Jamming percolation and glass transition in lattice models

C.Toninelli, IHES

G.Biroli, D.S.Fisher

Outline

- Physical motivations:
  phenomenology of liquid/glass transition;
  what is an ideal glass transition?

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  phenomenology of liquid/glass transition;
  what is an ideal glass transition?

- A new class of kinetically constrained models:
  existence of an ideal glass transition;
  ergodicity breaking transition;
  identification of ρ_c;
  first order/critical character of transition;
  a new percolation transition.

Liquid-Glass transition

- Liquid at $T > T_m \rightarrow$ fast cooling $\rightarrow$ avoided crystallization $\rightarrow$ supercooled liquid: dramatic slowing down without significant structural changes.

  Glass "transition" temperature: $\tau(T_g) = 10^3 s$

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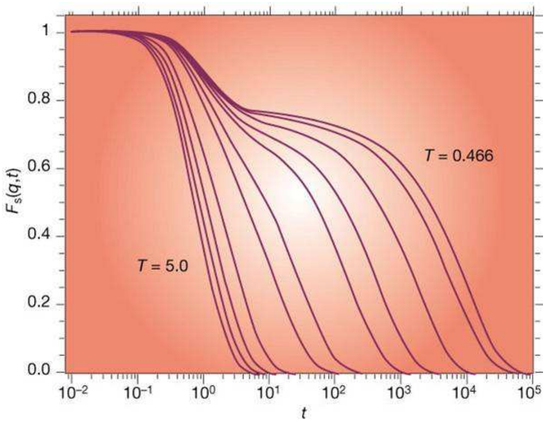
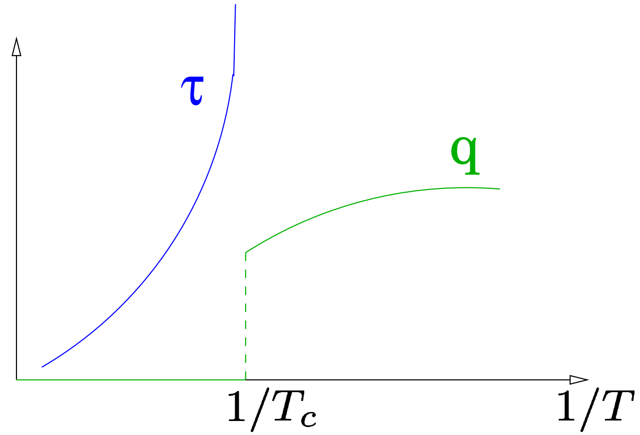
- • Is there a divergence of $\tau(T)$ at finite $T < T_g$?
  • Is there an equilibrium glass transition?
  • Which are the mechanisms causing the slowing down of dynamics and its heterogeneous character?
  • Which are the typical length/time scales?

Which kind of dynamical transition?

Mixed first order/critical properties





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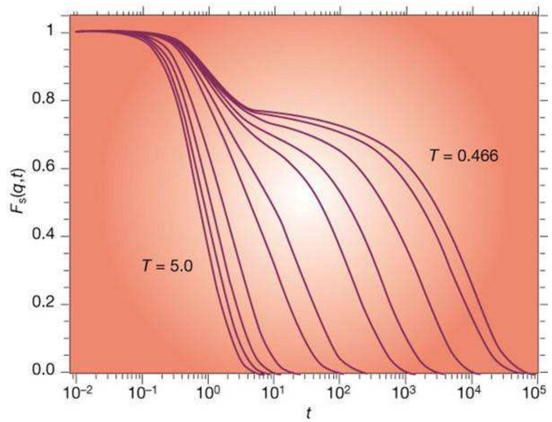

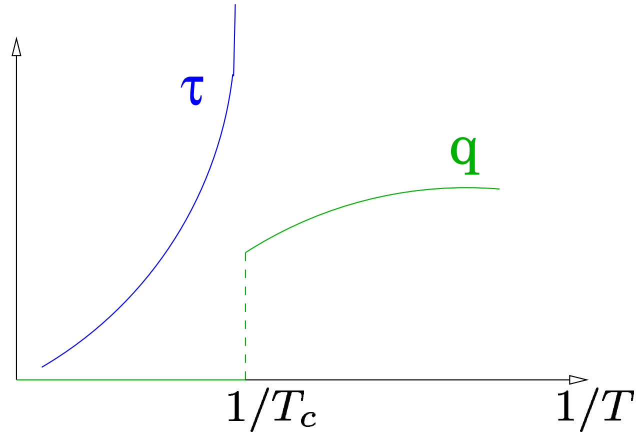

- Discontinuous order parameter:
  $q(T) = \lim_{t\to\infty} F(k,t) = \lim_{t\to\infty} F.T. < \rho(t,x)\rho(0,x) >_c$

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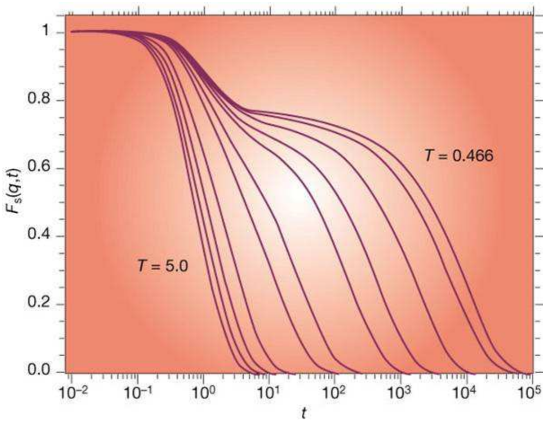

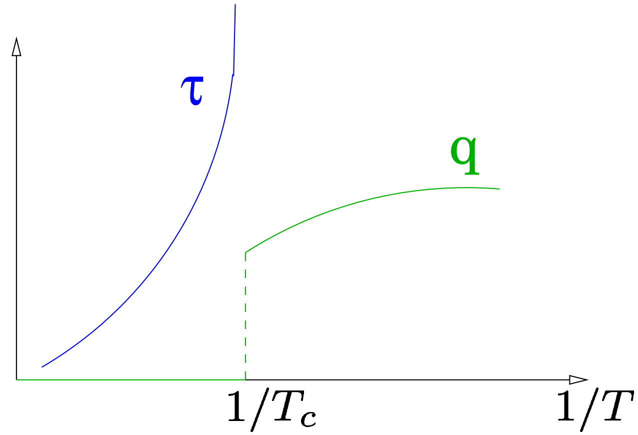

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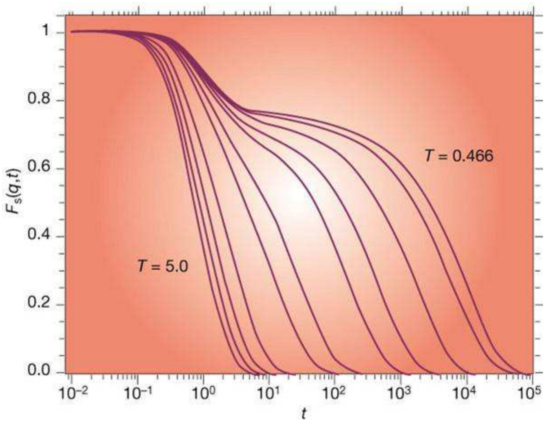

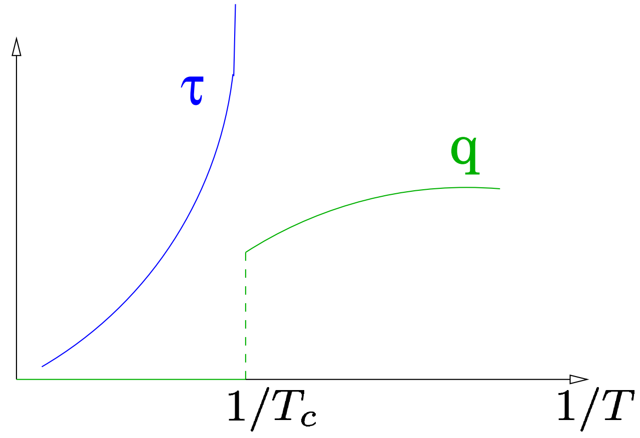

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- Superharrenius divergence: $\tau(T) \simeq \exp \frac{c}{T-T_c}$

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- Systems of particles with discrete positions on a lattice and hard core constraint;

- Stochastic conservative or non–conservative dynamics: sequence of jumps or birth/death of the particles;

- Additional constraints (besides hard core) to mimic cage effect $\rightarrow$ blocked configurations, slow dynamics, dynamical arrest, glassy phenomenology,. . . .

Kinetically constrained models II

Ex. Kob-Andersen '92:
Constraint: move allowed if jumping particle has ≤ 4 occupied n.n. both before and after moving.
Simulations: slow, glassy dynamics at high density
Conjecture: ergodicity breaking transition at $\rho_c < 1$

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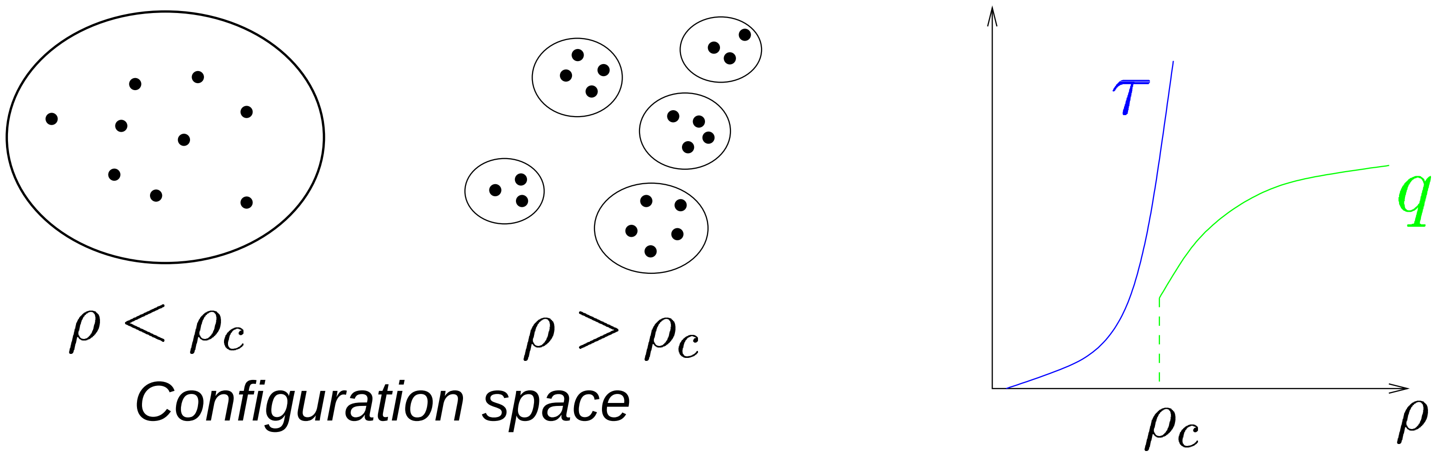

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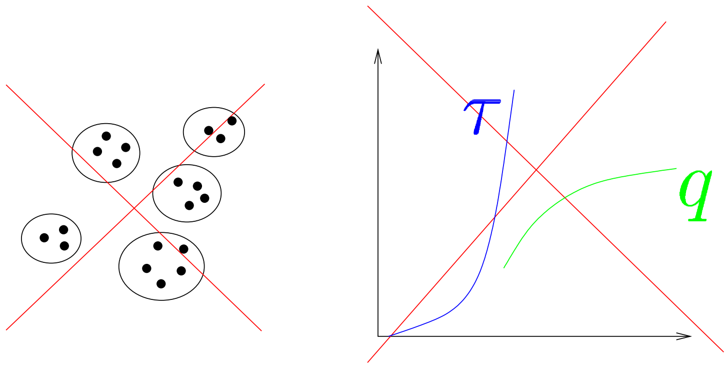
Rigorous results (G.Biroli, D.S.Fisher, C.T.)

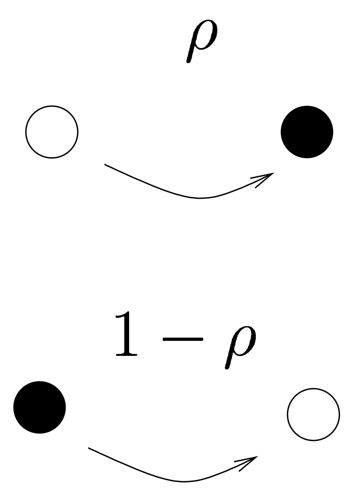


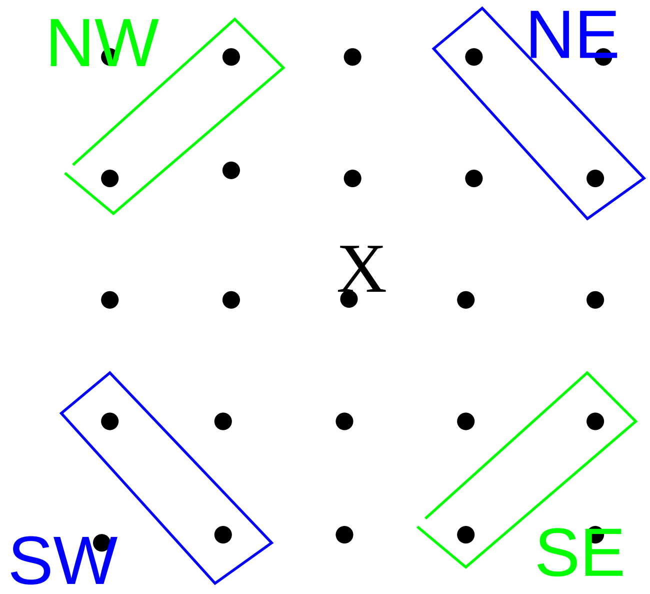
Large finite size effects $L_c(\rho) \propto \exp \exp \frac{c}{1-\rho}$
Relaxation: rearrangement of regions with diverging size and distance for $\rho \to 1$ $\quad \tau \propto L_c(\rho)^2$

