) \in \{0, 1\}$, where $\eta(x) = 0$ indicates the absence and $\eta(x) = 1$ the presence of a particle at x. A lattice-gas configuration is denoted by $\eta = \{\eta(x) : x \in \Lambda\}$ and is an element of the configuration space $\Omega = \{0, 1\}^\Lambda$.

0	0	1	0	0
0	0	0	1	0
0	1	1	0	0
0	1	1	0	0
0	0	0	0	0

A lattice-gas configuration.

With each configuration $\eta \in \Omega$ we associate an energy given by the Hamiltonian

$$H(\eta) = -U \sum_{\substack{x,y \in \Lambda^- \\ \|x-y\|=1}} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x), \tag{1.2}$$

where the interaction consists of a binding energy $-U < 0$ between neighbouring particles and an activation energy $\Delta > 0$ for single particles.

Kawasaki dynamics on Λ with an open boundary is the Metropolis dynamics driven by H at inverse temperature β with two types of allowed moves:

$$\eta \to \eta' \qquad \text{at rate} \qquad \mathrm{e}^{-\beta[H(\eta')-H(\eta)]_+} \tag{1.3}$$

for all η' obtainable from η via:

(1) *particle hop*: an exchange of occupation numbers between neighbouring sites in Λ.

(2) *particle creation or annihilation*: a raising or lowering of occupation numbers at single sites in $\partial^-\Lambda$.

We may think of $\mathbb{Z}^2\backslash\Lambda$ as an infinite reservoir that keeps the particle density inside Λ fixed at $\mathrm{e}^{-\beta\Delta}$. The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\mathrm{e}^{-\beta H(\eta)}, \qquad \eta \in \Omega, \tag{1.4}$$

and is the reversible equilibrium of the Kawasaki dynamics, describing the lattice gas when it is in equilibrium with the reservoir.

Let $\square, \blacksquare$ denote the configurations where Λ is empty, respectively, full. Let ℓ_c be the critical droplet size. We recall the following notation:

- Let $\mathcal{Q} = \bar{\mathcal{Q}} \cup \widetilde{\mathcal{Q}}$ be the set of canonical protocritical droplets. Here, $\bar{\mathcal{Q}}$ is the set of configurations consisting of an $(\ell_c - 1) \times \ell_c$ quasi-square with a protuberance attached to one of the longest sides, and $\widetilde{\mathcal{Q}}$ is the set of configurations consisting of an $(\ell_c - 1) \times \ell_c$ quasi-square with a protuberance attached to one of the shortest sides.

- Let $\mathcal{D} = \bar{\mathcal{D}} \cup \widetilde{\mathcal{D}}$ be the set of protocritical droplets defined by

$$\mathcal{D} = \mathcal{Q}^U, \tag{1.5}$$

  the set of configurations that can be reached from $\mathcal{Q}$ via a U-path, i.e., a path that begins and ends at the same energy and never exceeds U in energy.

- Let $\mathcal{D}^{\mathrm{fp}}$ be the set of critical droplets obtained from $\mathcal{D}$ by adding a free particle anywhere in Λ^-. The definition of $\mathcal{Q}^{\mathrm{fp}}$ is analogous.

1.2 Exercise

(i) Write down the formula for the energy E of a configuration where the particles form a single $\ell \times \ell$ square anywhere inside Λ^-.

(ii) Find local and global minima of E, and explain the role of the pair $(\square, \blacksquare)$ from the point of view of metastability. Find where the maximum is attained, and explain why $\Delta \in (U, 2U)$ is the metastable regime.

(iii) Compute $H(\mathcal{Q}^{\mathrm{fp}})$, show that it is equal to $H(\mathcal{D}^{\mathrm{fp}})$, and explain what it represents.

[Hint: Use the fact that

- $\bar{\mathcal{D}}$ is the set of configurations with a single cluster anywhere in Λ^- consisting of an $(\ell_c - 2) \times (\ell_c - 2)$ square with four bars of lengths $\bar{k}_i$, $i = 1, \ldots, 4$, attached to its four sides satisfying $1 \leq \bar{k}_i \leq \ell_c - 1$ and $\sum_{i=1}^4 \bar{k}_i = 3\ell_c - 3$,

- $\widetilde{\mathcal{D}}$ is the set of configurations with a single cluster anywhere in Λ^- consisting of an an $(\ell_c - 1) \times (\ell_c - 3)$ rectangle with four bars $\tilde{k}_i$, $i = 1, \ldots, 4$, attached to its four sides satisfying $1 \leq \tilde{k}_i \leq \ell_c - 1$ and $\sum_{i=1}^4 \tilde{k}_i = 3\ell_c - 2$,

provides a geometric description of the set of protocritical droplets. Notice that the four bars may be placed anywhere in the ring around the $(\ell_c - 2) \times (\ell_c - 2)$ square and that a bar may include a corner of the ring provided the neighbouring bar also includes this corner.]

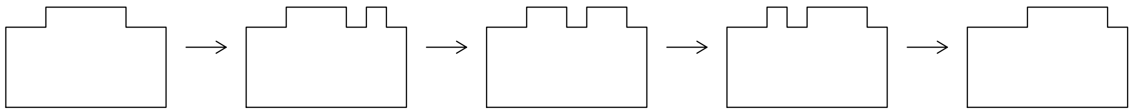

Figure 1: Translation of a bar on a side of a rectangle.

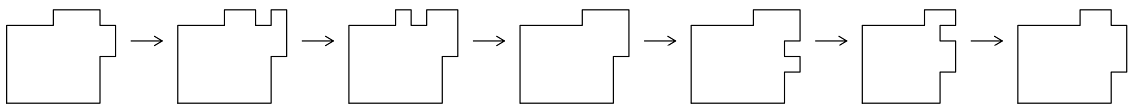

Figure 2: Motion of a particle around a corner of a rectangle.

2 Exercise 2: Motion along the border

In this exercise you will understand a special property of Kawasaki dynamics also found in den Hollander, Olivieri and Scoppola [2], namely, how the set of protocritical droplets arises from the set of canonical protocritical droplets via motion of particles along the border.

In Figure 1 you see a sequence of moves through which a bar on one side of a rectangle is shifted. In Figure 2 you see a sequence of moves through which a particle is moved around the corner of a rectangle.

(i) Write on top of the arrows the cost in energy to go from one configuration to the next.

(ii) Find out whether these motions are U-paths.

(iii) Explain in words why there is a degeneration of configurations on the "saddle point", which implies a large cardinality of the set of protocritical droplets.

[Hint: This is due to the fact that Kawasaki dynamics is conservative. Since the number of particles is conserved in the interior of the box, in order to produce growing or shrinking of the droplet, particles have to travel between the droplet and the boundary of the box.]

References

[1] A. Bovier and F. den Hollander. *Metastability: A Potential-Theoretic Approach*, Grundlehren der Mathematischen Wissenschaften, Vol. 351. Springer, 2015.

[2] F. den Holllander, E. Olivieri and E. Scoppola. *Metastability and nucleation for conservative dynamics*, J. Math. Phys. 41 (2000) 1424–1498.