LECTURE 8

Kawasaki dynamics on a box with open boundary.
Critical droplet and metastable crossover time.

§ TARGET

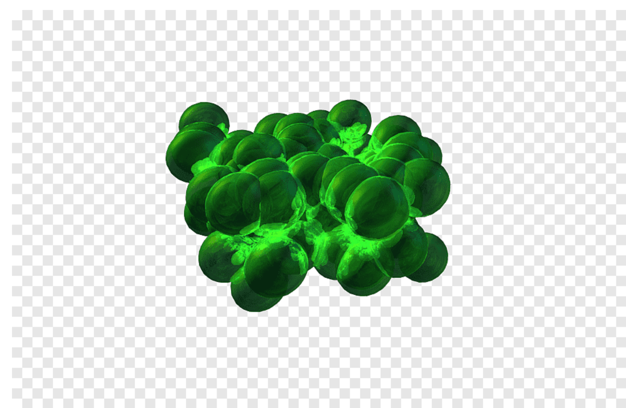
In this lecture we analyse metastability for the lattice gas in two and three dimensions subject to Kawasaki dynamics.

Particles live in a finite box, hop between nearest-neighbour sites, feel an attractive interaction when they sit next to each other, and are created, respectively, annihilated at the boundary of the box in a way that reflects the presence of an infinite gas reservoir.

We are interested in how the system nucleates, i.e., how the box fills up when it is initially empty.

Kawasaki dynamics is a conservative dynamics: particles are conserved in the interior of the box. Consequently, during the growing and the shrinking of droplets, particles must travel between the droplet and the boundary of the box, which causes several complications.

It turns out that, in the metastable regime of interest, particles move along the border of a droplet more rapidly than they arrive from the boundary of the box. This property leads to a shape of the critical droplet that is more complicated.



§ KAWASAKI DYNAMICS

1. Let $\Lambda \subset \mathbb{Z}^2$ be a large square box, centered at the origin. Let

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

be the internal boundary of Λ.

2. A configuration is denoted by $\eta \in \Omega = \{0,1\}^\Lambda$, where $\eta(x) = 0$ indicates the absence and $\eta(x) = 1$ the presence of a particle at x.

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.

3. Each configuration $\eta \in \Omega$ has an energy given by the Hamiltonian

$$H(\eta) = -U \sum_{\{x,y\} \in \Lambda^*} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x).$$

The interaction consists of a binding energy $-U < 0$ and an activation energy $\Delta > 0$.

4. There are two types of allowed moves:

(1) particle hop:
$0 \leftrightarrow 1$ between pairs of neighbouring vertices in Λ.

(2) particle creation or annihilation:
$0 \rightarrow 1$ or $1 \rightarrow 0$ at single vertices in $\partial\Lambda$.

Kawasaki dynamics is the Metropolis dynamics associated with H at inverse temperature β, i.e.,

$$\eta \to \eta' \text{ at rate } \exp\Big\{-\beta[H(\eta') - H(\eta)]_+\Big\}$$

for allowed moves.

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

Link between lattice gas and Ising spins:

$$\eta(x) \in \{0, 1\}, \qquad \sigma \in \{-1, +1\}.$$

Substitute $\eta(x) = \frac{1+\sigma(x)}{2}$ into the lattice gas Hamiltonian to get

$$H(\eta) = -U \sum_{\{x,y\} \in \Lambda^*} \frac{1+\sigma(x)}{2} \frac{1+\sigma(y)}{2} + \Delta \sum_{x \in \Lambda} \frac{1+\sigma(x)}{2}$$
$$= -\frac{U}{4} \sum_{\{x,y\} \in \Lambda^*} \sigma(x)\sigma(y) - \frac{2U - \Delta}{2} \sum_{x \in \Lambda} \sigma(x) + C,$$

where $C = C(U, \Delta, \Lambda)$ is a constant and we ignore details at the boundary. Hence we get the Ising spin Hamiltonian $H(\sigma)$ with