A new class of models

Configurations:
particles on a square lattice with hard core constraint

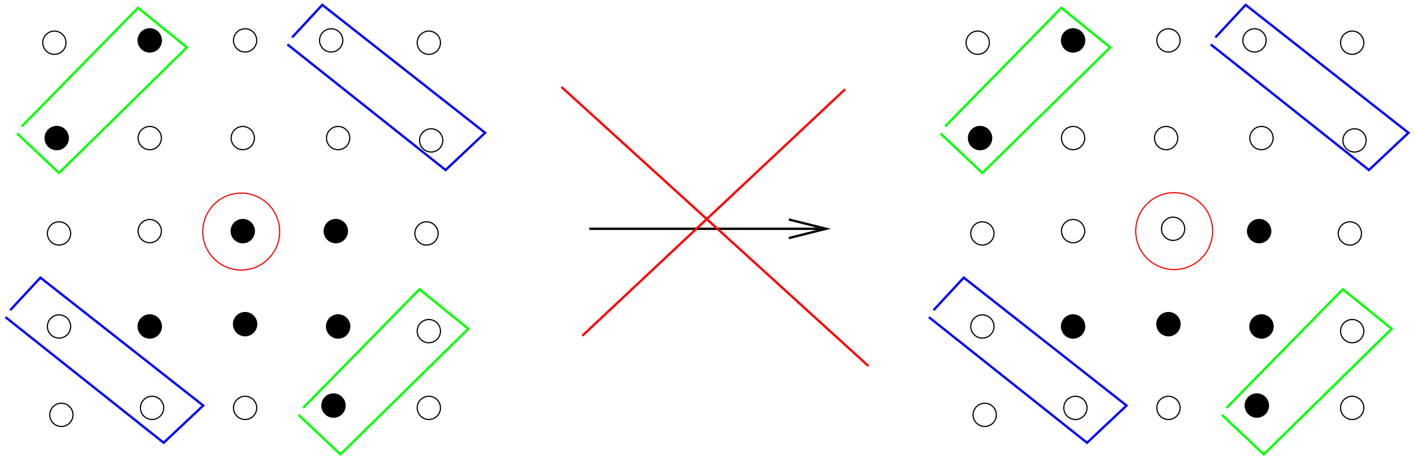
Dynamic: birth/death





(NE OR SW empty) AND (NW OR SE empty)

Rules



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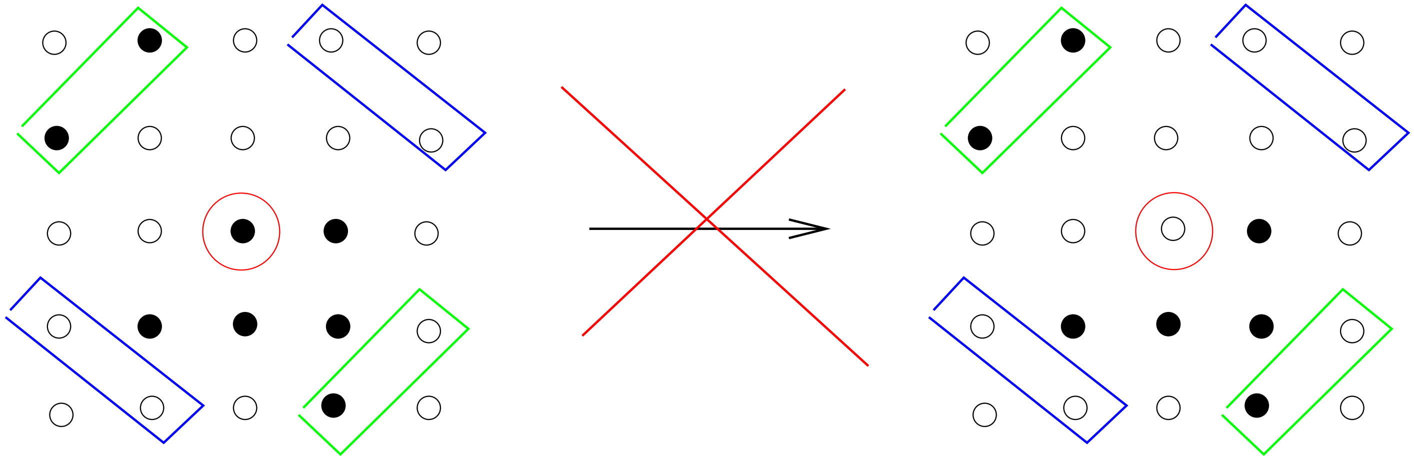

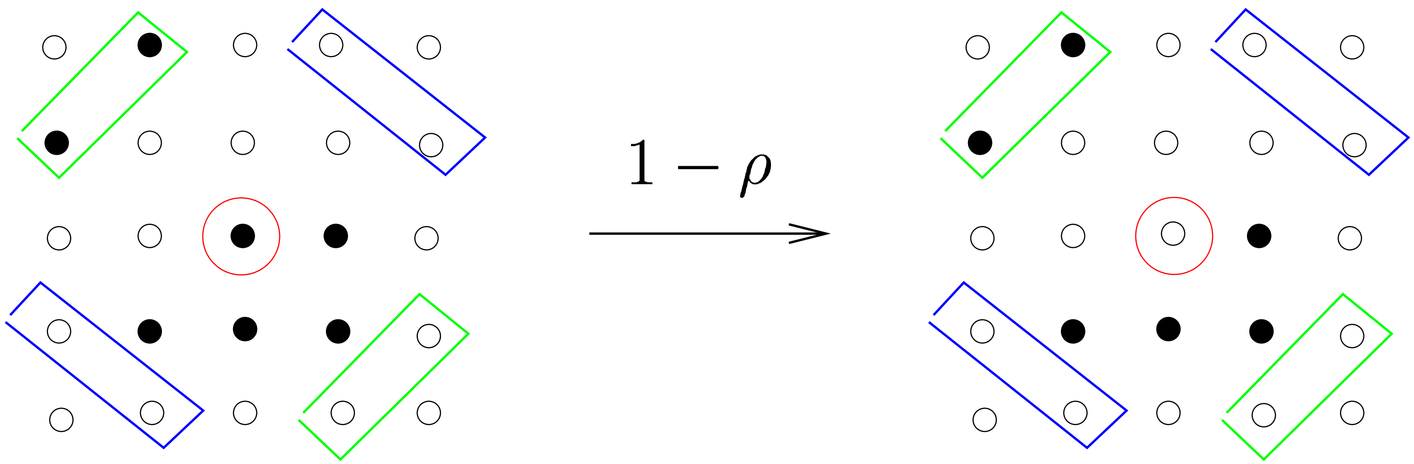

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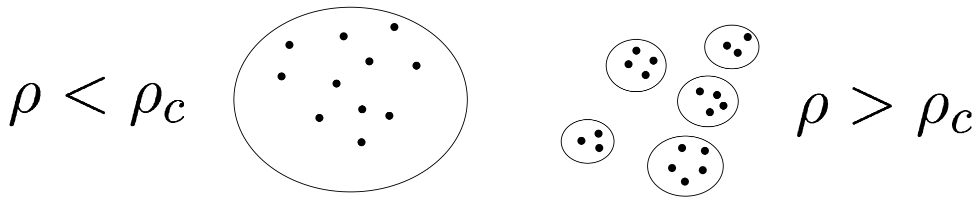

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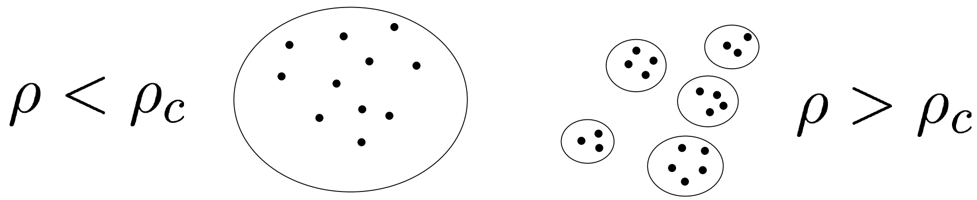

Configuration space

- Identification of ρ_c
  $=$ critical density of directed percolation in $d = 2$

Results II

- Critical properties $\rho \nearrow \rho_c$
  $L_c \simeq \exp(c\, \xi_{\|}^{1-z})$,
  $\xi_{\|} =$ correlation length of DP
  $\xi_{\|} \simeq 1/(\rho_c - \rho)^{\nu}$, $\nu \simeq 1.7$, $z \simeq 0.63$ anisotropy DP

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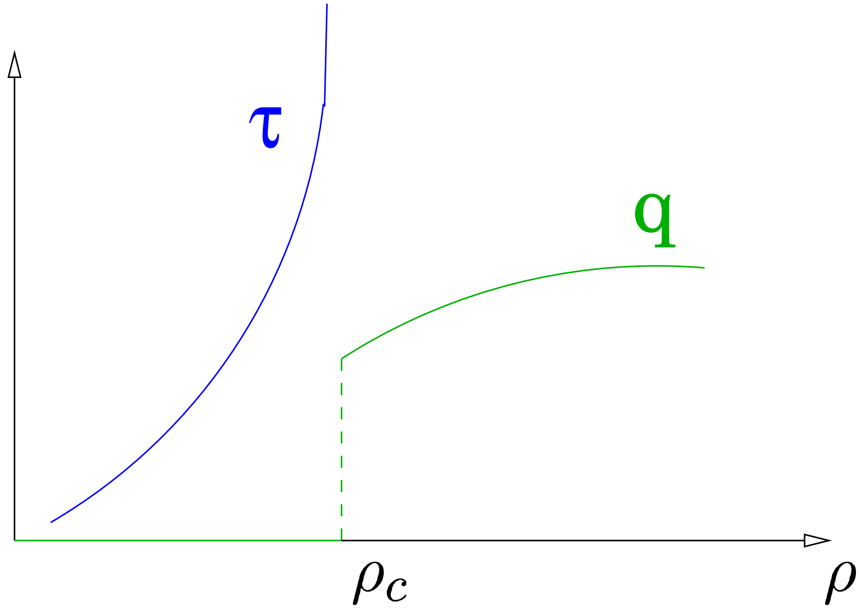
C.Toninelli, G.Biroli, D.S. Fisher *Phys. Rev. Lett* in press (cond-mat 0509661)

C.Toninelli, G.Biroli (cond-mat 0512335)

Results III



$\rightarrow$ Finite dimensional model with ideal glass transition

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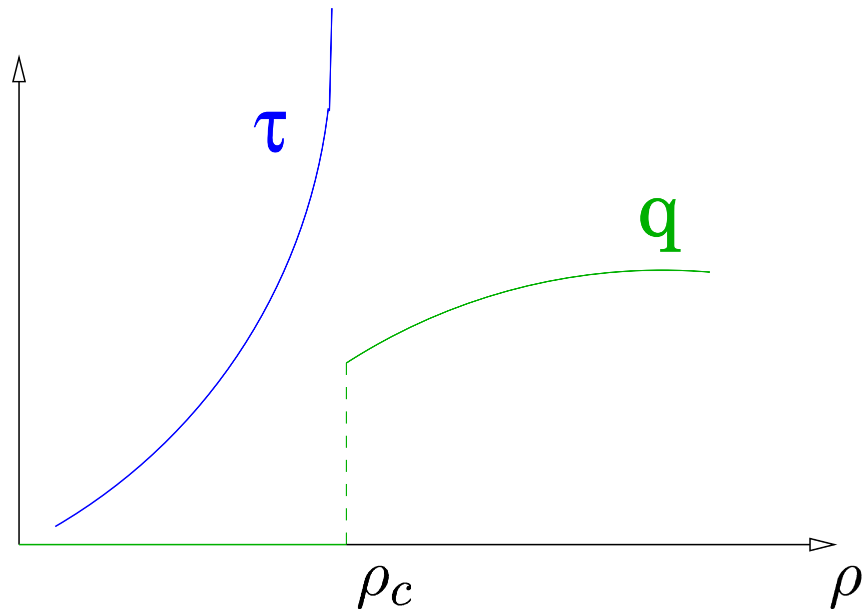
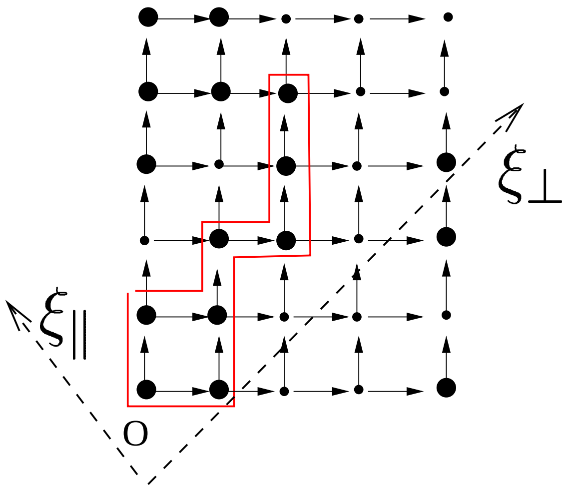
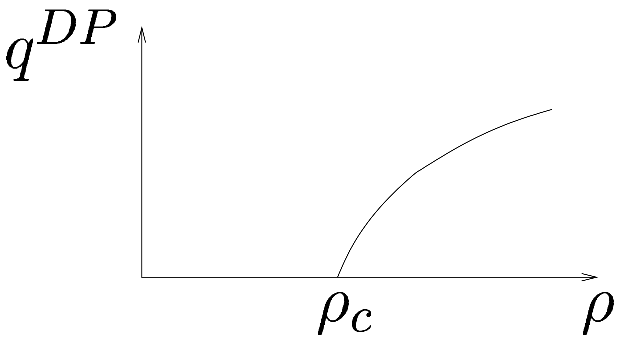


$\rightarrow$ Finite dimensional model with ideal glass transition

$\rightarrow$ A new percolation transition:
discontinuous + anomalous critical properties
Jamming percolation

Directed Percolation





q^{DP}= density of infinite clusters following arrows

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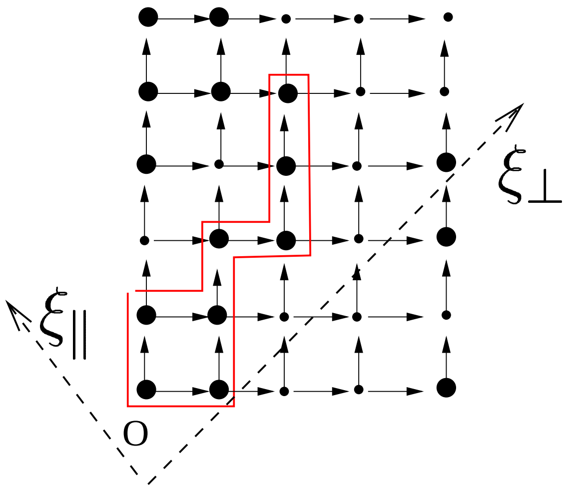

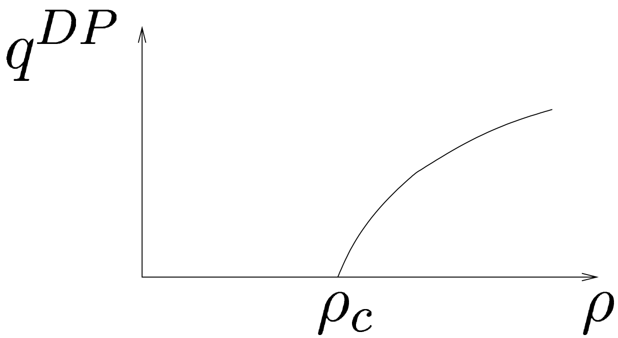

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Continuous transition à $\rho_c \simeq 0.7$

