Universality results for IPS with kinetic constraints

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Kinetically Constrained Models, a.k.a. KCM

Configurations : $\eta \in \Omega := \{0,1\}^{\mathbb{Z}^2}$, $0 =$ empty, $1 =$ occupied

Fix a density parameter $q \in [0,1]$ and an update family $\mathcal{U}$ with

$$\mathcal{U} = \{U_1, \ldots, U_m\}, \quad U_i \subset \mathbb{Z}^2 \setminus 0, \quad |U_i| < \infty, \quad m < \infty$$

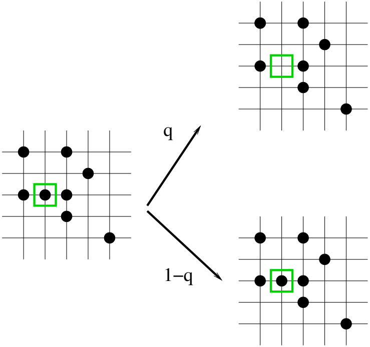
i.e. $\mathcal{U}$ is a finite collection of local neighbourhoods of the origin

Fix $\eta \in \Omega$ and $x \in \mathbb{Z}^2$: "the constraint is satisfied at x" iff at least one of the translated sets $U_i + x$ is completely empty

Dynamics: each site with the constraint satisfied is updated to empty at rate q and to occupied at rate $1 - q$

An example: 2-neighbour KCM a.k.a. FA-2f model

$\mathcal{U}$ = collection of sets containing 2 nearest neighb. of the origin



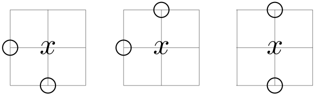
Other popular KCM

- FA-jf model:
  $\mathcal{U}$ = all sets containing j nearest neighbours of the origin

- East model: $\mathcal{U} = \{U_1, U_2\}$ with $U_1 = (0, -1)$, $U_2 = (-1, 0)$

- North-East model: $\mathcal{U} = \{U_1\}$ with $U_1 = \{(0, 1), (1, 0)\}$

- Duarte model: $\mathcal{U} = \{U_1, U_2, U_3\}$ with



U_1 U_2 U_3

Kinetically Constrained Models, a.k.a. KCM

KCM are a class of IPS with Glauber dynamics featuring:

- reversibility w.r.t. μ_q, the product measure of density $1-q$;
- non attractive dynamics ;
- blocked structures and blocked configurations;
- several invariant measures;
- anomalous divergence of time scales for $q \downarrow 0$.

Kinetically Constrained Models, a.k.a. KCM

- non attractive dynamics ;
  - $\rightarrow$ injecting more vacancies has unpredictable consequences
  - $\rightarrow$ coupling and censoring arguments fail
- blocked structures and blocked configurations;
  - $\rightarrow$ relaxation is not uniform on the initial condition
  - $\rightarrow$ worst case analysis is too rough
  - $\rightarrow$ coercive inequalities fail
- anomalous divergence of time scales for $q \downarrow 0$.

$\Rightarrow$ many standard IPS tools fail for KCM $\rightarrow$ new tools needed!

Origins of KCM

Introduced in the '80's to model the liquid/glass transition

- understanding this transition is a major open problem in condensed matter physics;
- sharp divergence of timescales;
- no significant structural changes.

$\Rightarrow$ kinetic constraints mimic *cage effect* :
if temperature is lowered free volume shrinks ($q \leftrightarrow e^{-1/T}$)

$\Rightarrow$ trivial equilibrium and yet sharp divergence of timescales when $q \downarrow 0$, aging, heterogeneities, ... $\rightarrow$ glassy dynamics

Blocked clusters and bootstrap percolation

Choose a configuration $\eta \in \Omega$.
Is η blocked? does it contain a subset of blocked particles?

A deterministic discrete time algorithm:

- kill particles on all sites that have the constraint satisfied;
- iterate until reaching a stable configuration.

- Clusters of particles in the stable configuration $\leftrightarrow$ blocked clusters of η
- the algorithm is $\mathcal{U}$-Bootstrap Percolation (BP) [Bollobás, Smith, Uzzell CPC '15]
- For FA-jf the corresponding algorithm is j-neighbour BP.