$$J = \frac{U}{2}, \qquad h = 2U - \Delta.$$

§ METASTABLE REGIME

The metastable regime of interest turns out to be

$$\Delta \in (U, 2U), \qquad \beta \to \infty.$$

A key role is played by what we call the critical droplet size

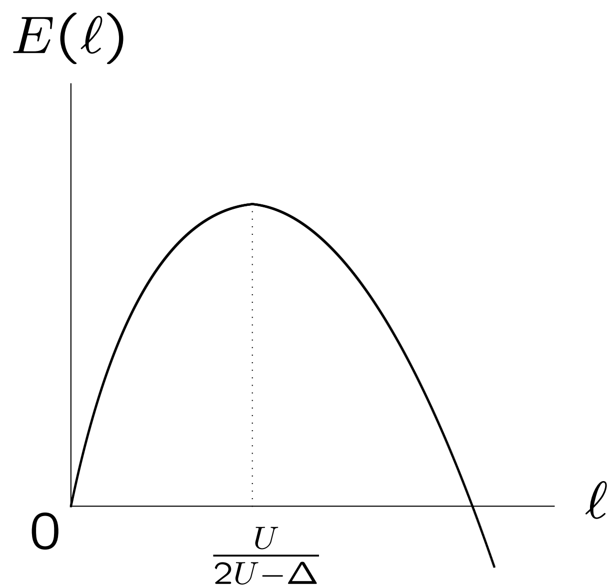
$$\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil,$$

where for convenience we assume that

$$\frac{U}{2U - \Delta} \notin \mathbb{N}.$$

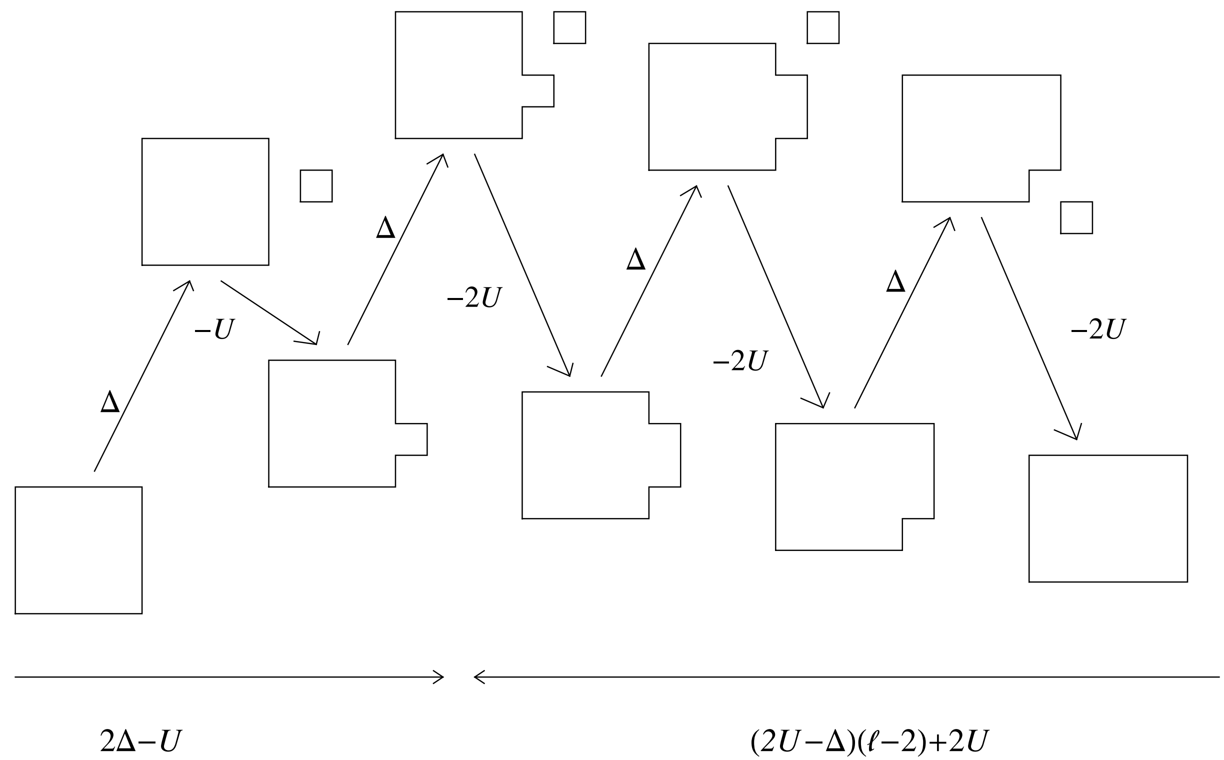
The energy of an $\ell \times \ell$ droplet equals