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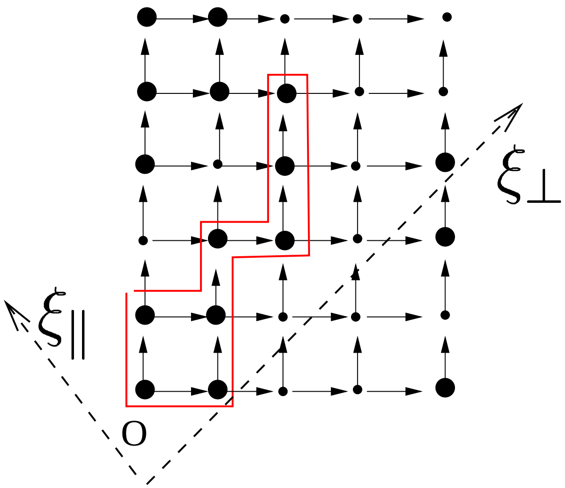

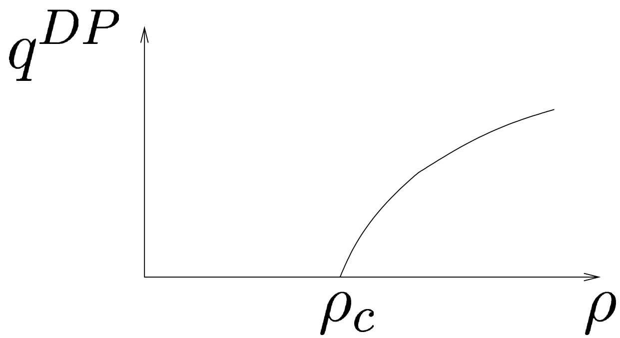

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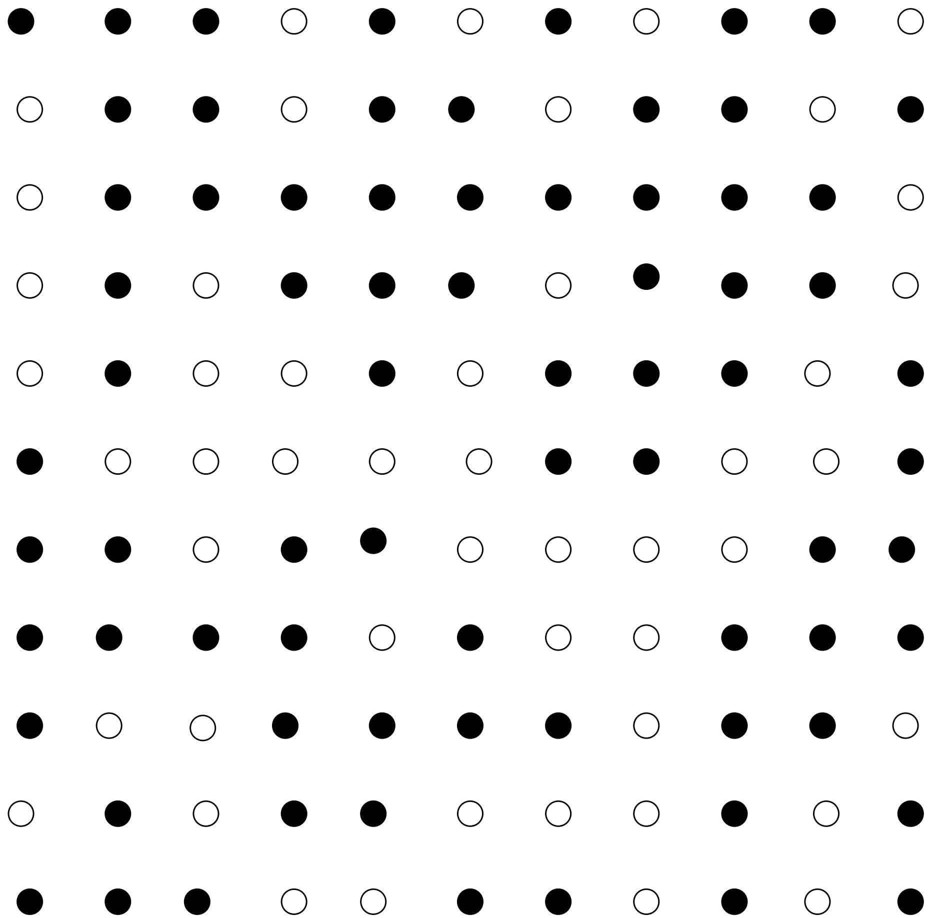
Continuous transition à $\rho_c \simeq 0.7$

Asymmetry: two diverging lengths

$\xi_{||} \simeq (\rho - \rho_c)^{\nu_{||}} \qquad \xi_\perp \simeq (\rho - \rho_c)^{\nu_\perp}$,

$\nu_{||} \simeq 1.73 \qquad \nu_\perp \simeq 1.09$

Ergodicity breaking $\rho > \rho_c$



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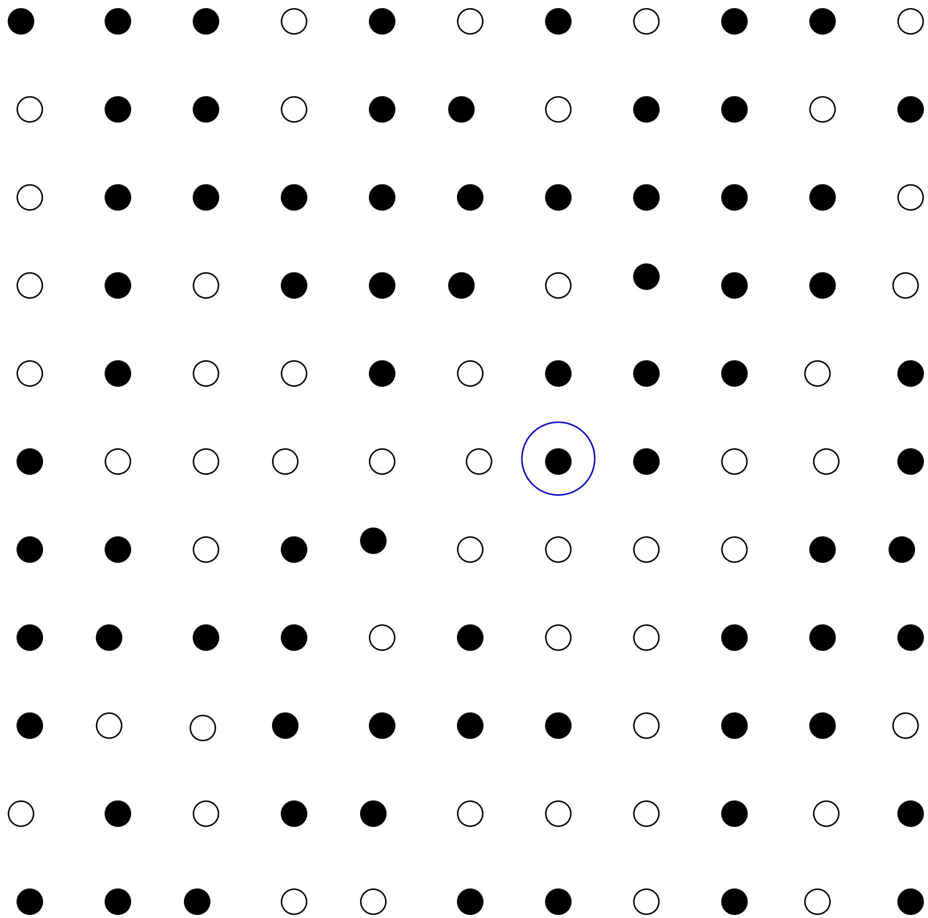

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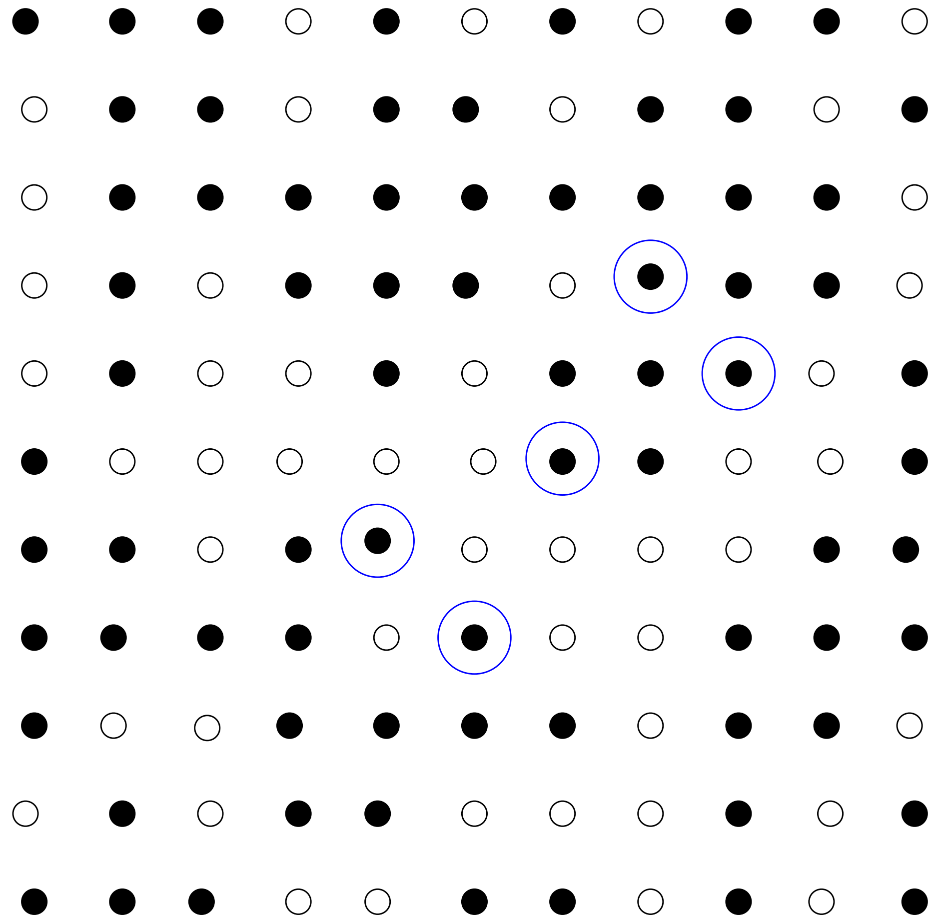

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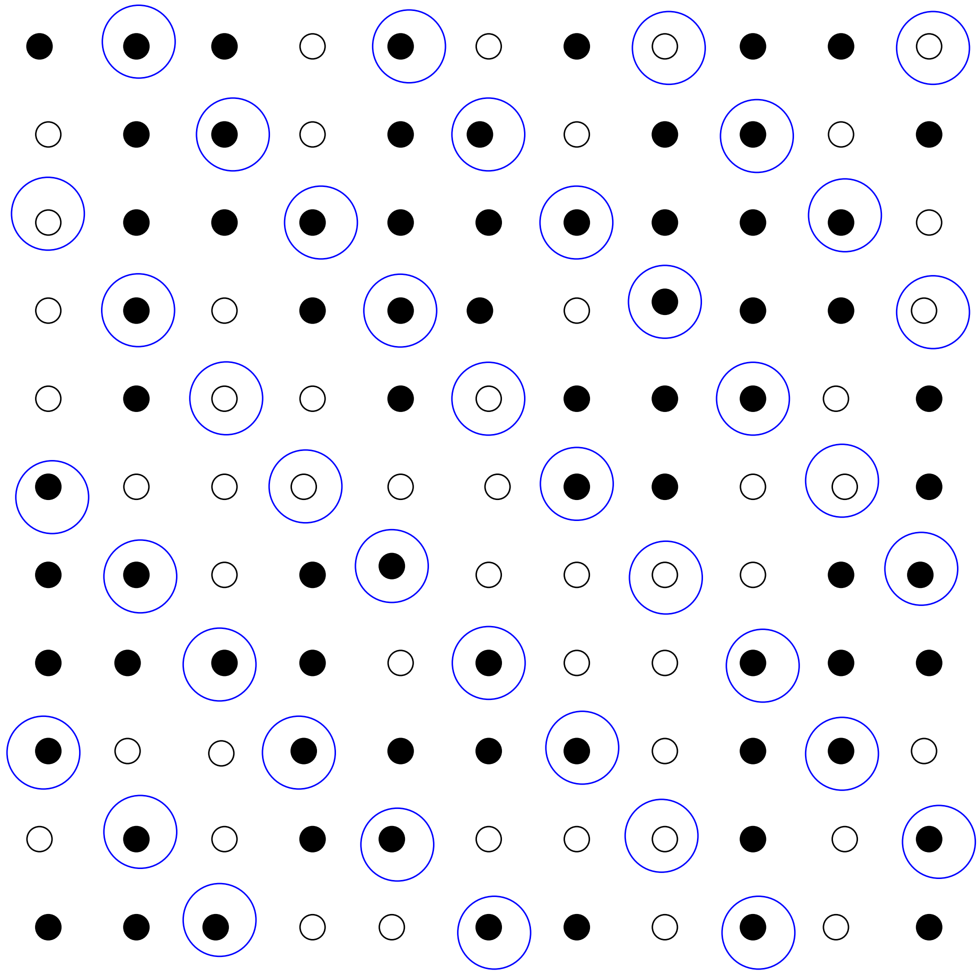