BP: critical density and infection time

- *Is the whole lattice empty in the stable configuration? What happens typically if η is distributed with μ_q, $\eta \sim \mu_q$?*

  $q_c := \inf\{q \in [0,1] : \mu_q(\text{origin is emptied eventually}) = 1\}$

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  $q_c := \inf\{q \in [0,1] : \mu_q(\text{origin is emptied eventually}) = 1\}$

- *How many steps do we need to empty the origin?*

  $\tau_0^{\mathrm{BP}} =$ first time at which origin is emptied

  How does τ_0^{BP} behave if $\eta \sim \mu_q$ and $q \downarrow q_c$?

Three universality classes

- Supercritical: $q_c = 0, \quad \tau_0^{\text{BP}}(q) = 1/q^{\Theta(1)}$ w.h.p. as $q \downarrow 0$
- Critical: $q_c = 0, \quad \tau_0^{\text{BP}}(q) = \exp(1/q^{\Theta(1)})$ w.h.p. as $q \downarrow 0$
- Subcritical: $q_c > 0$

Easy-to-use criterion to determine the class of any $\mathcal{U}$
(m simple geometric checks, m= # of rules)

[Bollobás, Smith, Uzzell CPC '15 + Balister, Bollobás, Przykucki, Smith TAMS '16]

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- East and FA-1f are supercritical;
- Duarte and FA-2f are critical;
- North-East is subcritical.

KCM: time scales

τ_0:= first time at which origin is emptied

- How does τ_0 diverge under μ_q when $q \downarrow q_c$?
- How does it compare with τ_0^{BP}?

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An (easy) lower bound:

Let $T^{\text{BP}}(q) := \inf\{t \geq 0 : \ \mu(\tau_0^{\text{BP}} \geq t) \leq 1/2\}$, then

$$\mathbb{E}_{\mu_q}(\tau_0) \geq c\, T^{\text{BP}}(q) \quad \text{for } q \text{ small enough}$$

General, but it does not capture the correct behavior

Supercritical KCM : a refined classification

We identify 2 subclasses: supercritical rooted and unrooted

Easy-to-use criterion to check the subclass of each $\mathcal{U}$

Theorem [Martinelli, Morris, C.T. CMP '19, Marêché, Martinelli, C.T. AoP '20]

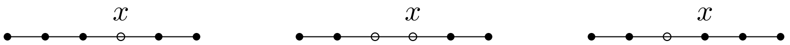
- for all supercritical unrooted models $\mathbb{E}_{\mu_q}(\tau_0) = 1/q^{\Theta(1)}$
- for all supercritical rooted models $\mathbb{E}_{\mu_q}(\tau_0) = 1/q^{\Theta(\log(1/q))}$

$\longrightarrow$ For supercritical rooted $\mathbb{E}_{\mu_q}(\tau_0) \gg T^{\text{BP}} = 1/q^{\Theta(1)}$

- FA-1f is supercritical unrooted
- East model is supercritical rooted

The FA-1f mechanism

Constraint = to be update we need an empty nearest neighbour



- a vacancy can move of one step by creating one additional vacancy $\rightarrow$ $\sim$ r.w. of rate q^{-1};

$\rightarrow$ $d = 1$ $\quad \mathbb{E}_{\mu_q}(\tau_0) \sim q^{-1}(1/q)^2 = q^{-3}$;

$\rightarrow$ $d = 2$ $\quad q^{-2} \leq \mathbb{E}_{\mu_q}(\tau_0) \leq q^{-2}|\log q|$;

$\rightarrow$ $d \geq 3$ $\quad \mathbb{E}_{\mu_q}(\tau_0) \sim q^{-1}(1/q^{1/d})^d = q^{-2}$

[Cancrini, Martinelli, Roberto, C.T. PTRF '08 + Shapira JSP '20]

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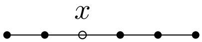
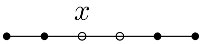
- If we start from a single vacancy 

  and we can create 1 zero we reach only 

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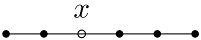
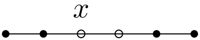
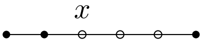
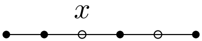
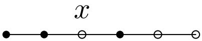
- If we start from a single vacancy 

  and we can create 1 zero we reach only 

- if we can create up to 2 simultaneous additional zeros we reach also:







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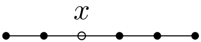
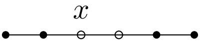
- If we start from a single vacancy 

  and we can create 1 zero we reach only 

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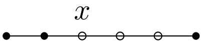

