

CROSSING A PHASE TRANSITION OUT OF EQUILIBRIUM

Alberto Sicilia Garcia

Phases of matter

Matter can be found in many different phases.

• Characterize the phases of matter is a central problem in many fields of physics.

Some examples:

**Energy
scale.**



- Cosmology: Phases of matter in the first instants of the universe.
- QCD: gluon-plasma phase transition.
- Biophysics: phases of polymers in a solution.
- Condensed matter: insulator/conductor/superconductor.

Out of equilibrium dynamics

- **Great advances have been made in the study of equilibrium properties of phase transitions.**
- **A natural step forward:** what happens if we force the system to cross out of equilibrium a phase transition?

How?

- Changing abruptly a control parameter (ex. the temperature).
 - Changing abruptly a microscopical parameter (ex. a coupling constant).
- **The system will evolve on time until reaching its new equilibrium state. Slow dynamics (“aging”).**

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 - **Note that this is only a particular example of an out of equilibrium process. One can also study, for example, out of equilibrium stationary states:**
 - Coupling the system at two thermal reservoirs at different temperatures.
 - Constantly injecting energy to the system (“shaking”).

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Defect formation

- **When crossing a phase transition out of equilibrium, defects are created.**
- **On the subsequent time evolution, defects will progressively disappear until the system reaches the new equilibrium state.**
- **A possible way to study the out of equilibrium evolution of the system is then to focus on defect dynamics.**

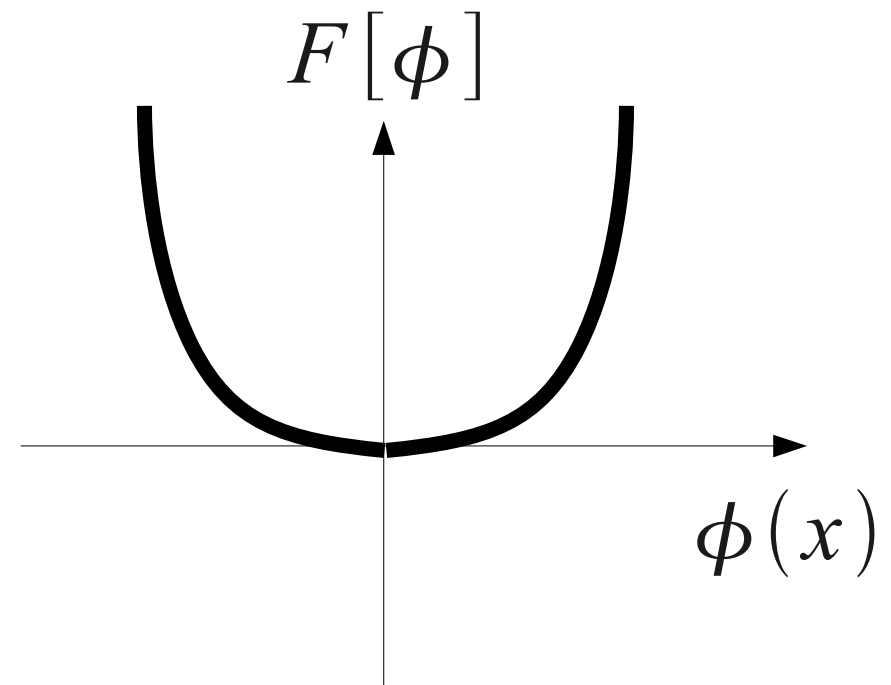
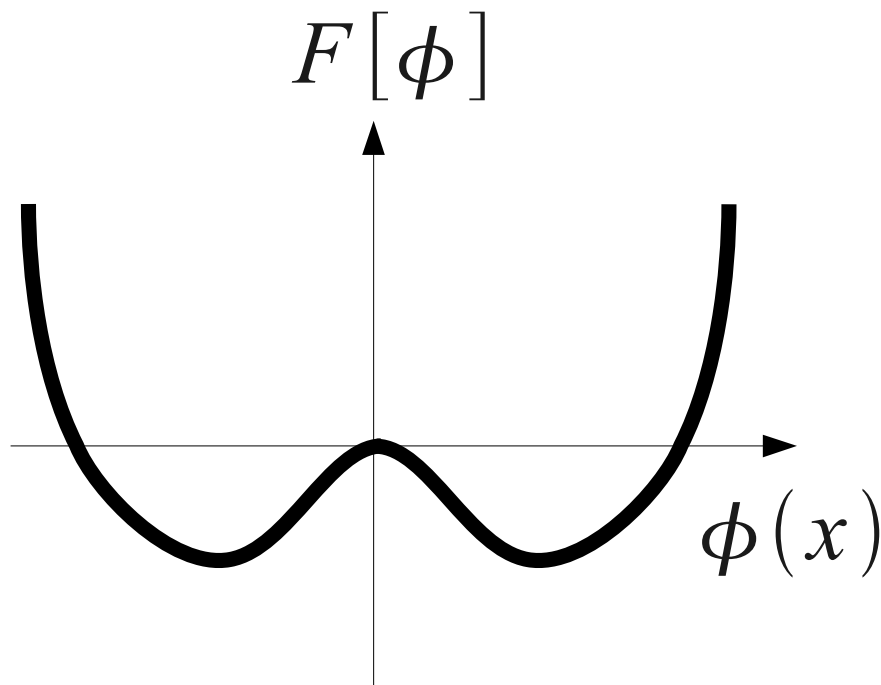
But...

- What defects are?
- Why are they created when crossing a phase transition?