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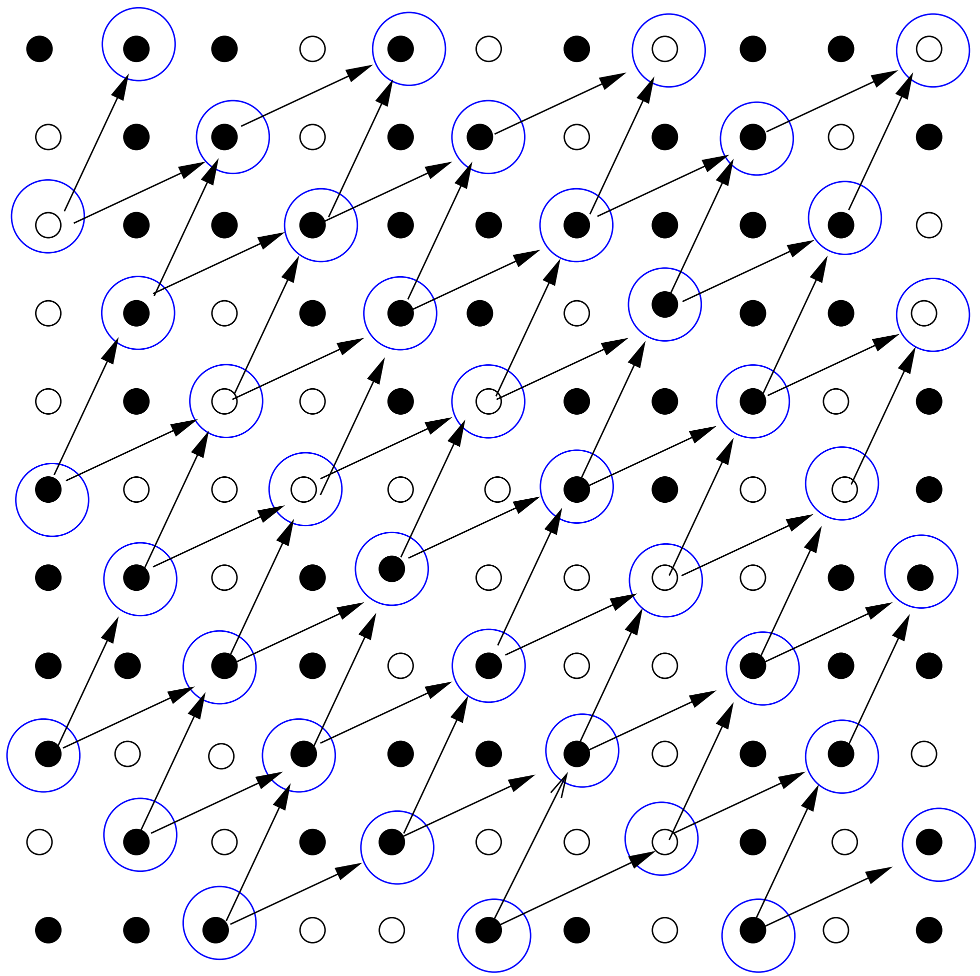

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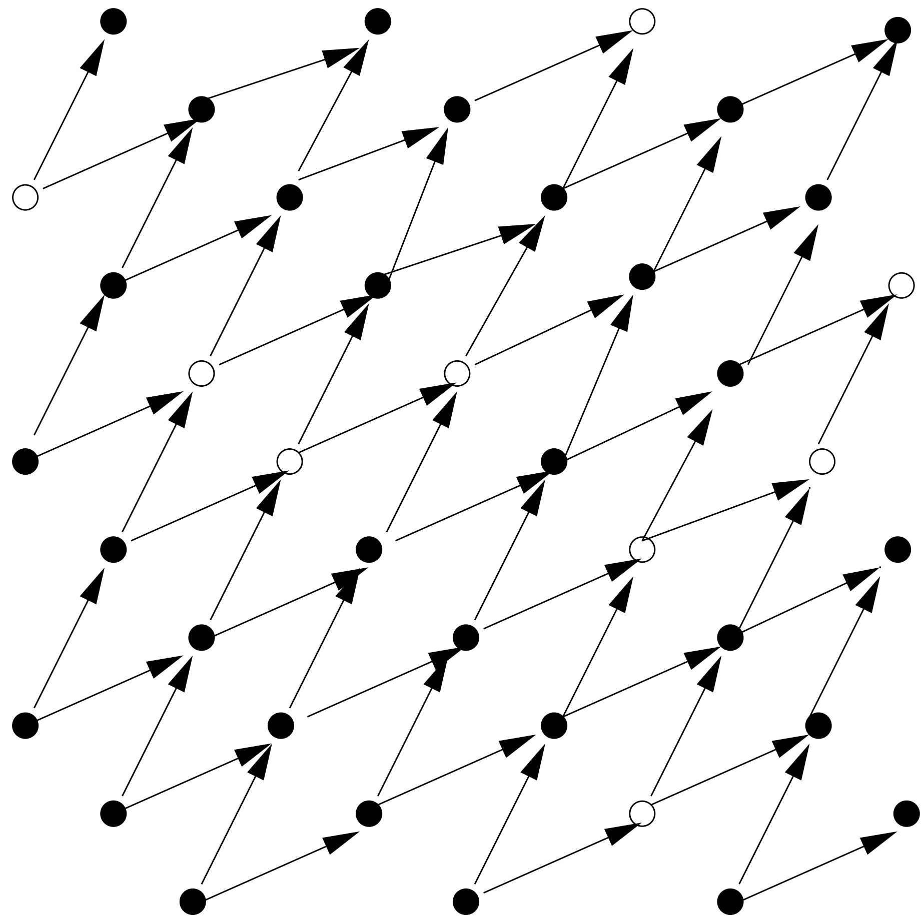

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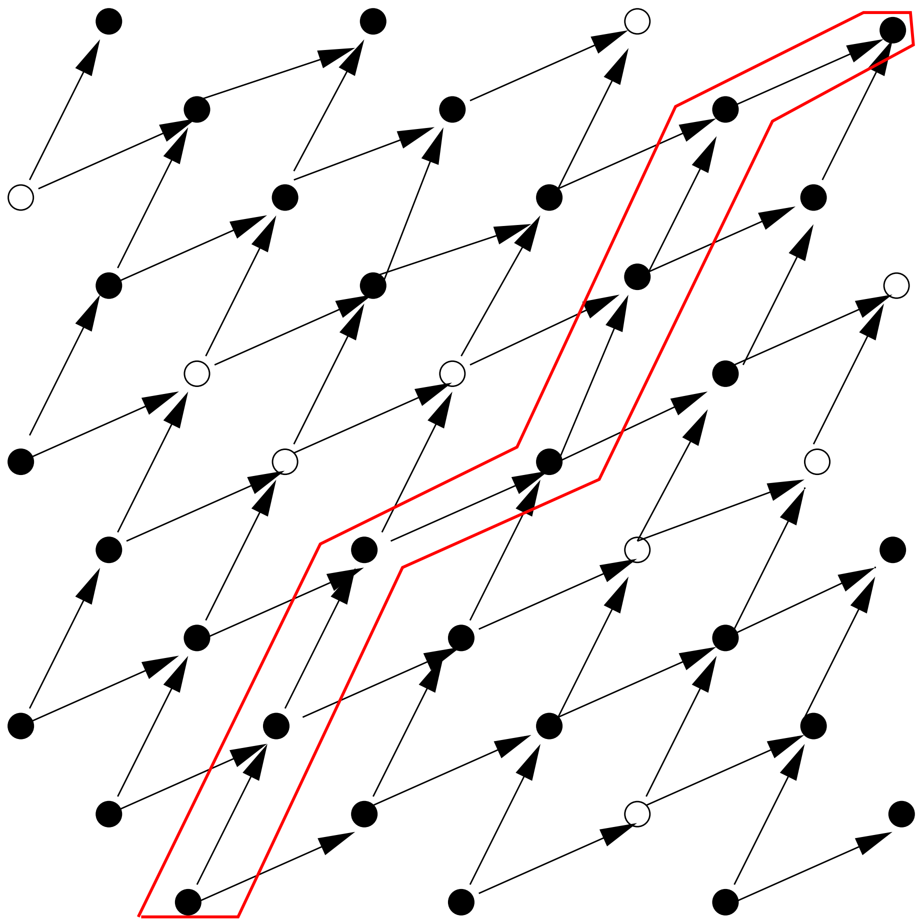

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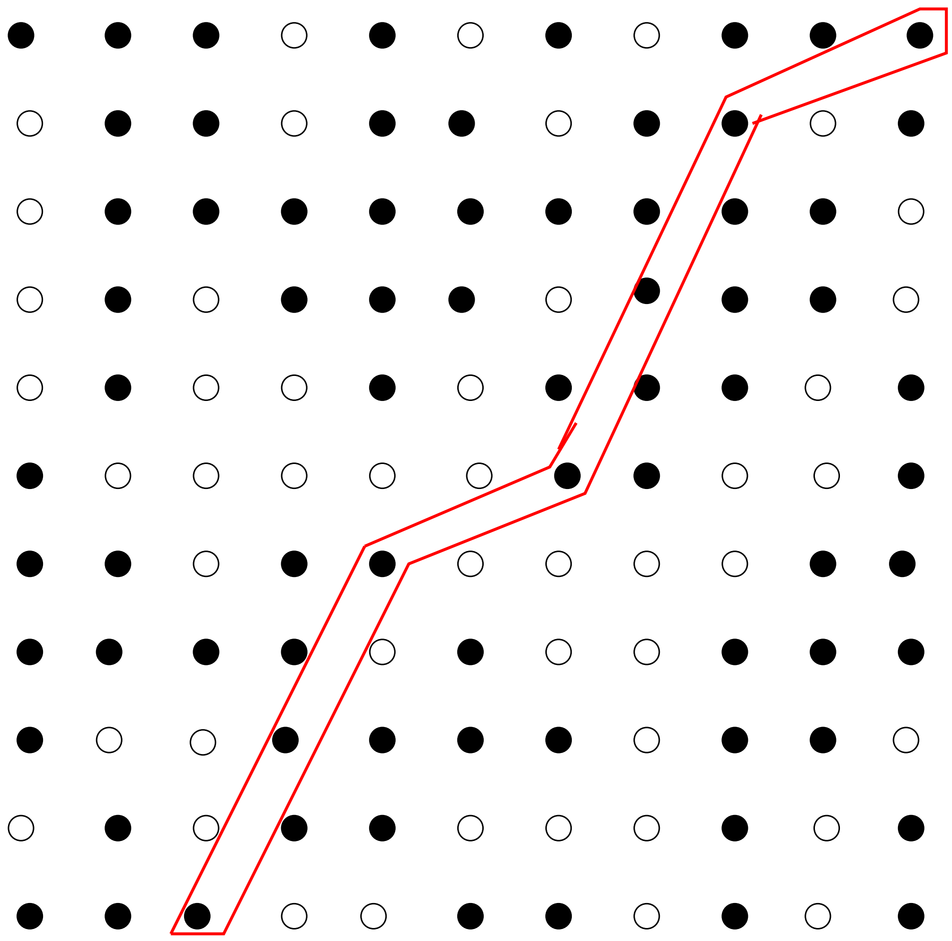

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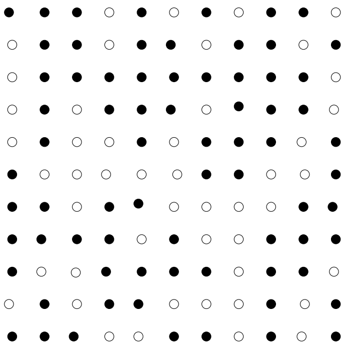

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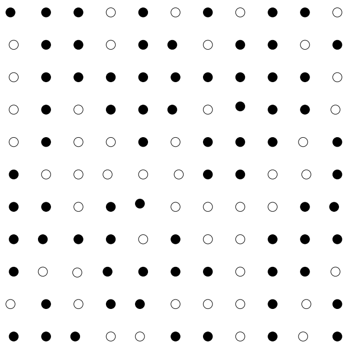

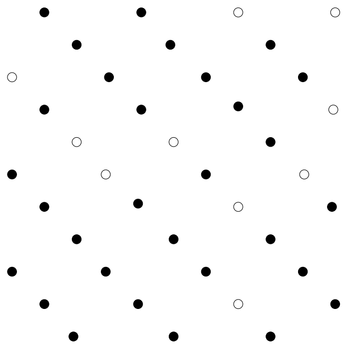

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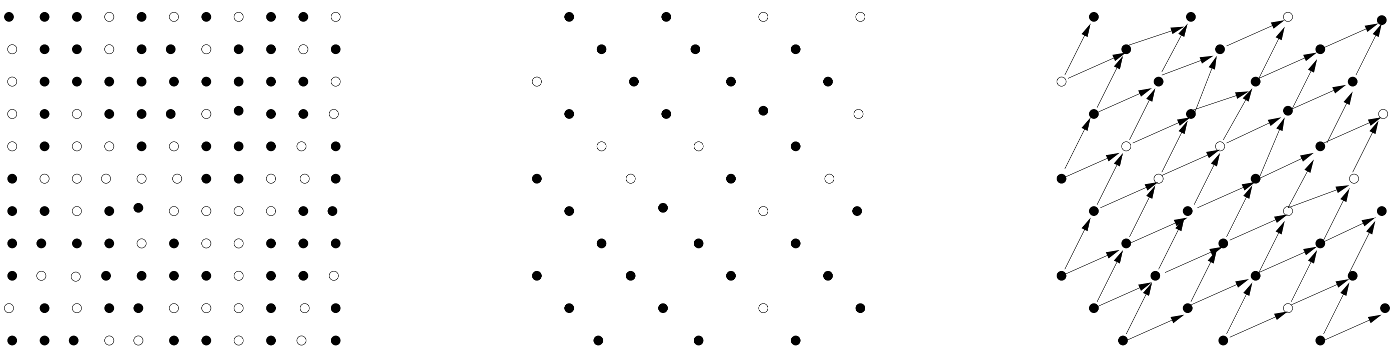

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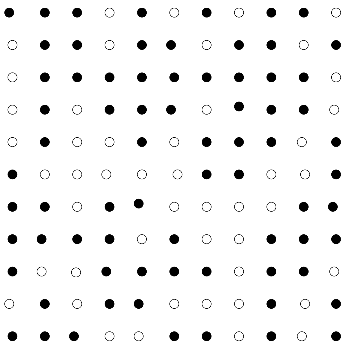