$$E(\ell) = -U[2\ell(\ell-1)] + \Delta\ell^2. \qquad \text{EXERCISE!}$$



$$\ell_c = \left\lceil \frac{U}{2U-\Delta} \right\rceil$$

An $(\ell_c - 1) \times (\ell_c - 1)$ droplet is subcritical while an $\ell_c \times \ell_c$ droplet is supercritical.



Add or remove a bar of length ℓ.

Note: The costs match when $\ell = \frac{U}{2U-\Delta}$.

§ NUCLEATION

The nucleation proceeds in four steps:

(1) Creation of a canonical protocritical droplet: a quasi-square with a single protuberance.

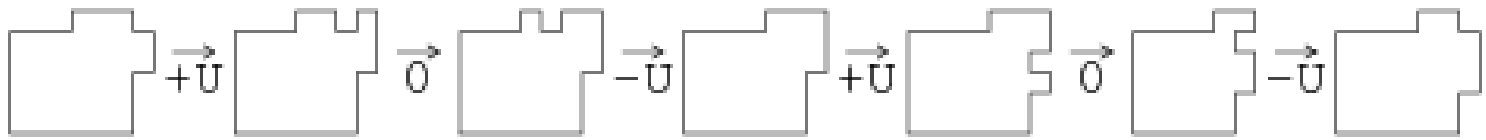
(2) Particles move along the border of the droplet: all the other protocritical droplets are visited.

(3) A free particle moves from the boundary of the box to the protocritical droplet.

(4) The free particle attaches itself to the protocritical droplet.

After these four steps are completed, the dynamics is over the hill and proceeds downwards in energy to fill up the box.

Step (2) of the nucleation is specific to Kawasaki dynamics:



Motion of a particle around a corner of a rectangle at cost U.

This motion leads to deformation of protocritical droplets before they turn into critical droplets via the arrival of a free particle from $\partial\Lambda$.

§ PROTOCRITICAL DROPLETS

DEFINITION 8.1:

(a) Let $\square, \blacksquare$ denote the configurations where Λ is empty, respectively, full.

(b) Let $\mathcal{Q} = \bar{\mathcal{Q}} \cup \tilde{\mathcal{Q}}$ be the set of canonical protocritical droplets defined by

- $\bar{\mathcal{Q}}$ 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.
- $\tilde{\mathcal{Q}}$ 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.

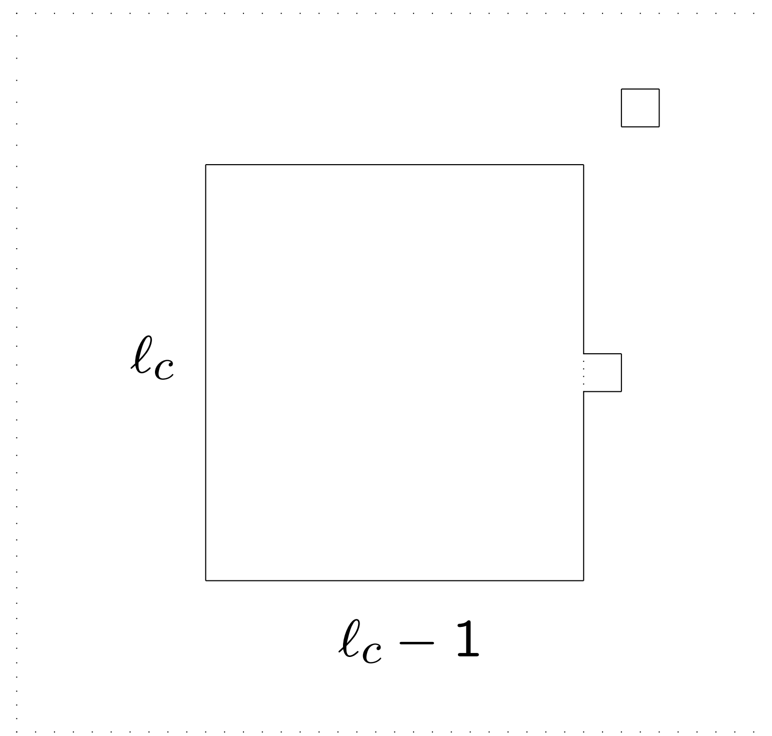
(c) Let $\mathcal{D}$ be the set of protocritical droplets defined by