Defect formation

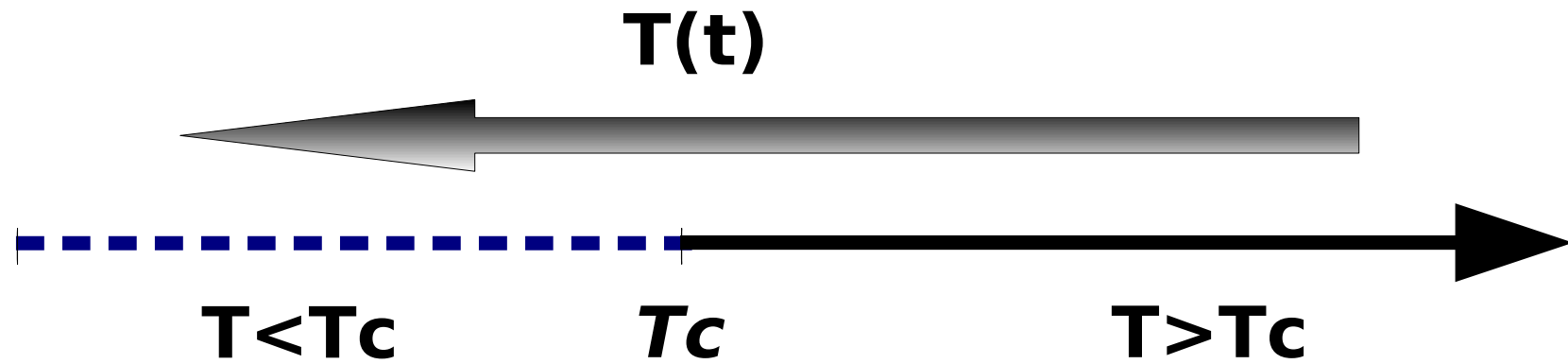
FERRO

PARAMAGNETIC

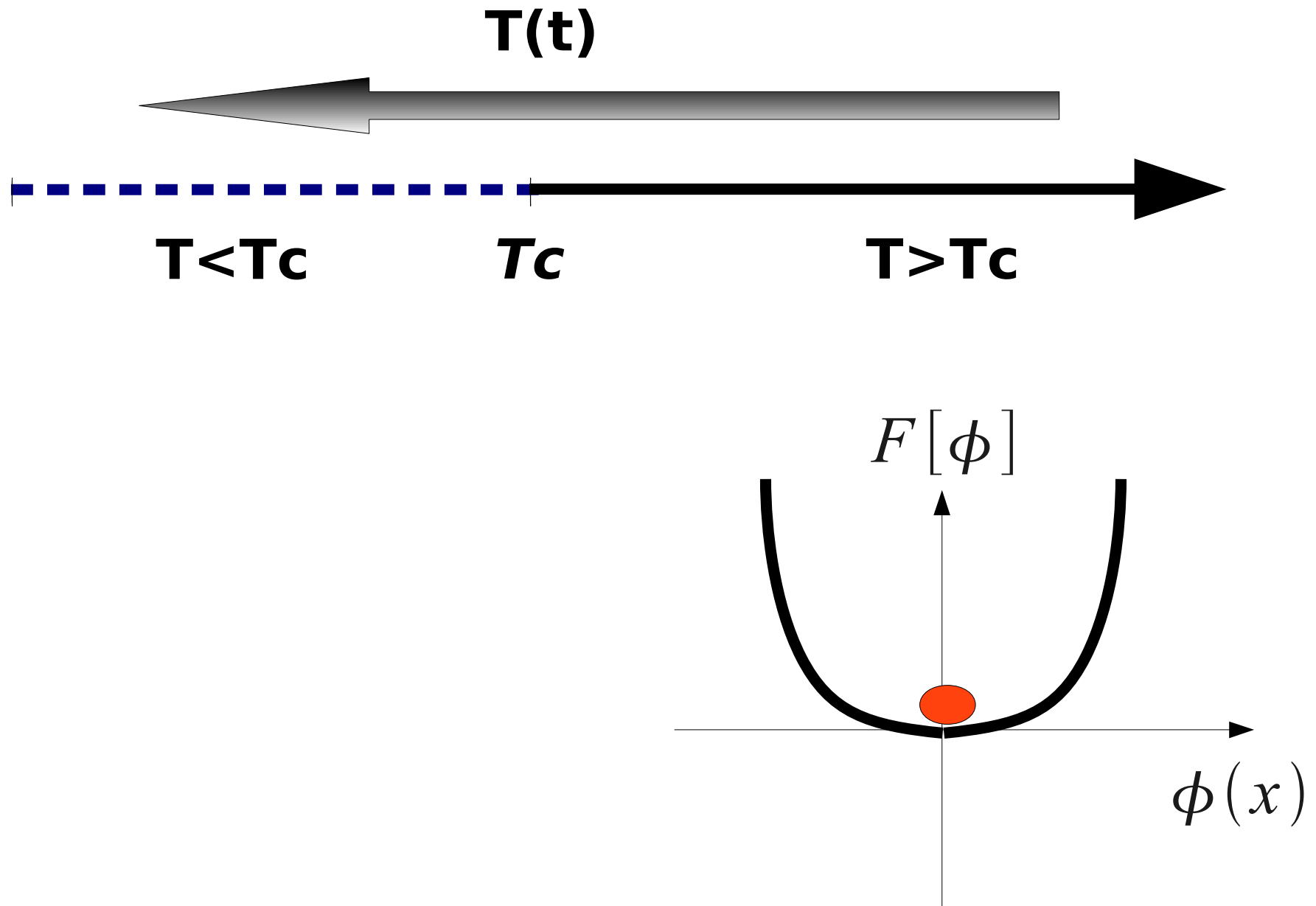


Crossing a phase transition out of equilibrium

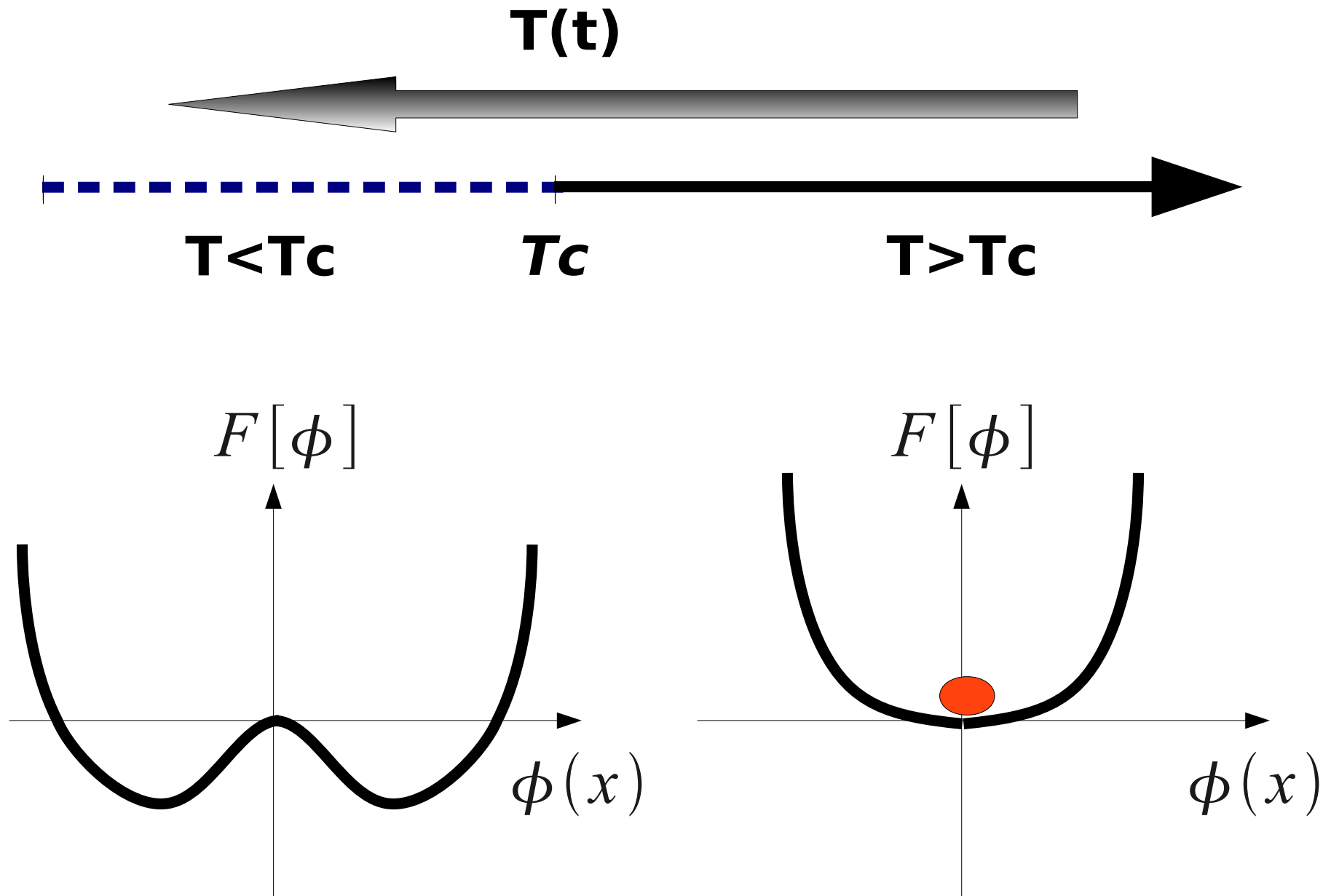
Defect formation



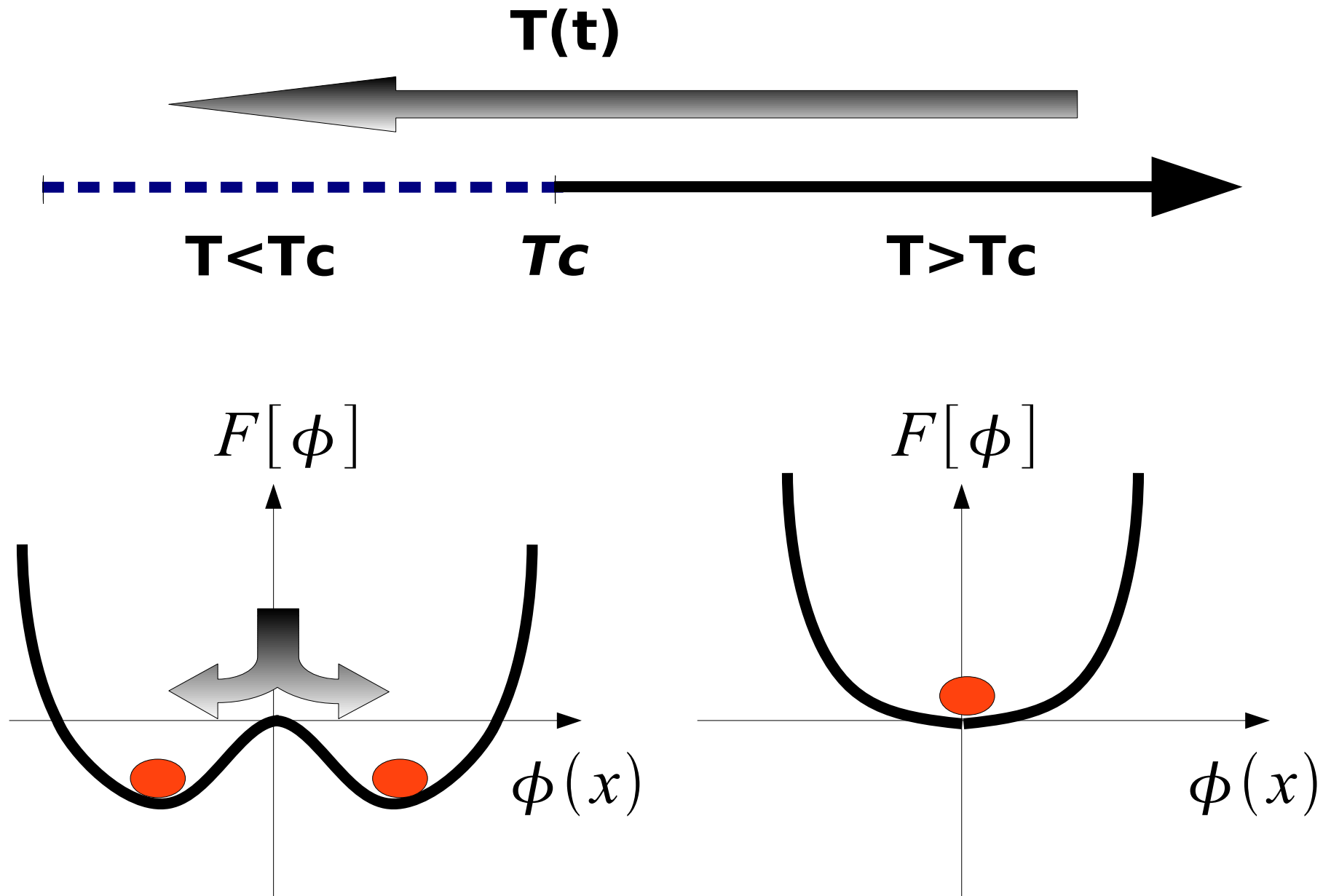
Defect formation



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Defect formation

- Below T_c , the order parameter must choose a vacuum.
- But in different regions of the space, the order parameter chooses different vacua...