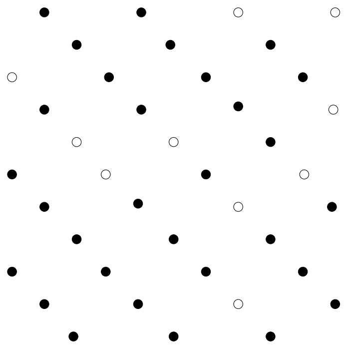

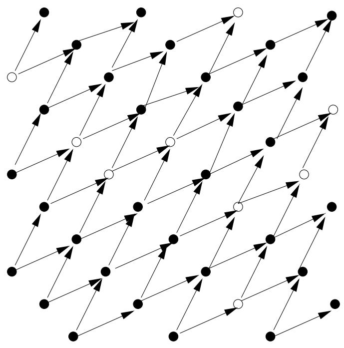

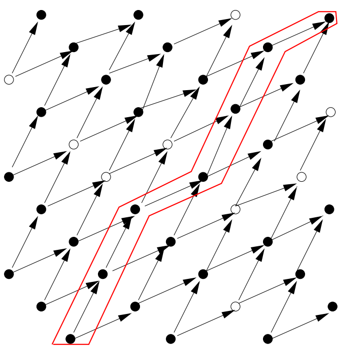

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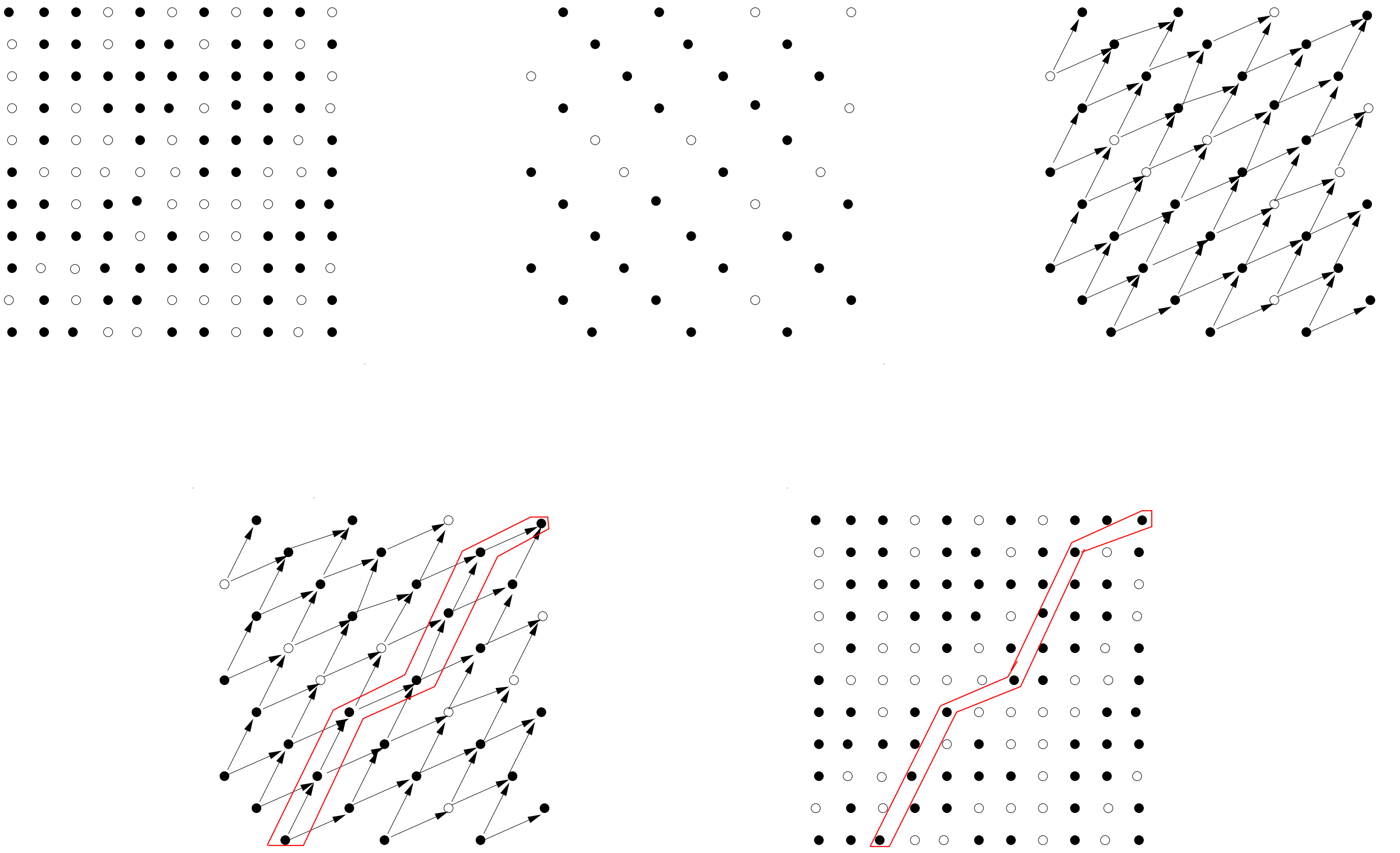

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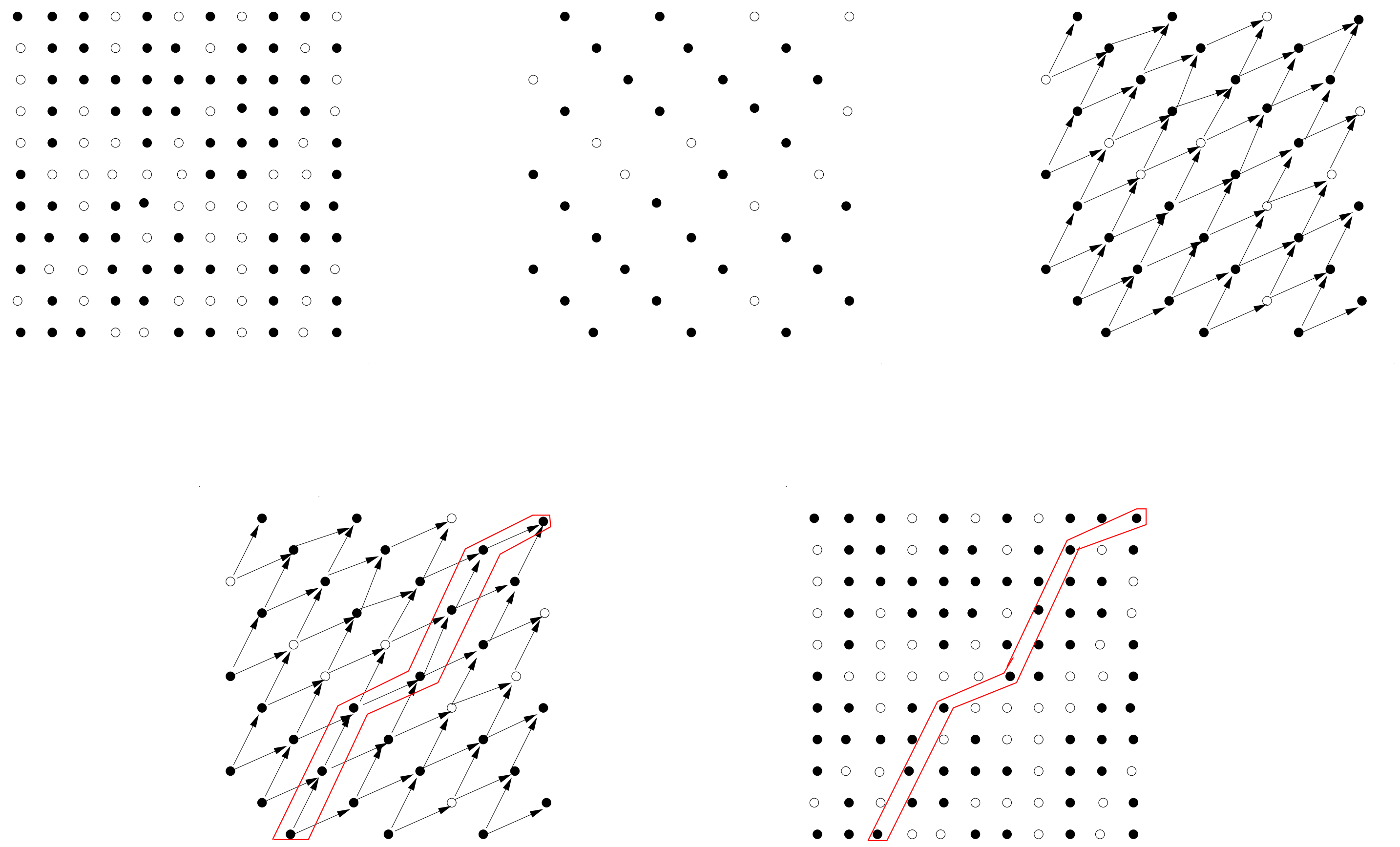

Percolation of blocked clusters $\rightarrow$ ergodicity breaking

T-Junctions

DP spanning clusters $\rightarrow$ blocked

Blocked cluster $\not\rightarrow$ DP spanning cluster

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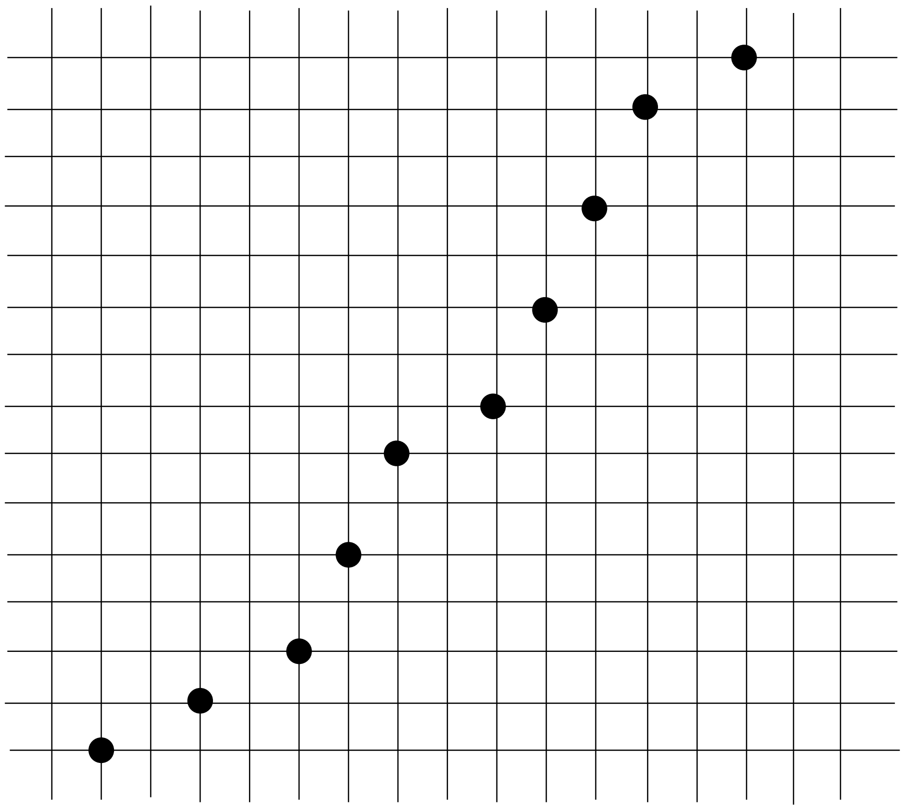

Percolating NE-SW cluster $\rightarrow$ blocked

T-Junctions

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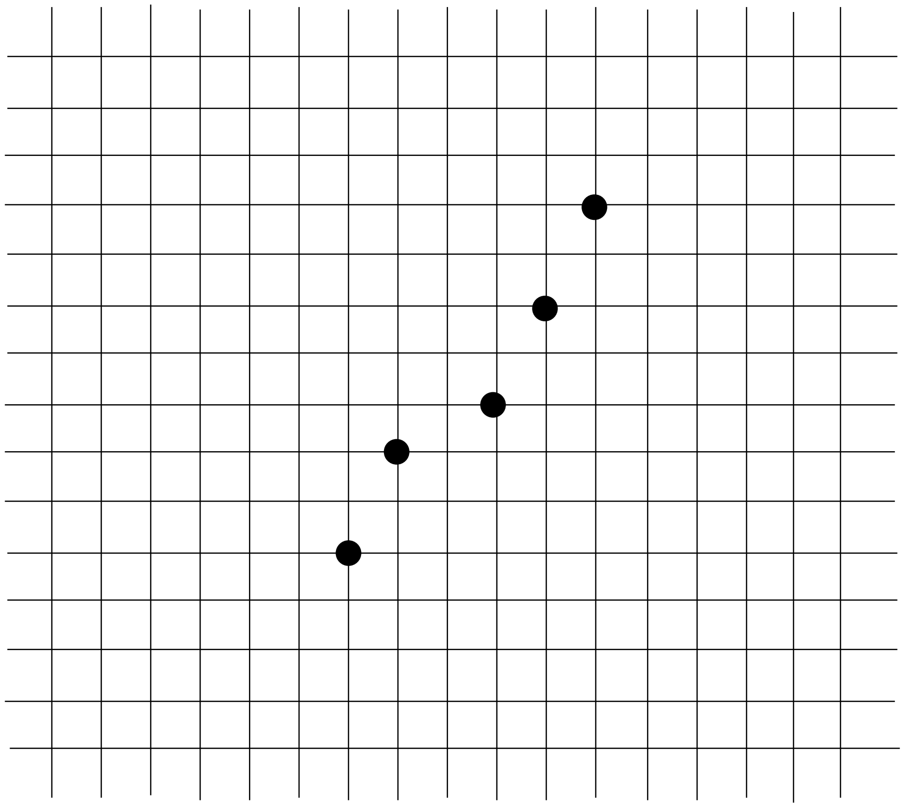
Blocked cluster $\not\rightarrow$ DP spanning cluster



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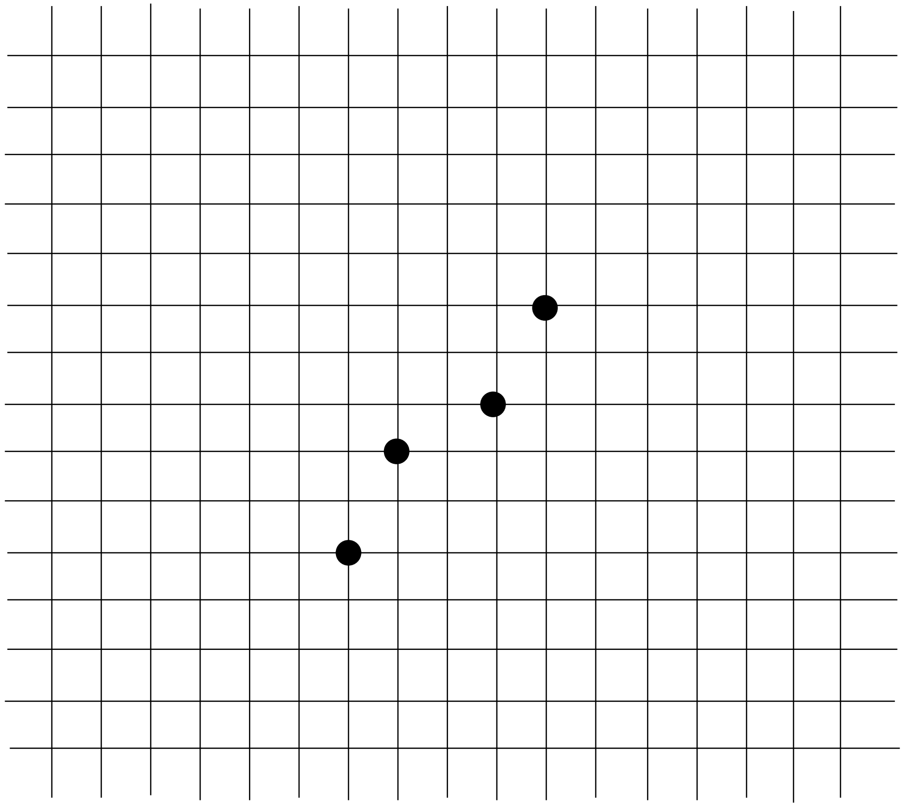