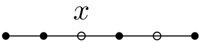

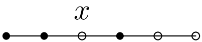

- if we can create up to n simultaneous additional zeros
  - one of the configurations that we can reach has its rightmost vacancy at $x + (2^n - 1)$;
  - all the others have rightmost vacancy in $[x, x + (2^n - 1)]$

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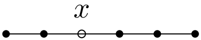

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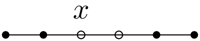

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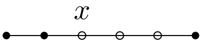

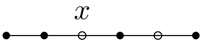

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$\Rightarrow$ the East model has logarithmic energy barriers

The East mechanism in $d = 1$

- The first vacancy at the left of origin is at $\ell \sim 1/q$
- Trivially, $\tau_0^{\rm BP} = \ell$ and $T^{\rm BP} \sim 1/q$
- $\mathbb{E}_{\mu_q}(\tau_0) \sim$ time to create $\log_2(\ell)$ empty sites
- $\to \mathbb{E}_{\mu_q}(\tau_0) = 1/q^{\Theta(1)|\log q|}$ [Aldous, Diaconis JSP '02]

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- $\rightarrow \mathbb{E}_{\mu_q}(\tau_0) = 1/q^{\Theta(1)|\log q|}$ [Aldous, Diaconis JSP '02]
- Sharp result (taking entropy into account) in $d \geq 1$

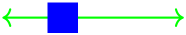
$$\lim_{q \to 0} \frac{\log \mathbb{E}_{\mu_q}(\tau_0)}{|\log q|^2} = (2d \log 2)^{-1}$$

[Cancrini, Martinelli, Roberto, C.T. PTRF '08] for $d = 1$

[Chleboun, Faggionato, Martinelli AoP '16] for $d \geq 2$

Supercritical models

- Unrooted: large empty droplet can move back and forth



→ renormalise to an FA-1f with effective density $q_{\text{eff}} = q^{\Theta(1)}$

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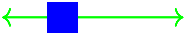

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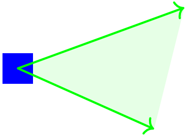
- Rooted: any empty droplet can move only inside a cone



$\Longrightarrow$ logarithmic energy barriers as for East [Marêché SIDMA '20]

$\rightarrow$ renormalise to an East with effective density $q_{\text{eff}} = q^{\Theta(1)}$

$\rightarrow$ $\mathbb{E}_{\mu_q}(\tau_0) \sim q_{\text{eff}}^{\Theta(|\log q_{\text{eff}}|)} = e^{\Theta(\log q)^2}$

Critical models: more on BP results

- an empty droplet cannot expand unless it has external help
- α = difficulty of the update family $\sim$ minimal number of empty sites a droplet should meet to expand
- α is model dependent, $\alpha = 1$ for 2-neighbour and Duarte

$$T^{\text{BP}}(q) = \exp\left(\frac{|\log q|^{O(1)}}{q^{\alpha}}\right)$$

$\sim$ distance from origin to nearest "easily expandable" droplet

$$\text{i.e. empty region of size} \sim \frac{|\log q|^{O(1)}}{q^{\alpha}}$$

[Bollobás, Duminil-Copin, Morris, Smith, '16]

Critical KCM: a refined classification

We identify 2 subclasses: finitely critical and infinitely critical

Theorem [Martinelli, Morris, C.T. CMP '19 + Hartarsky, Marêché, C.T. PTRF '20, Hartarsky, Martinelli, C.T. AoP '21+]

For critical KCM it holds

$$\mathbb{E}_{\mu_q}(\tau_0) = \exp\left(\frac{|\log q|^{O(1)}}{q^{\nu}}\right)$$

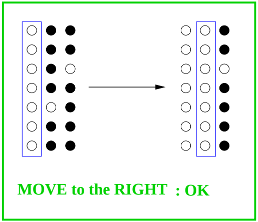
- $\nu = \alpha$ for finitely critical models;
- $\nu = 2\alpha$ for infinitely critical models

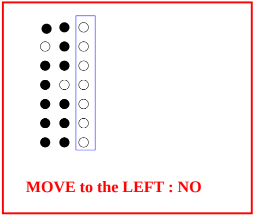
Easy geometric criterion to distinguish the two subclasses:

- FA-2f model is finitely critical $\rightarrow \nu = \alpha = 1$
- Duarte model is infinitely critical $\rightarrow \nu = 2\alpha = 2$

Duarte model

Constraint at x: at least 2 vacancies in $\{x - \vec{e}_1, x + \vec{e}_2, x - \vec{e}_2\}$





An empty segment of length $\ell = 1/q\,|\log q|$ can (typically) create an empty segment to its right, but never to its left!