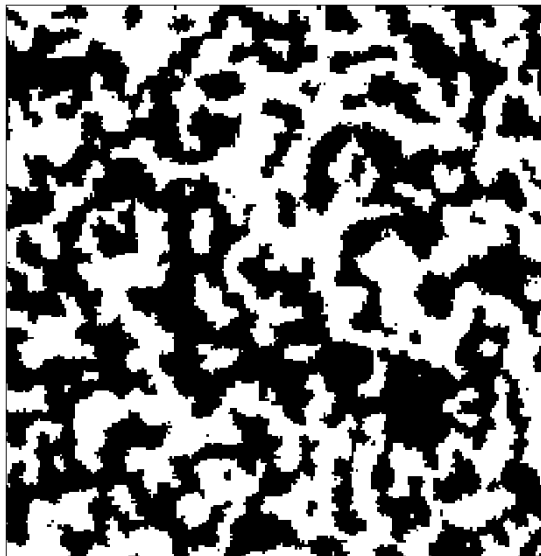
⇒ Formation of **TOPOLOGICAL** defects.

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⇒ Formation of TOPOLOGICAL defects.

- An Example of topological defects.



Domain Walls: Closed hypersurfaces in $d-1$ dimensions.

Defect formation

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Domain Walls: Closed hypersurfaces in $d-1$ dimensions.

Defect formation

➤ Depending on...