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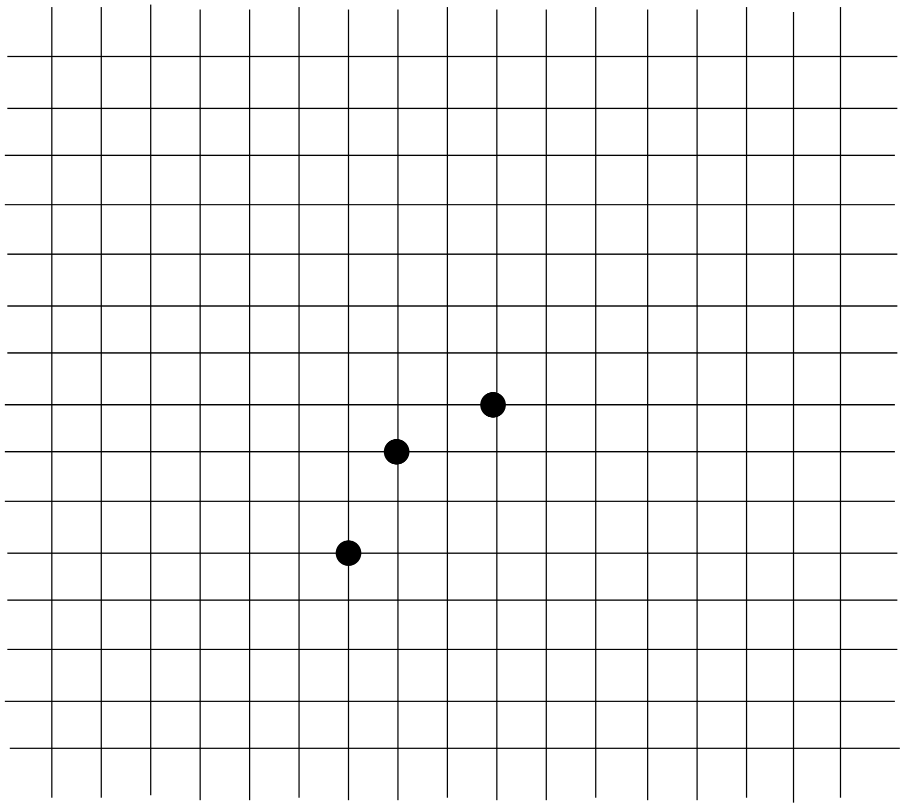

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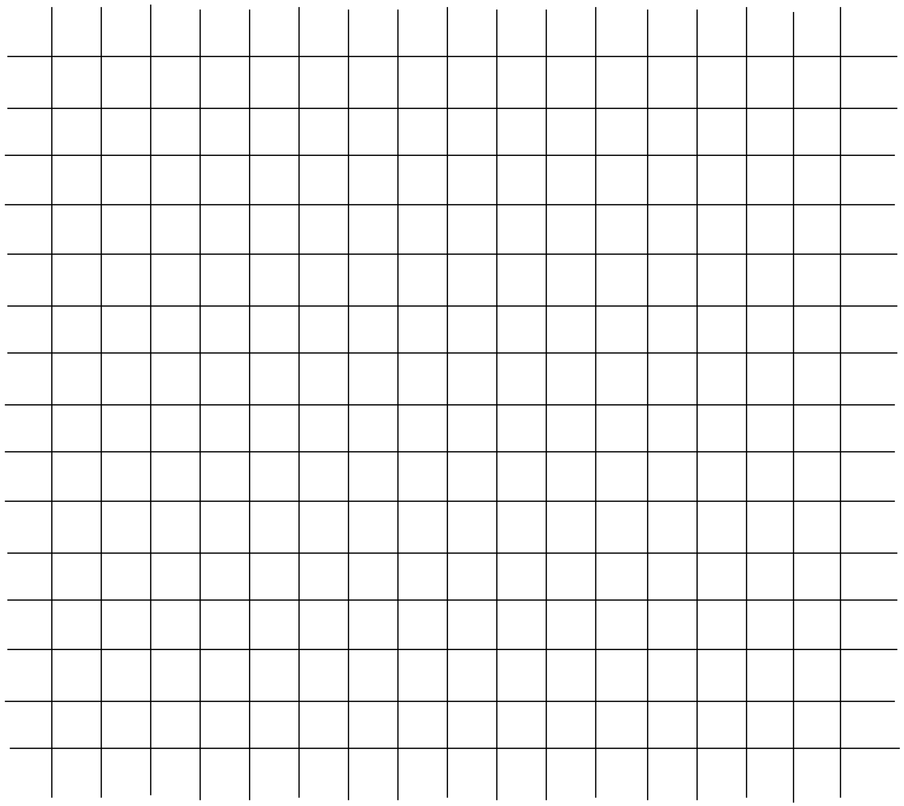
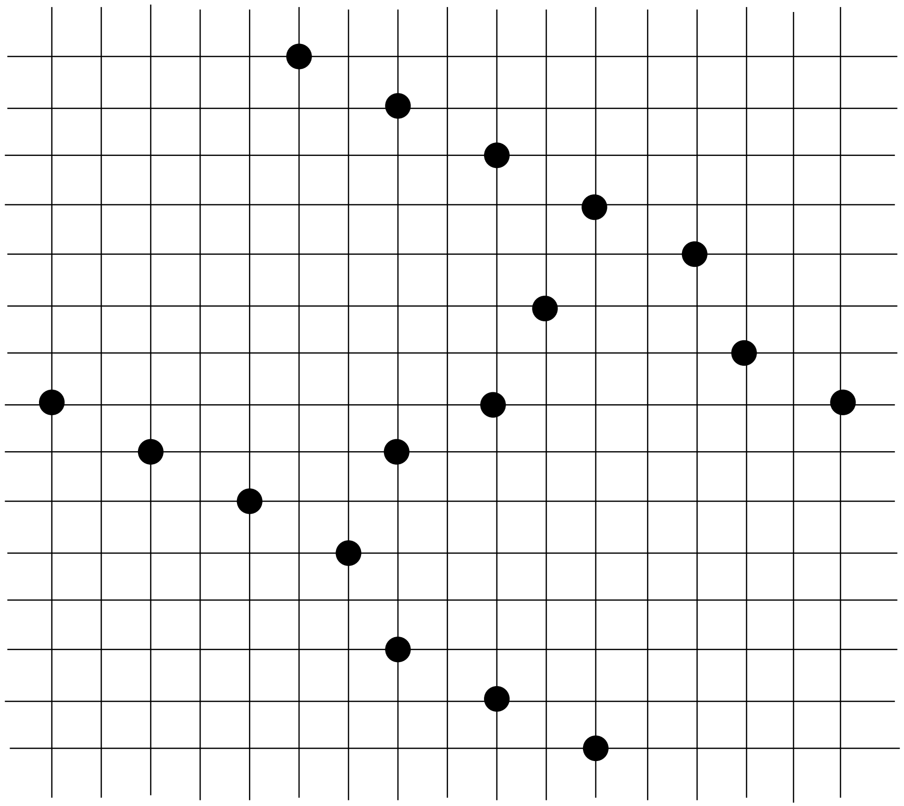


Non percolating NE-SW cluster $\rightarrow$ non blocked

T-Junctions

DP spanning clusters $\longrightarrow$ blocked

Blocked cluster $\not\longrightarrow$ DP spanning cluster

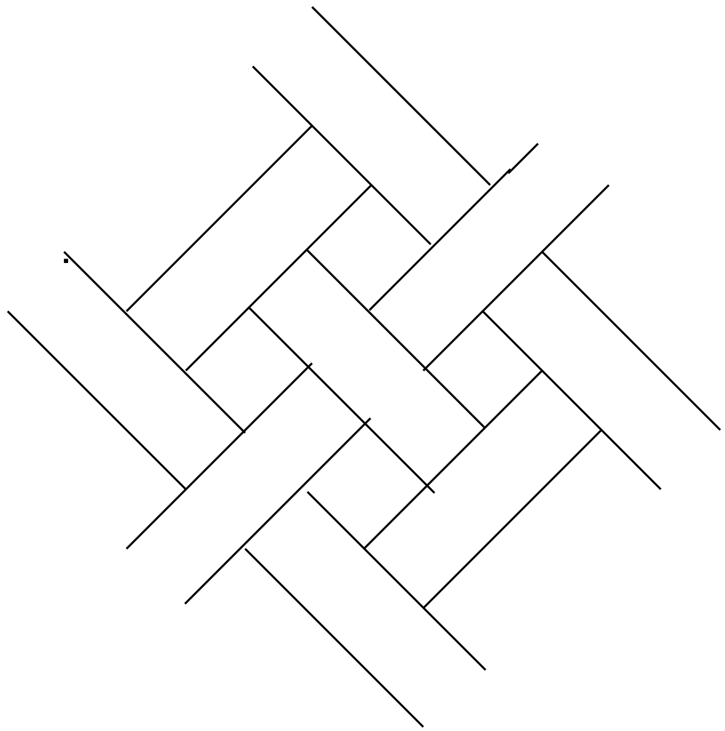


NE-SW cluster blocked by T-junction with NW-SE percolating cluster

T-Junctions

DP spanning clusters $\rightarrow$ blocked

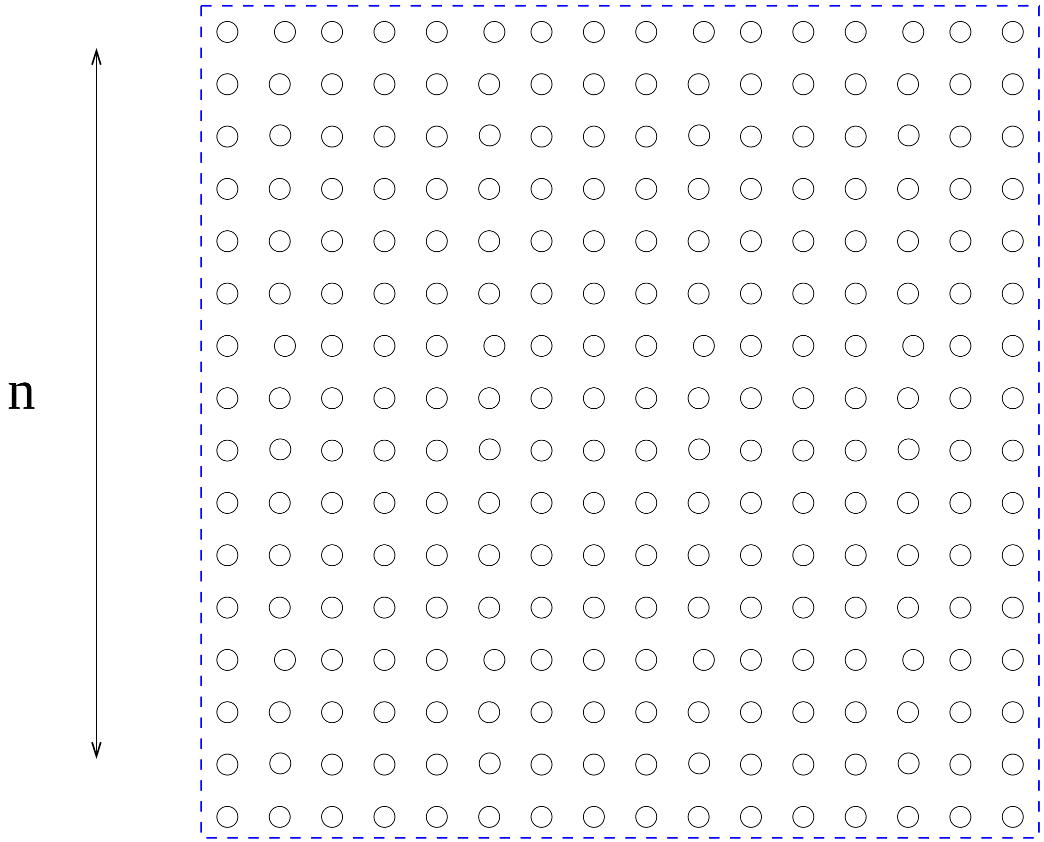
Blocked cluster $\not\rightarrow$ DP spanning cluster



Lines = NE-SW or NW-SE clusters

Ex. Blocked structures without NW-SE nor NE-SW percolating clusters

Ergodicity $\rho < \rho_c$



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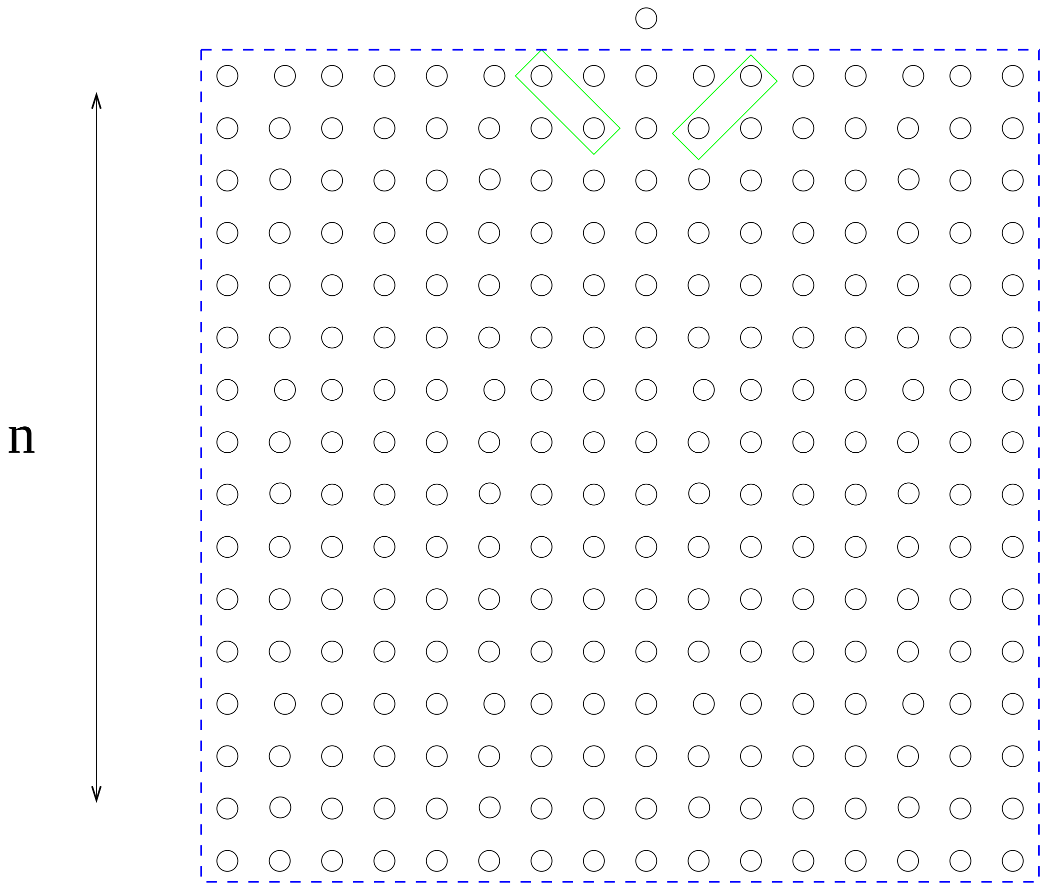