$\rightarrow$ it is a mobile droplet with East-like dynamics and

density $q_{\text{eff}} = q^{\ell} = e^{-\Theta(\log q)^2/q}$

Duarte model: heuristics

- nearest empty droplet to the origin is at distance $L \sim q_{\text{eff}}^{-1}$

$\to$ $T^{\text{BP}} \sim L = \exp\left(\frac{\Theta(1)|\log q|^2}{q}\right)$

[Mountford SPA '95]

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$\rightarrow$ $T^{\text{BP}} \sim L = \exp\left(\frac{\Theta(1)|\log q|^2}{q}\right)$
[Mountford SPA '95]

- Duarte droplets move East like $\rightarrow$ to empty the origin we have to create $\log(L)$ simultaneous droplets

$\rightarrow$ $\mathbb{E}_{\mu_q}(\tau_0) \sim q_{\text{eff}}^{-\log L} \sim \exp\left(\frac{\Theta(1)|\log q|^4}{q^2}\right) \gg T^{\text{BP}}$

[Martinelli, Morris, C.T. CMP '19 + Marêché, Martinelli, C.T. AoP '20]

Upper bound: main obstacles and tools

- droplets move only on a good environment
- the environment evolves and can ”lose its goodness”
- no monotonicity $\rightarrow$ we cannot ”freeze” the environment
- the motion of droplets is not random walk like
- it is very difficult to use canonical path arguments

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→ a very flexible long range Poincaré inequality
[Martinelli, C.T. AoP ’19]

→ renormalisation

→ Matryoshka Dolls: a new technique to compare Dirichlet forms avoiding canonical paths
[Martinelli, Morris, C.T. CMP ’19]

Lower bound: how do we exclude a smarter mechanism?

Constructing a bottleneck involving $\log(L)$ droplets

Key difficulty: droplets cannot be "rigid objects"

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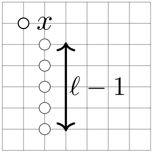
Suppose we say ” droplet = empty column of height $\geq \ell$ ”

- in this config. there are no droplets (only sites with a circle are empty);
- x has Duarte constraint satisfied;
- if we flip site x we create a droplet;



- so we have created a droplet from nowhere . . . it is not an East dynamics, and does not have log barriers!!

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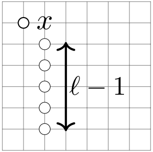

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Solution: a subtle algorithmic identification of droplets [Marêché, Martinelli, C.T. '18]

The general critical case

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$$\rightarrow \tau_0 \sim q_{\text{eff}}^{\Theta(|\log q_{\text{eff}}|)} = \exp\left(\frac{|\log q|^{O(1)}}{q^{2\alpha}}\right)$$

- For finitely critical KCM the droplet motion is a subtle combination of East on mesoscopic scales $\left(L \sim q^{-\Theta(1)}\right)$ and FA-1f on macroscopic scales $(\sim q_{\text{eff}}^{-1})$

$$\rightarrow \tau_0 \sim q_{eff}^{\Theta(\log L)} = \exp\left(\frac{|\log q|^{O(1)}}{q^{\alpha}}\right)$$

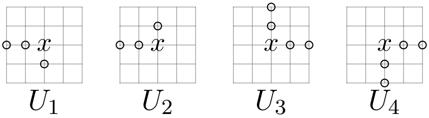
Summary

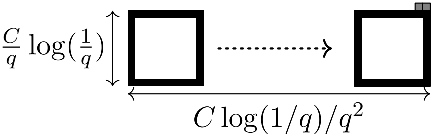
- KCM are the stochastic counterpart of BP
- time scales for KCM and BP can diverge very differently
  - τ_0^{BP} = length of the optimal path to empty origin
  - τ_0^{KCM} = time to overcome energy barriers of optimal path
- we establish the universality picture for KCM in $d = 2$
- the results are novel also for the physicists: KCM time scales are very difficult to guess from numerical simulations!

Thanks for your e-attention !