- **The nature of the order parameter** (space and field dimensionalities, scalar/vector, real/complex...).
- **How the symmetry is broken.**

⇒ Different kinds of topological defects!

- **Domain walls.**
- **Strings.**
- **Monopoles.**
- **Textures.**

GOAL OF THIS THESIS:

“Gain some understanding in the dynamics of systems forced to cross a phase transition out of equilibrium.”

In particular, study this problem from a geometrical point of view: focusing on defect dynamics.

Particular problems we studied

An equilibrium prelude:

- Geometrical properties of critical parafermionic models.

with R. Santachiara and M. Picco.

Out-of-equilibrium dynamics:

- Geometry of domain growth in 2d.

with J. Arenzon, A. Bray, LFC, I. Dierking and Y. Sarrazin.

- Relaxation in spatially extended chaotic systems: coupled map lattices.

with E. Katzav and LFC.

- Coarsening in the Potts model.

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- Revision of the classical Kibble-Zurek mechanism.

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- Equilibrium and out-of-equilibrium dynamics of the Blume-Capel model.

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SUMMARY OF THE TALK

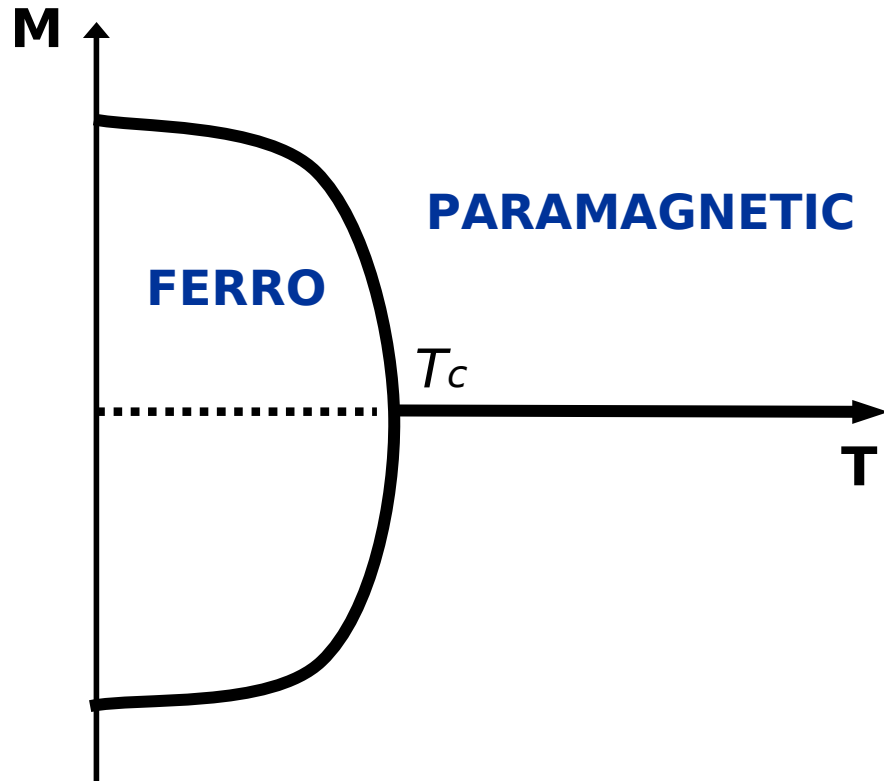
1.- Phenomenology of “domain growth” (“coarsening”, “phase ordering dynamics”).

2.- OUR WORK: Geometrical description of 2d domain growth.

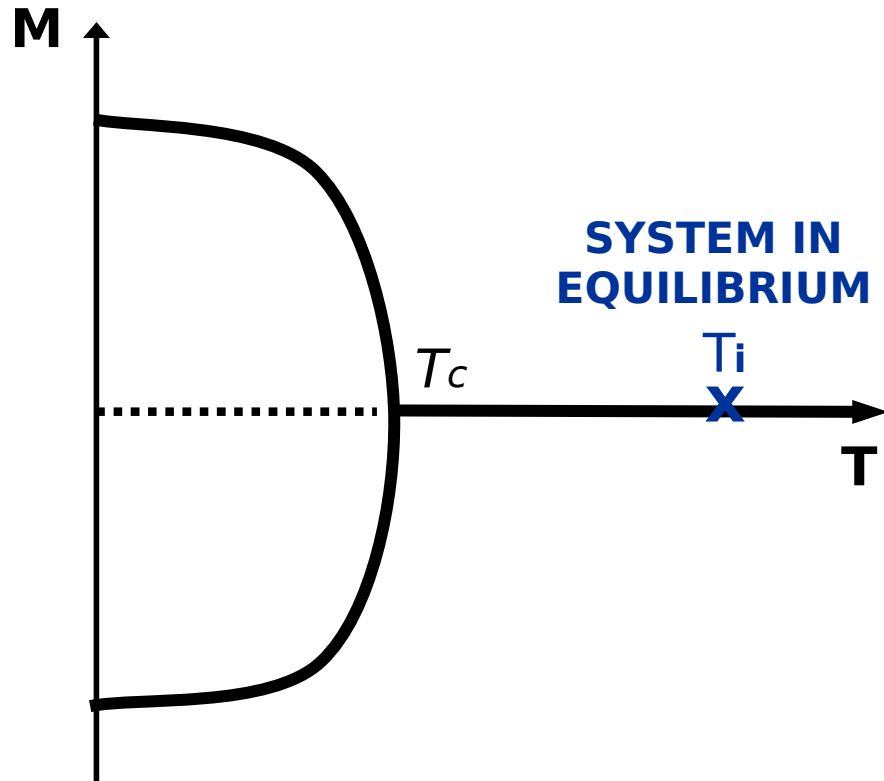
3.- Conclusions.