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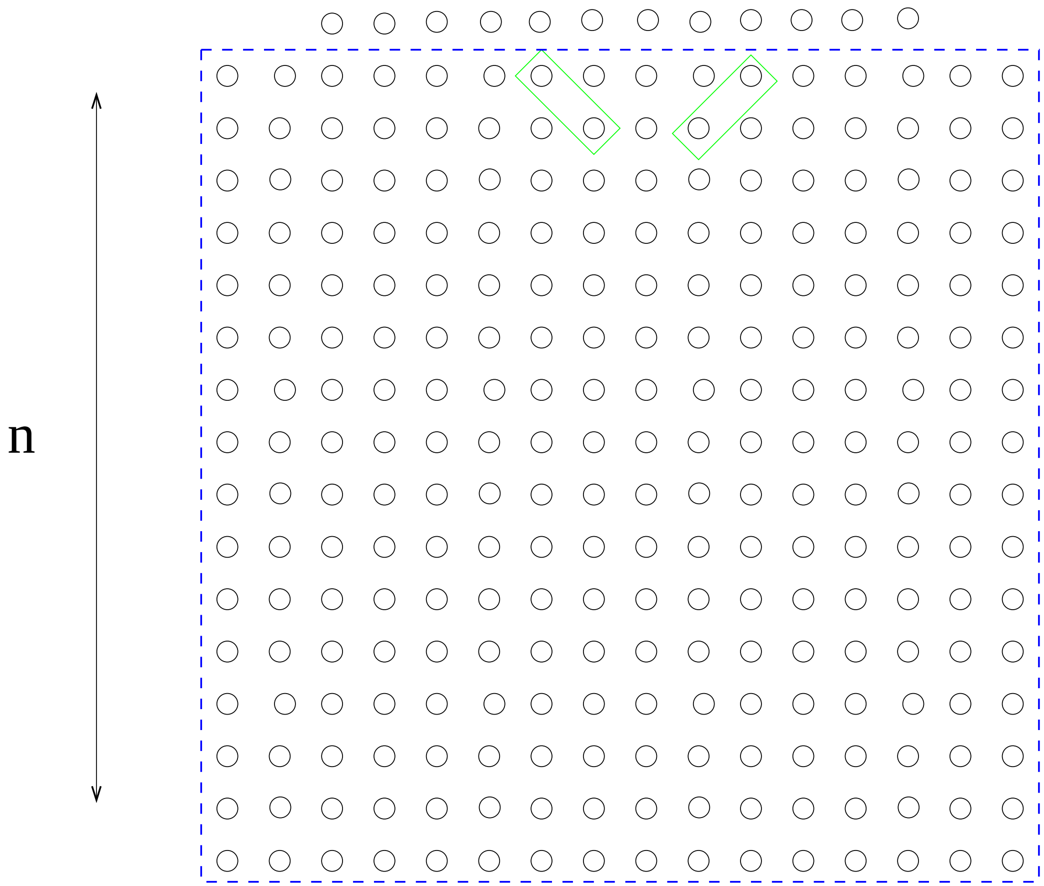

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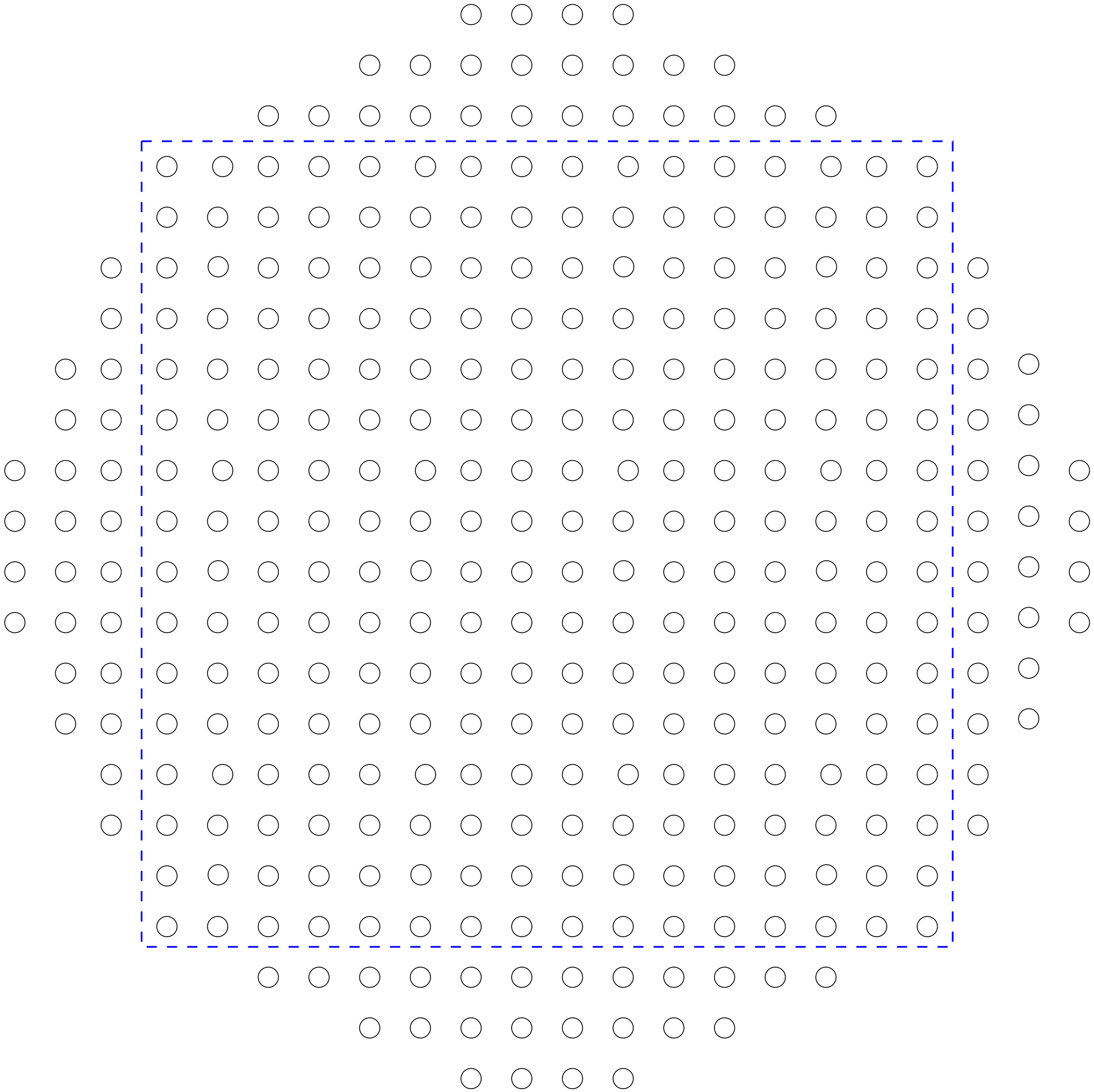

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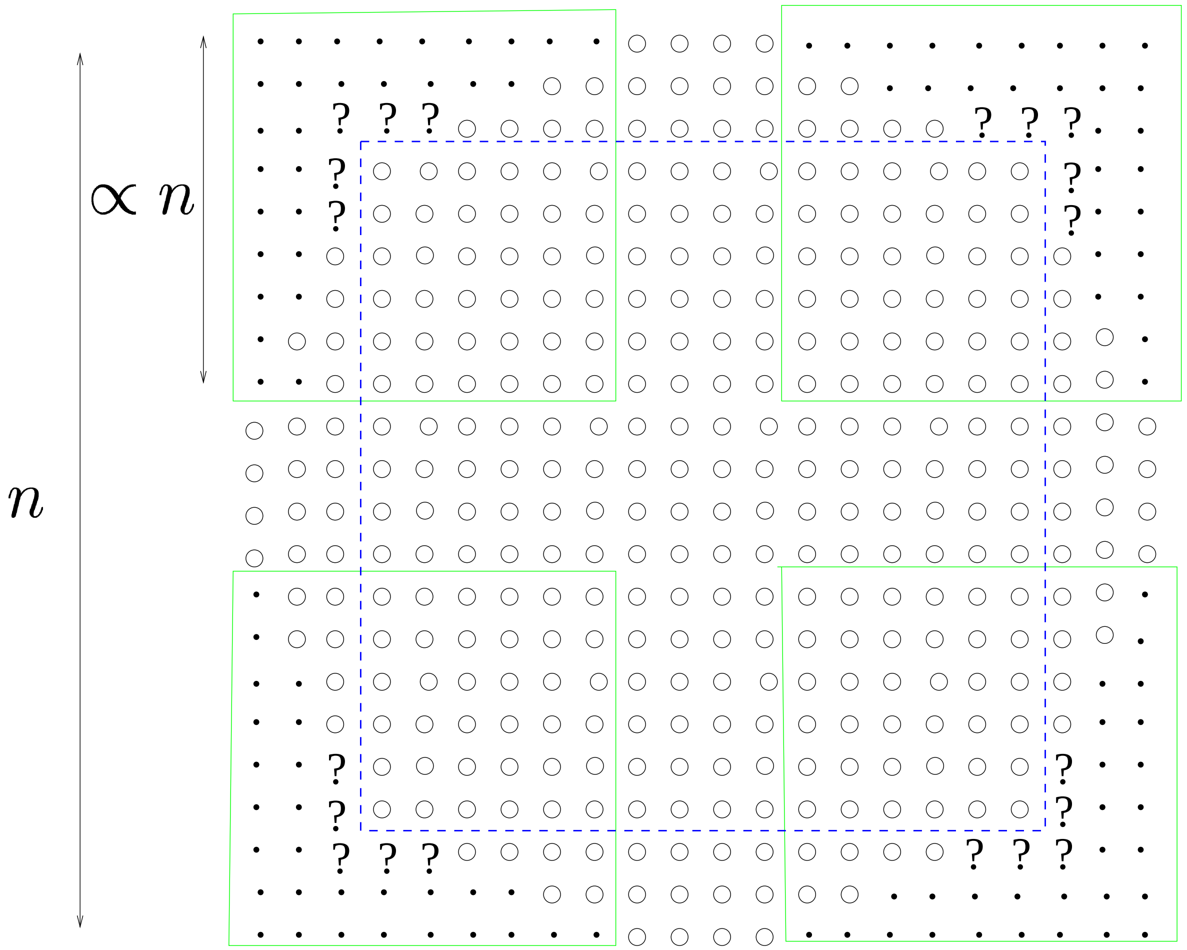

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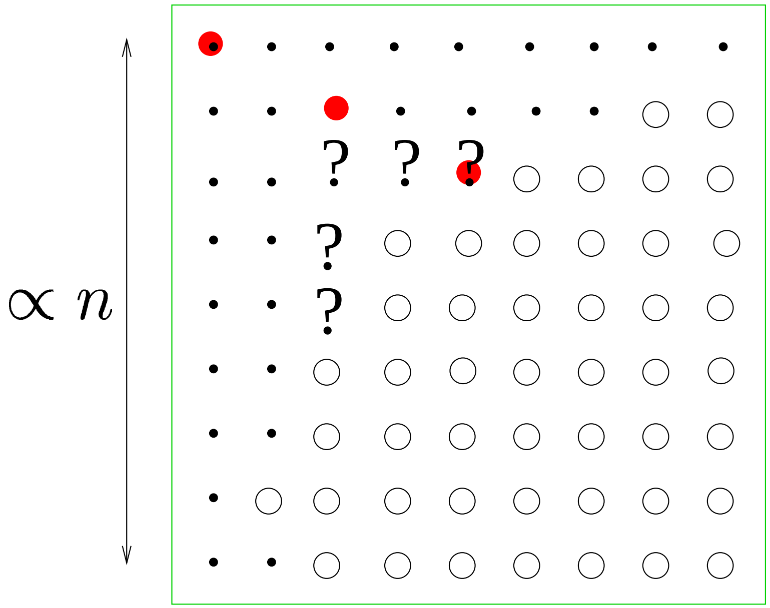

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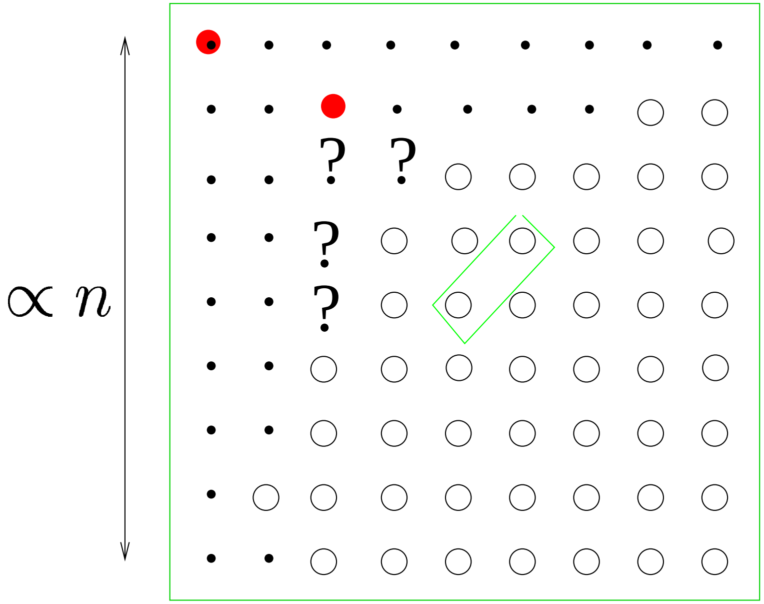