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

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 does not exceed U in energy.

(d) Let $\mathcal{D}^{\text{fp}}$ be the set of critical droplets obtained from $\mathcal{D}$ by adding a free particle anywhere in Λ.

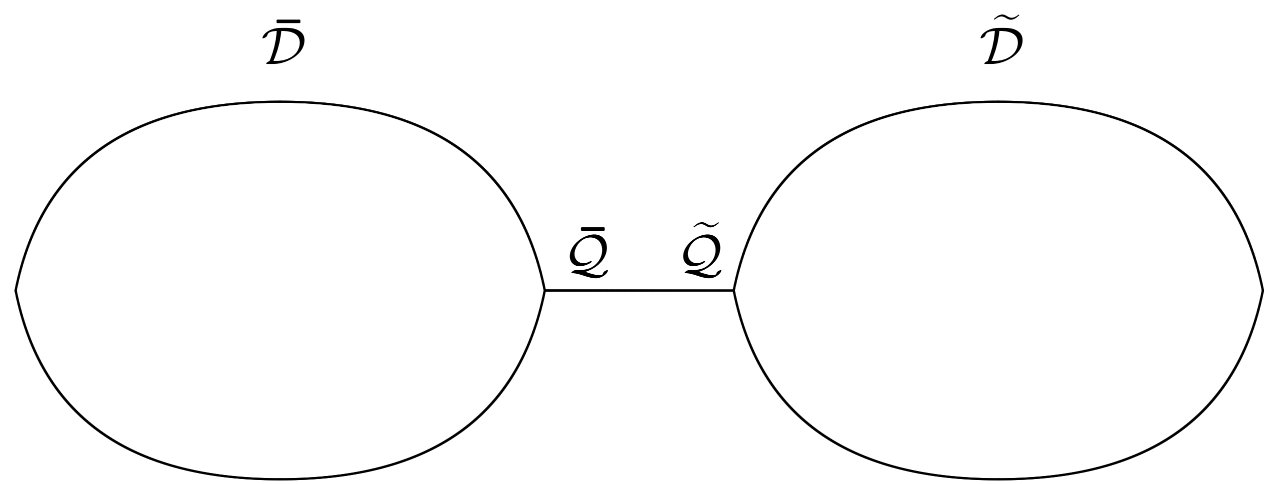
discrete isoperimetric inequalities



An example of a canonical critical droplet.

EXERCISE!