1.- PHENOMENOLOGY OF DOMAIN GROWTH

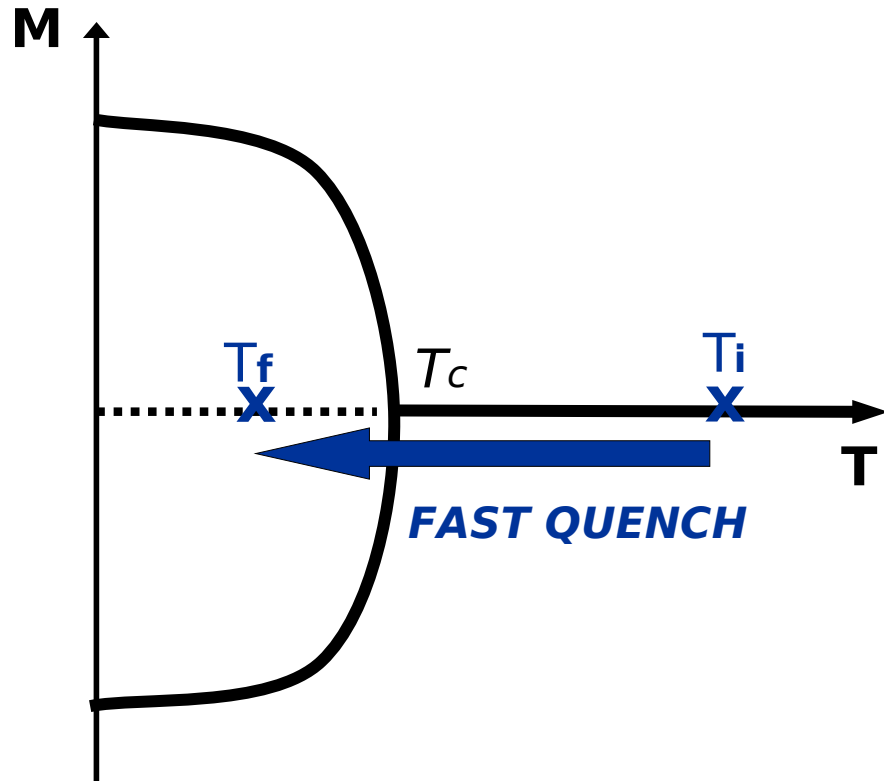
What is domain growth?



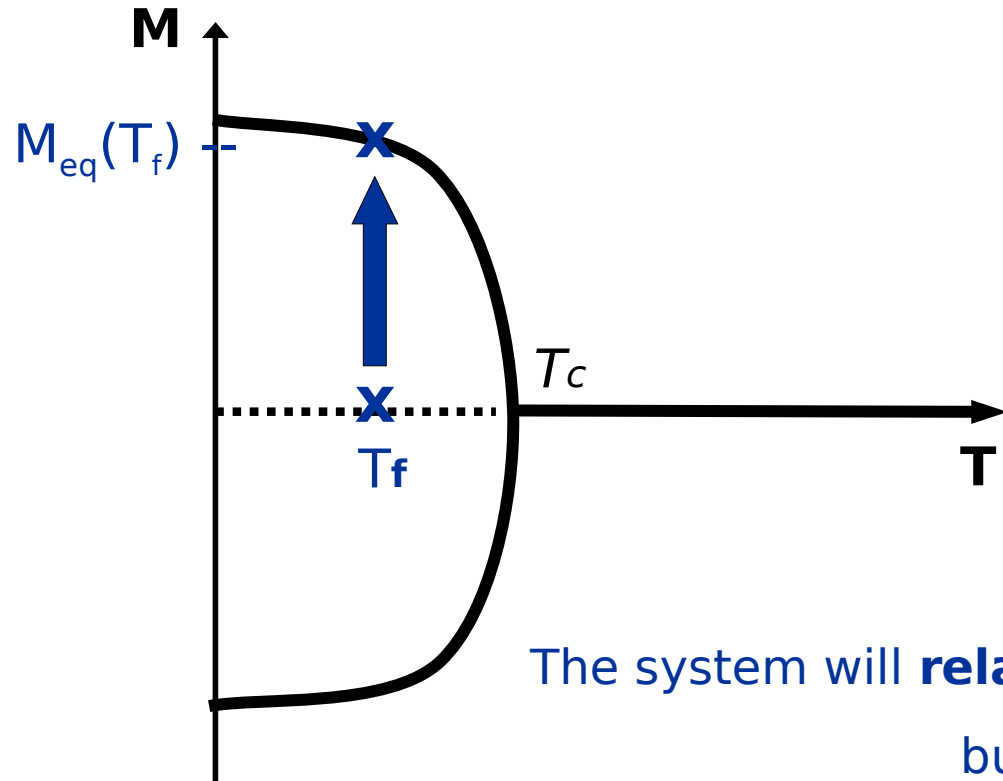
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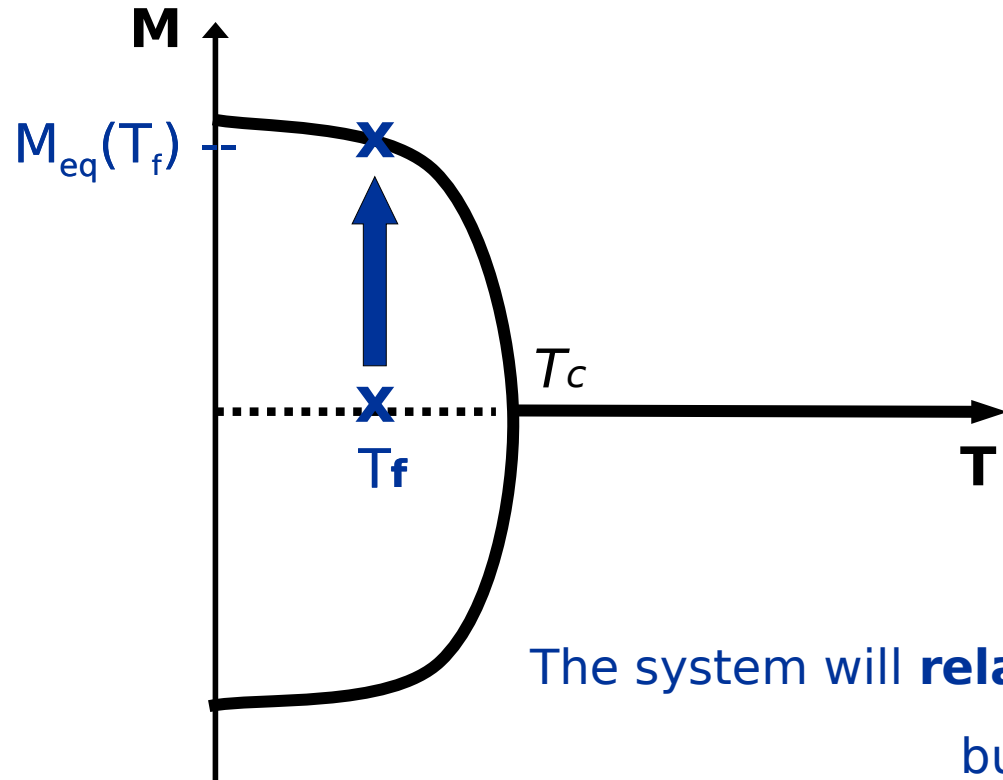
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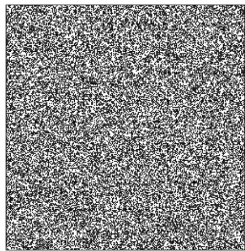