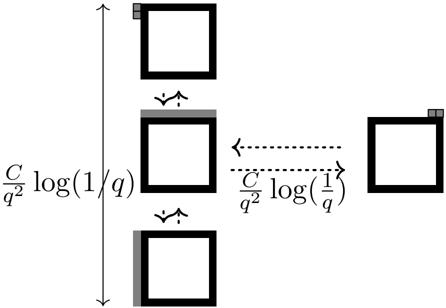
Addenda

Finitely critical $\mathcal{U}$: an example





To move of one step towards $\vec{e}_2$ the droplet has to move East-like to the right till reaching the first infected pair of empty sites

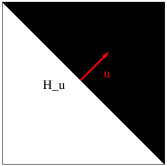


The move of one step in the $-\vec{e}_1$ direction the droplet has to move in the direction $\vec{e}_2$ until reaching the first infected pair of empty sites. A subtle hierarchical combination of East paths. . .

How can you identify the universality class of $\mathcal{U}$?

We need the notion of stable and unstable directions

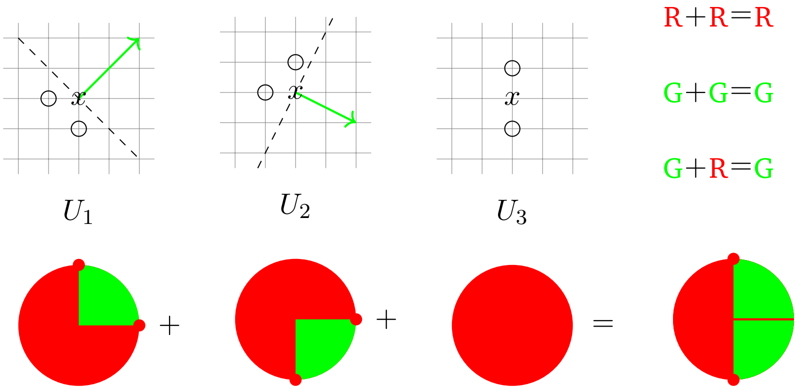
- Fix a direction $\vec{u}$
- Start from a configuration which is
  - completely empty on the half plane perpendicular to $\vec{u}$ in the negative direction (H_u)
  - filled otherwise
- Run the bootstrap dynamics



$$\vec{u} \text{ is } \begin{cases} \text{stable} & \text{if no other site can be emptied} \\ \text{unstable} & \text{otherwise} \end{cases}$$

How to easily identify all stable and unstable directions

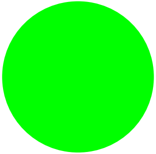
Draw the half planes H_u and $\mathbb{Z}^2 \setminus H_u$ so that the separation line contains the origin. $\vec{u}$ is unstable iff $U_i \subset H_u$ for at least one i



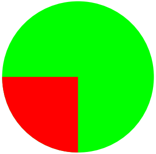
$\mathcal{U}$ is supercritical iff there exists an open semicircle $\mathcal{C}$ which does not contain stable directions.

A supercritical model is

- rooted if it has at least 2 non opposite stable directions
- unrooted otherwise



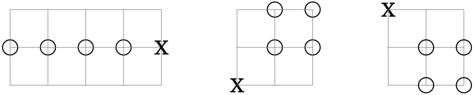
FA-1f
Unrooted



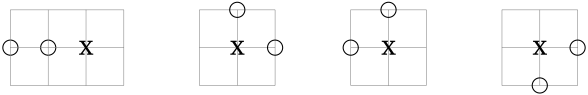
East
Rooted

Guess who is rooted...?

Model A



Model B



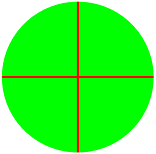
Lesson: rooted models are not necessarily oriented ($\neq$ East)!

Critical universality class

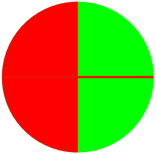
$\mathcal{U}$ is critical if it is not supercritical and there exists an open semicircle $\mathcal{C}$ with only a finite number of stable directions

A critical model is

- finitely critical if it has a finite number of stable directions
- infinitely critical otherwise



FA-2f
Finitely critical



Duarte
Infinitely critical

Subcritical universality class

Two equivalent definitions

$\mathcal{U}$ is subcritical iff it is neather supercritical nor critical

or

$\mathcal{U}$ is subcritical iff each open semicircle has infinite stable directions

$\Rightarrow \quad q_c > 0$: blocked clusters percolate at $q < q_c$

Example: North East model