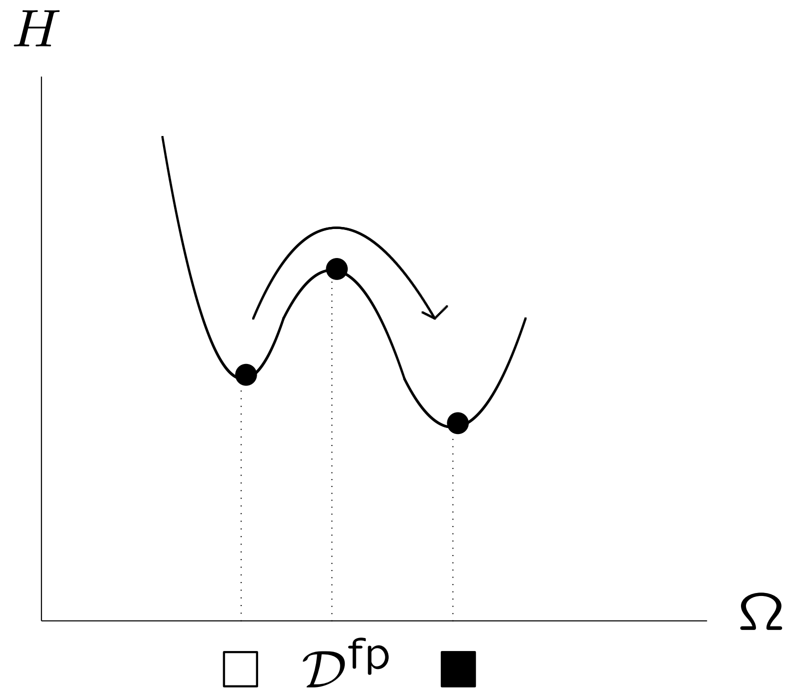
The configurations in $\mathcal{D}$ arise from each other via motion of particles along the border of the droplet: because $\Delta > U$, all protocritical droplets are explored before the free particle arrives and attaches itself.



Dumb-bell shape: $\mathcal{D} = \bar{\mathcal{D}} \cup \tilde{\mathcal{D}}$

$\bar{\mathcal{Q}}$ and $\tilde{\mathcal{Q}}$ are the gateways between $\bar{\mathcal{D}}$ and $\tilde{\mathcal{D}}$.

EXERCISE!



Nucleation for Kawasaki dynamics.

THEOREM 8.2:

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = [1 + o(1)] K \mathrm{e}^{\beta \Gamma^\star}, \qquad \beta \to \infty,$$

with

$$\begin{aligned} \Gamma^\star &= H(\mathcal{D}^{\mathrm{fp}}) - H(\square) = H(\mathcal{D}) + \Delta \\ &= -U[(\ell_c - 1)^2 + \ell_c(\ell_c - 2) + 1] + \Delta[\ell_c(\ell_c - 1) + 2] \end{aligned}$$

and $K = K(\Lambda)$ *satisfying*

$$\lim_{\Lambda \to \mathbb{Z}^2} \frac{4\pi|\Lambda|}{\log|\Lambda|} K(\Lambda) = \frac{1}{N(\ell_c)}$$

with

$$N(\ell_c) = \sum_{k=1,2,3,4} \binom{4}{k} \left[\binom{\ell_c + k - 2}{2k - 1} + 2\binom{\ell_c + k - 3}{2k - 1} \right]$$

the cardinality of $\mathcal{D}$ *modulo shifts.*

The prefactor K can be expressed in terms of capacities associated with two-dimensional simple random walk on Λ moving from $\partial\Lambda$ to a protocritical droplet in the interior of Λ.

No easily computable expression is available for K for finite Λ, but at least a sharp asymptotics is available as $\Lambda \to \mathbb{Z}^2$.

discrete isoperimetric inequalities
Alonso and Cerf 1996

§ EXTENSION TO THREE DIMENSIONS

We briefly indicate how to extend the main results from two to three dimensions.

Let $\Lambda \subset \mathbb{Z}^3$ be a large cubic box, centred at the origin. The metastable regime is

$$\Delta \in (2U, 3U), \qquad \beta \to \infty,$$

and we assume that

$$\frac{U}{3U - \Delta} \notin \mathbb{N}, \qquad \frac{2U}{3U - \Delta} \notin \mathbb{N}.$$

DEFINITION:

(a) Let $\mathcal{Q}$ be the set of canonical protocritical droplets consisting of:

- $(m_c - 1) \times (m_c - \delta_c) \times m_c$ quasi-cube
- attached to one of the faces: $(\ell_c - 1) \times \ell_c$ quasi-square
- attached to one of the sides: single protuberance.