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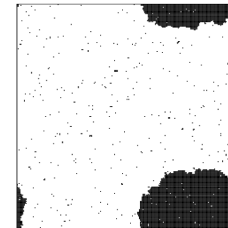
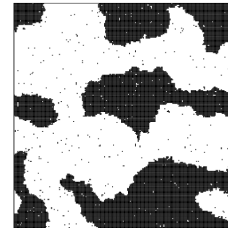
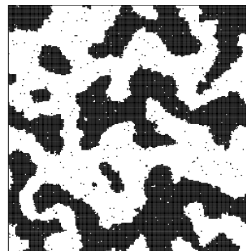
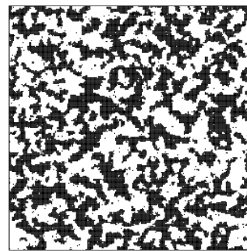


The system will **relax to the new equilibrium state...**
but **HOW???**

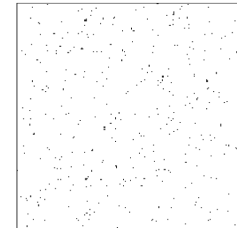
Equilibrium T_i



$t=0$



Equilibrium T_f



$t=t_{eq.}$

time

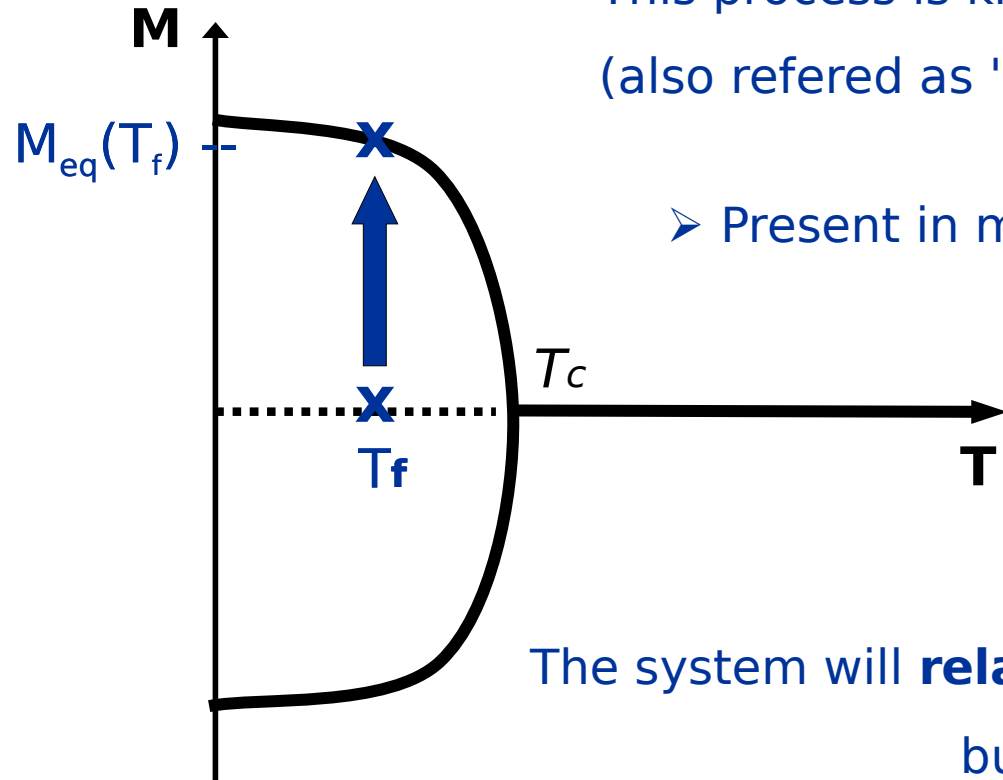
Crossing a phase transition out of equilibrium

What is domain growth?

This process is known as **DOMAIN GROWTH**

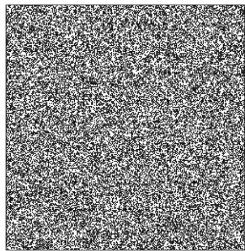
(also referred as 'phase ordering' or 'coarsening').

➤ Present in many different systems.

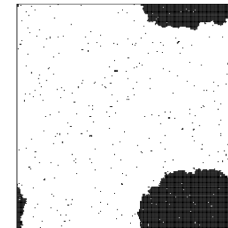
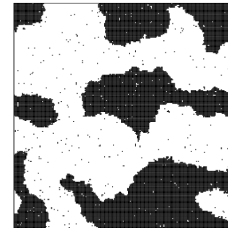
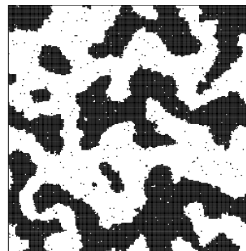
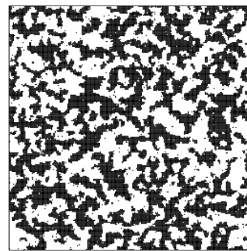


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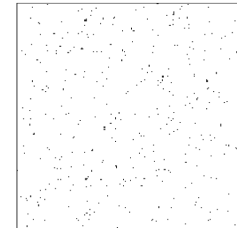
Equilibrium T_i



t=0



Equilibrium T_f



t=teq.

time

Crossing a phase transition out of equilibrium

What is domain growth?

DYNAMICAL SCALING HYPOTHESIS

- There exists a **characteristic length scale $R(t)$** :

If we measure all distances in units of $R(t)$, the system is statistically the same at any time.

$$R(t) \sim t^{1/2}$$

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- **There was no analytical proof in 2d.**

3.- OUR WORK:
GEOMETRICAL DESCRIPTION OF 2D
DOMAIN GROWTH

Mathematical formalism

- Mathematical model we used: Langevin equation.

$$\frac{\partial \phi(\vec{x}, t)}{\partial t} = -\frac{\delta H[\phi]}{\delta \phi(\vec{x}, t)} + \eta(\vec{x}, t)$$

$$\langle \eta(\vec{x}, t) \rangle = 0 \quad \langle \eta(\vec{x}, t) \eta(\vec{x}', t') \rangle = 2T \delta(\vec{x} - \vec{x}') \delta(t - t')$$

$$H[\phi] = \int d^d x \left[\frac{1}{2} (\nabla \phi)^2 + \frac{r}{2} \phi^2 + \frac{g}{4} \phi^4 \right]$$

- There are other mathematical models one could consider.

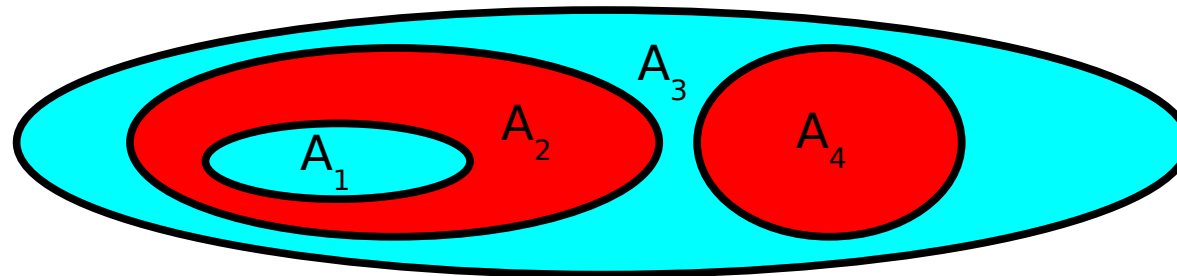
Examples:

- Instead of a coarse-grained field, a more microscopical approach.
- Instead of a continuous order parameter, a lattice model.
- Instead of a Langevin equation, a master equation.
- Instead of stochastic dynamics, deterministic dynamics (Hamilton eqs.).
- Instead of a classical system, a quantum system.