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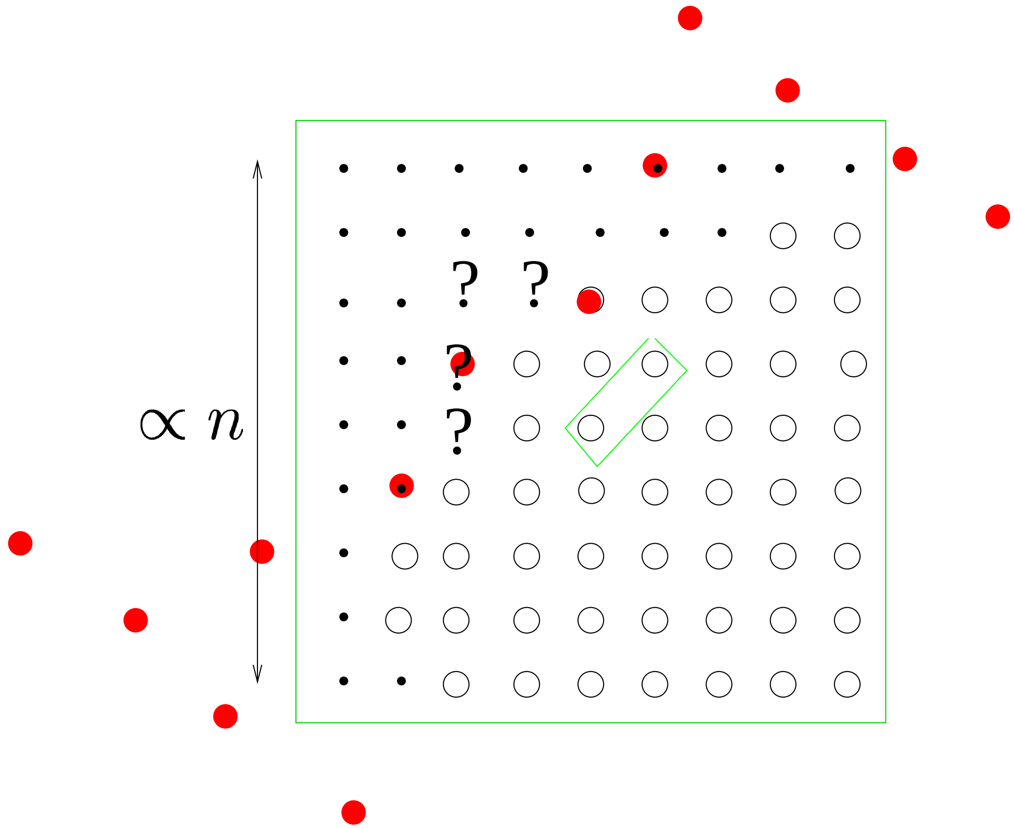

To block ? we need a NE-SW of length $\propto n$

Ergodicity $\rho < \rho_c$

Proba (empty square $n \times n \;\rightarrow\; (n+2) \times (n+2)) \propto$

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$(1 - A \exp^{-n/\xi_{\|}})$, $\quad \xi_{||}(\rho)$= DP correlation length

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$\prod_n^{\infty}$=P (empty $n \times n \rightarrow$ empty lattice)$> \exp(-c\, \xi_{\|}^{1-z})$

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- Ergodicity in infinite volume $\rho < \rho_c$
- Ergodicity breaking at ρ_c
- Critical length $\rho \nearrow \rho_c$: $L_c(\rho) \simeq \exp(\xi_{\|}^{1-z})$

  $\xi \propto 1/(\rho_c - \rho)^{\nu}$, $\nu \simeq 1.73$, $z \simeq 0.63$

  Critical properties different from DP
  Enormous finite size effects

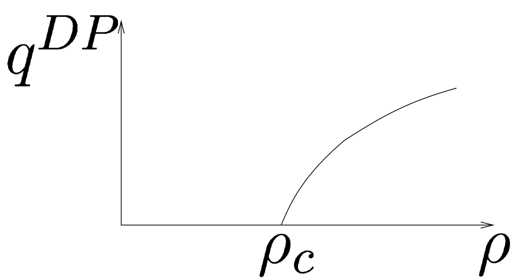
Discontinuity I

Order parameter: density of blocked clusters

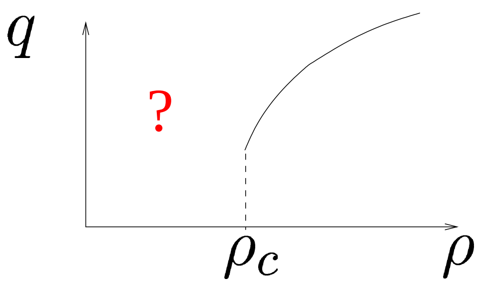
$$\rho < \rho_c\text{: } q(\rho) = 0; \quad \rho > \rho_c\text{: } q(\rho) > 0$$

$q(\rho_c) > 0$?

$q(\rho_c) \geq q^{DP}(\rho_c) = 0$ ($q^{DP}(\rho_c) = 0$: DP cluster fractal)

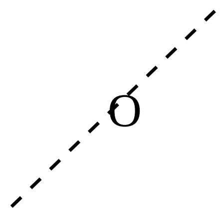


DP: continuous

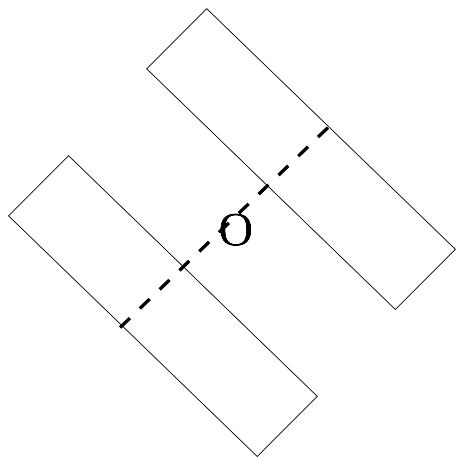


Jamming: discontinuos?

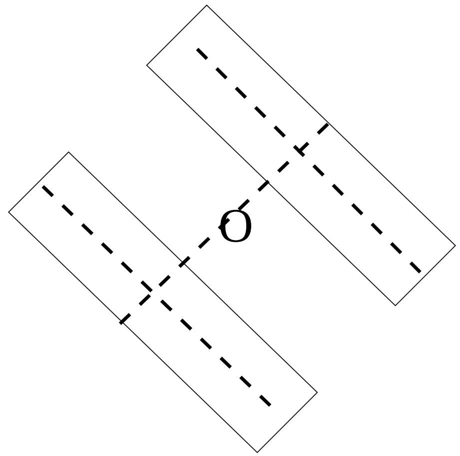
Discontinuity II



Discontinuity II



Discontinuity II



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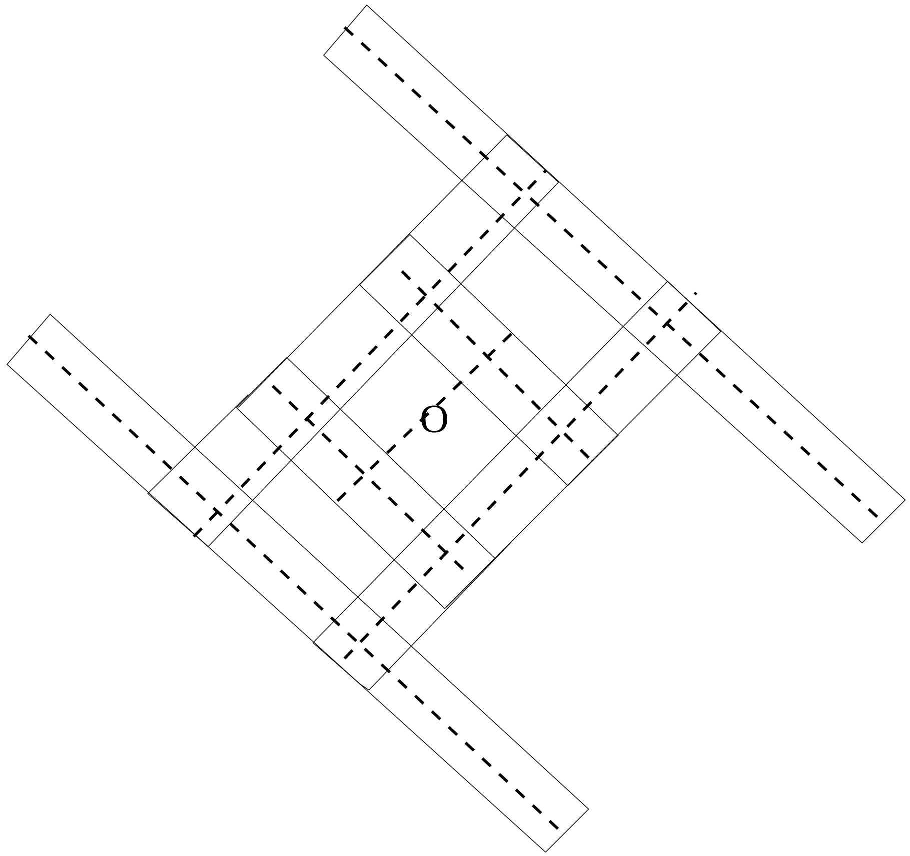
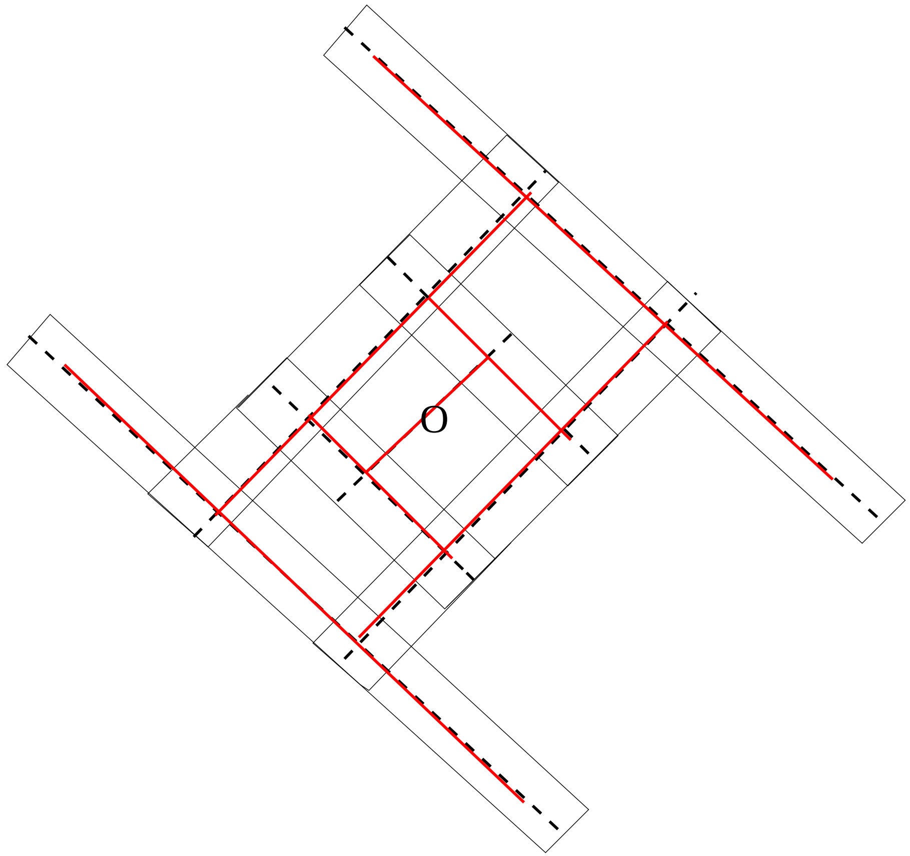


Discontinuity II



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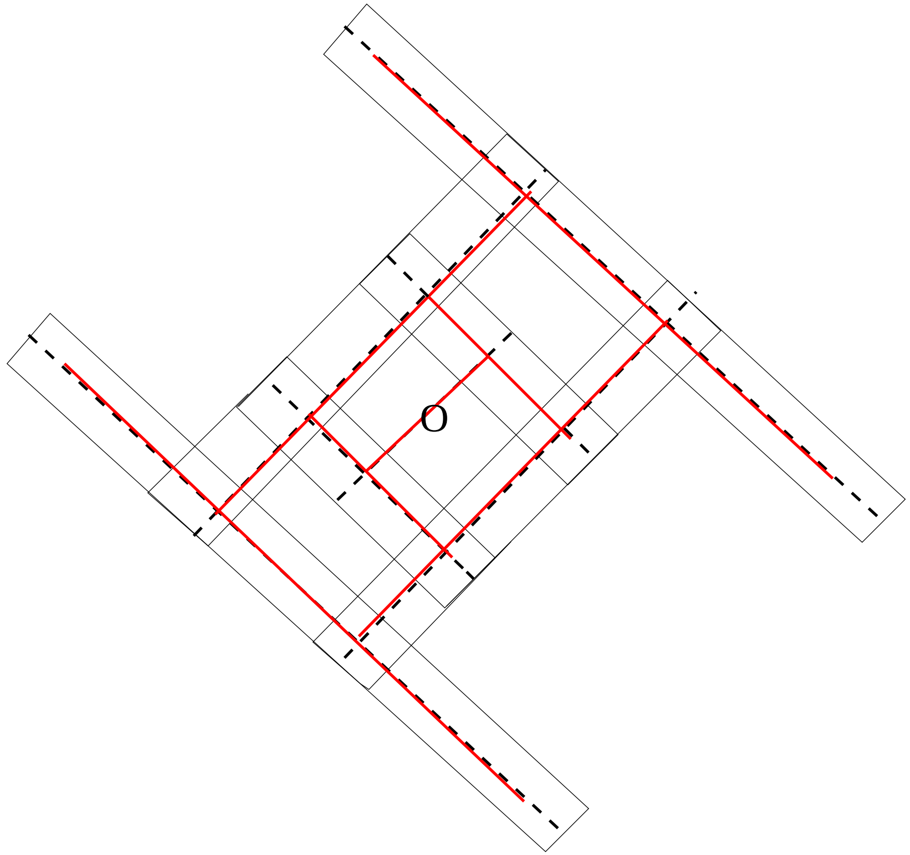

$\lim_{L\to\infty}$ Proba ($\exists$ cluster DP in $L \times cL$) $\to 1$

$\to q(\rho)$= $\prod_L^\infty > 0$

Clusters are compact at $\rho_c \to$ discontinuous percolation

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- New percolation transition: discontinuous + anomalous critical properties
- Relation with experimental data (colloidal suspensions, jamming for granular media . . .);
- Out of equilibrium dynamics: aging, driven non-equilibrium.