Here, $\delta_c \in \{0, 1\}$ depends on the arithmetic properties of U and Δ, while

$$\ell_c = \left\lceil \frac{U}{3U - \Delta} \right\rceil, \qquad m_c = \left\lceil \frac{2U}{3U - \Delta} \right\rceil,$$

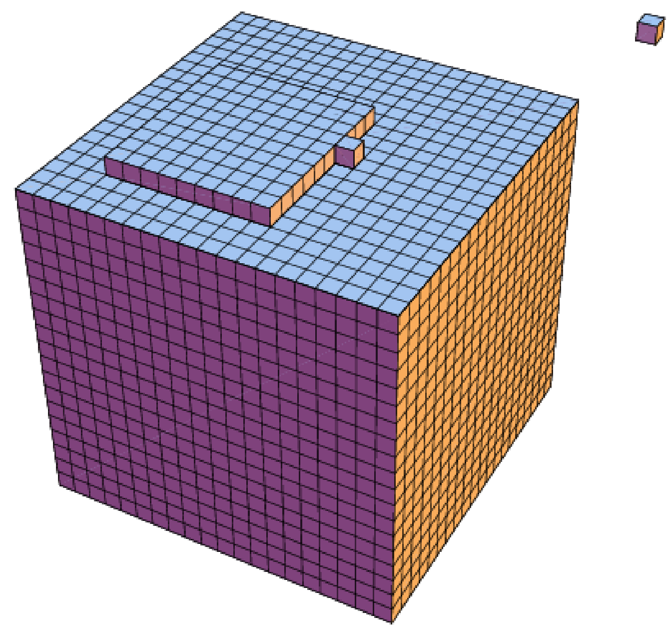
denote the two-dimensional critical droplet size on a face, respectively, the three-dimensional critical droplet size.

(b) Let $\mathcal{D}$ be the set of protocritical droplets consisting of configurations that can be reached from $\mathcal{Q}$ via a $2U$-path.

(c) Let $\mathcal{D}^{\mathrm{fp}}$ be the set of critical droplets obtained from $\mathcal{D}$ by adding a free particle anywhere in Λ.

(d) Let

$$\begin{aligned}\Gamma^\star &= H\left(\mathcal{D}^{\mathrm{fp}}\right) = H\left(\mathcal{D}\right) + \Delta = H(\mathcal{Q}) + \Delta \\ &= U[m_c(m_c-\delta_c) + m_c(m_c-1) + (m_c-\delta_c)(m_c-1) \\ &\qquad\qquad + 2\ell_c + 3] \\ &\quad - (3U-\Delta)[m_c(m_c-\delta_c)(m_c-1) \\ &\qquad\qquad + \ell_c(\ell_c-1) + 2].\end{aligned}$$



An example of a canonical critical droplet:

$\ell_c = 10$, $m_c = 20$, $\delta_c = 0$.

The main theorem for the average metastable crossover time carries over:

THEOREM 8.3:

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = [1 + o(1)]\, K\, \mathrm{e}^{\beta \Gamma^\star}, \qquad \beta \to \infty.$$

Unfortunately, the geometry of the set of critical droplets has not been fully identified. This is due to the fact that the motion of particles along the border of the droplet is much more complex in three than in two dimensions.

Consequently, only crude bounds are known for K.

discrete isoperimetric inequalities

PAPERS:

(1) F. den Hollander, E. Olivieri, E. Scoppola,
Metastability and nucleation for conservative dynamics,
J. Math. Phys. 41 (2000) 1424–1498.

(2) F. den Hollander, F.R. Nardi, E. Olivieri, E. Scoppola,
Droplet growth for three-dimensional Kawasaki dynamics,
Probab. Theory Relat. Fields 125 (2003) 153–194.

(3) A. Bovier, F. den Hollander, F.R. Nardi,
Sharp asymptotics for Kawasaki dynamics on a finite box with open boundary,
Probab. Theory Relat. Fields 135 (2006) 265–310.

LITERATURE:

Chapter 18 in Bovier and den Hollander 2015, and references therein.