Distribution of areas in quenches to $T=0$

Geometrical Description of 2D Domain Growth

- Our defects are the domain walls (a.k.a. “hulls”).
- Two different areas associated to each domain wall.



➤ Domain area.

There are 4 domains with areas:

A_1 A_2 A_3 A_4

➤ Hull enclosed area.

There are 4 hulls with enclosed areas:

A_1 A_1+A_2 A_4 $A_1+A_2+A_3+A_4$

$n_d(\mathbf{A},t)$

Area distributions densities (and per unit area of the system).

$n_h(\mathbf{A},t)$

Distribution of areas in a quench to $T=0$

- From Langevin equation at $T=0$, Allen and Cahn (1979),

$$v = -\frac{\lambda_h}{2\pi} \kappa$$

- The velocity of a wall in each point is proportional to its local curvature.
- Velocity points in the direction of reducing curvature.

Coarsening does not proceed by coalescence of small domains.

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- Integrating the Allen-Cahn eq. around a hull:

$$\oint v \, dl = -\frac{\lambda_h}{2\pi} \oint \kappa \, dl$$
$$\frac{dA_h}{dt} = -\frac{\lambda_h}{2\pi} \oint \kappa \, dl \quad ???$$

Distribution of areas in a quench to $T=0$

$$\frac{dA_h}{dt} = -\frac{\lambda_h}{2\pi} \oint \kappa dl \quad ???$$

- We can use the Gauss-Bonnet th.

$$\int_M K_g dS + \oint_{\partial M} \kappa dl = 2\pi \chi(M)$$

- Hull-enclosed areas are flat 2d manifolds with no holes.

$$K_g = 0 \quad \chi(M) = 1 \quad \oint_{\partial M} \kappa dl = 2\pi$$

- Evolution equation for hull-enclosed areas:

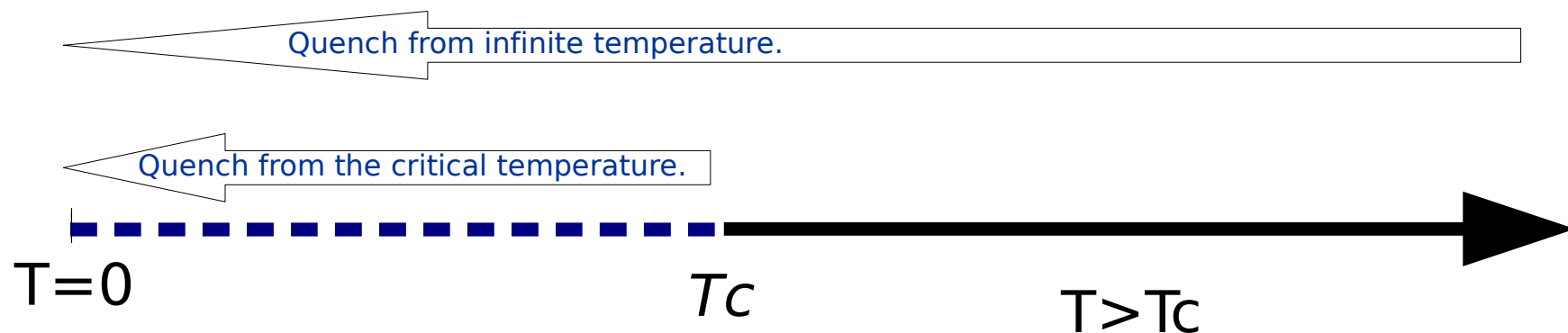
$$\frac{dA_h}{dt} = -\lambda_h \quad A_h(t, A_i) = A_i - \lambda_h(t - t_i)$$

- Hull enclosed areas **evolve independently one from another**.
- They **all shrink at a constant rate**, independently of their size.

Distribution of areas in a quench to $T=0$

$$\begin{aligned} n_h(A, t) &= \int_0^\infty dA_i \delta(A - A_i + \lambda_h(t - t_i)) n_h(A_i, t_i) \\ &= n_h(A + \lambda_h(t - t_i), t_i) . \end{aligned}$$

- If you **know the distribution at initial time**, when the system is quenched, you **know the distribution at any time during the evolution**.
- Remember, we are quenching our system to $T=0$.
- Before the quench, the system is in equilibrium at some temperature $T > T_c$.
- The two extreme cases are:



Distribution of areas in a quench to $T=0$

- We are lucky, because the equilibrium distributions for both initial cases are known (Cardy and Ziff, 2002):

$$n_h(A, 0) \sim \begin{cases} 2c_h/A^2 & \text{Critical percolation} \Leftrightarrow T_0 = \infty \\ c_h/A^2 & T_0 = T_c \end{cases} \quad c_h = 1/8\pi\sqrt{3}$$

- Plugging-in these initial distributions into the evolution equation:

$$n_h(A, t) = \frac{2c_h}{(A + \lambda_h t)^2} \quad \text{Quench to } T=0 \text{ from } T_0 = \infty$$

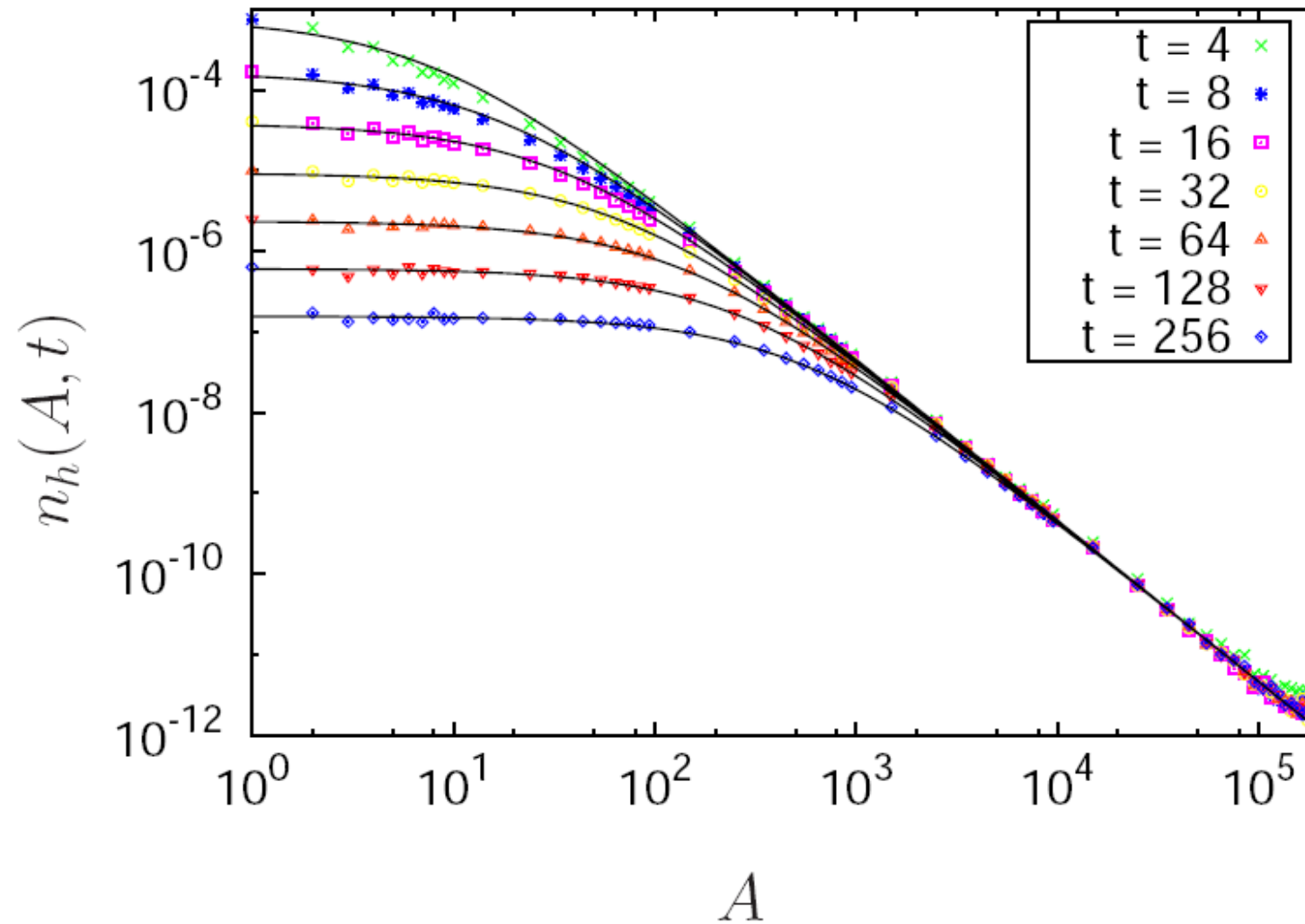
$$n_h(A, t) = \frac{c_h}{(A + \lambda_h t)^2} \quad \text{Quench to } T=0 \text{ from } T_0 = T_c$$

- The distributions have the scaling form,

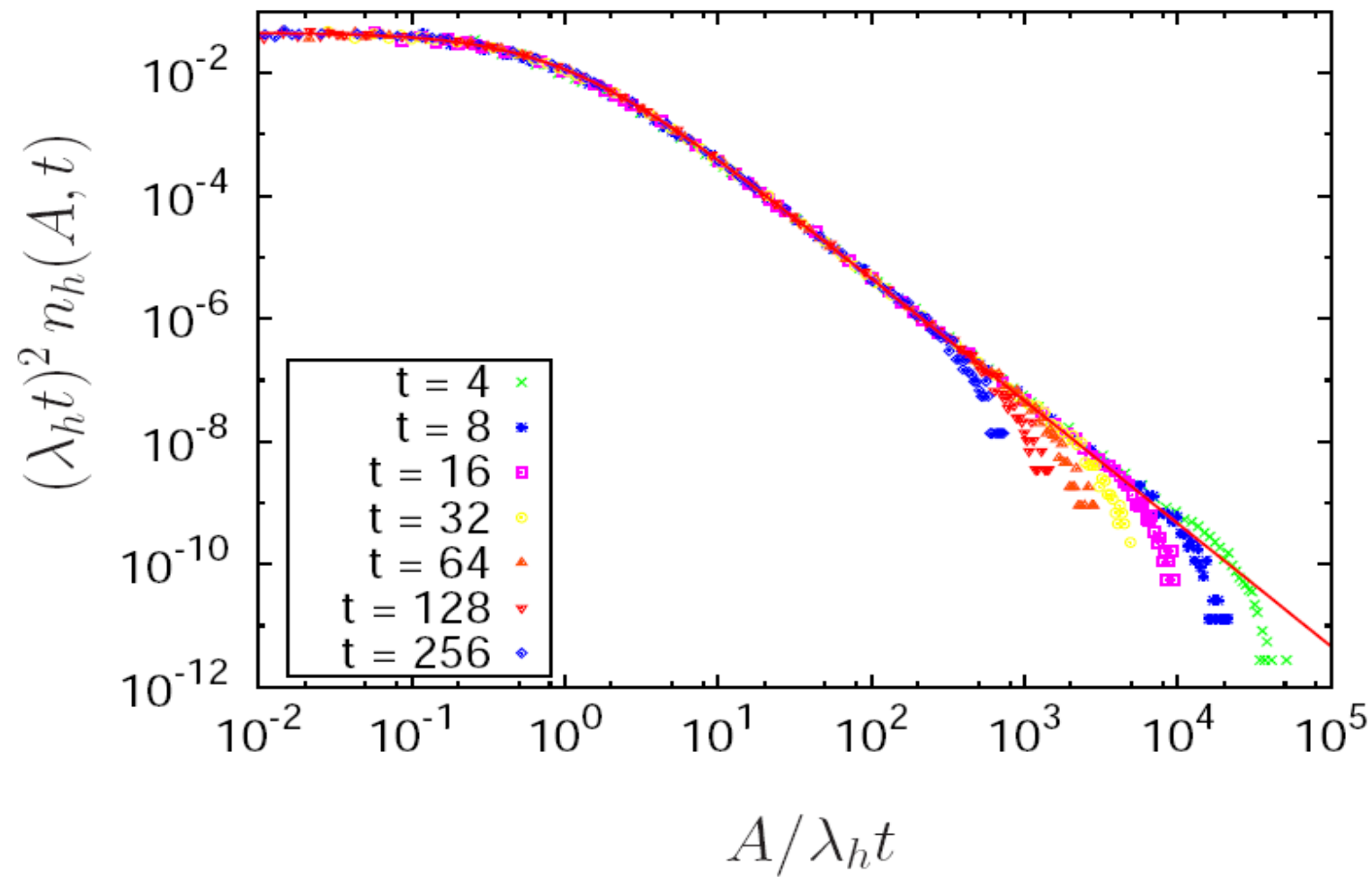
$$n_h(A, t) = t^{-2} f(A/t)$$

Scaling dynamical hypothesis is recovered from calculation!

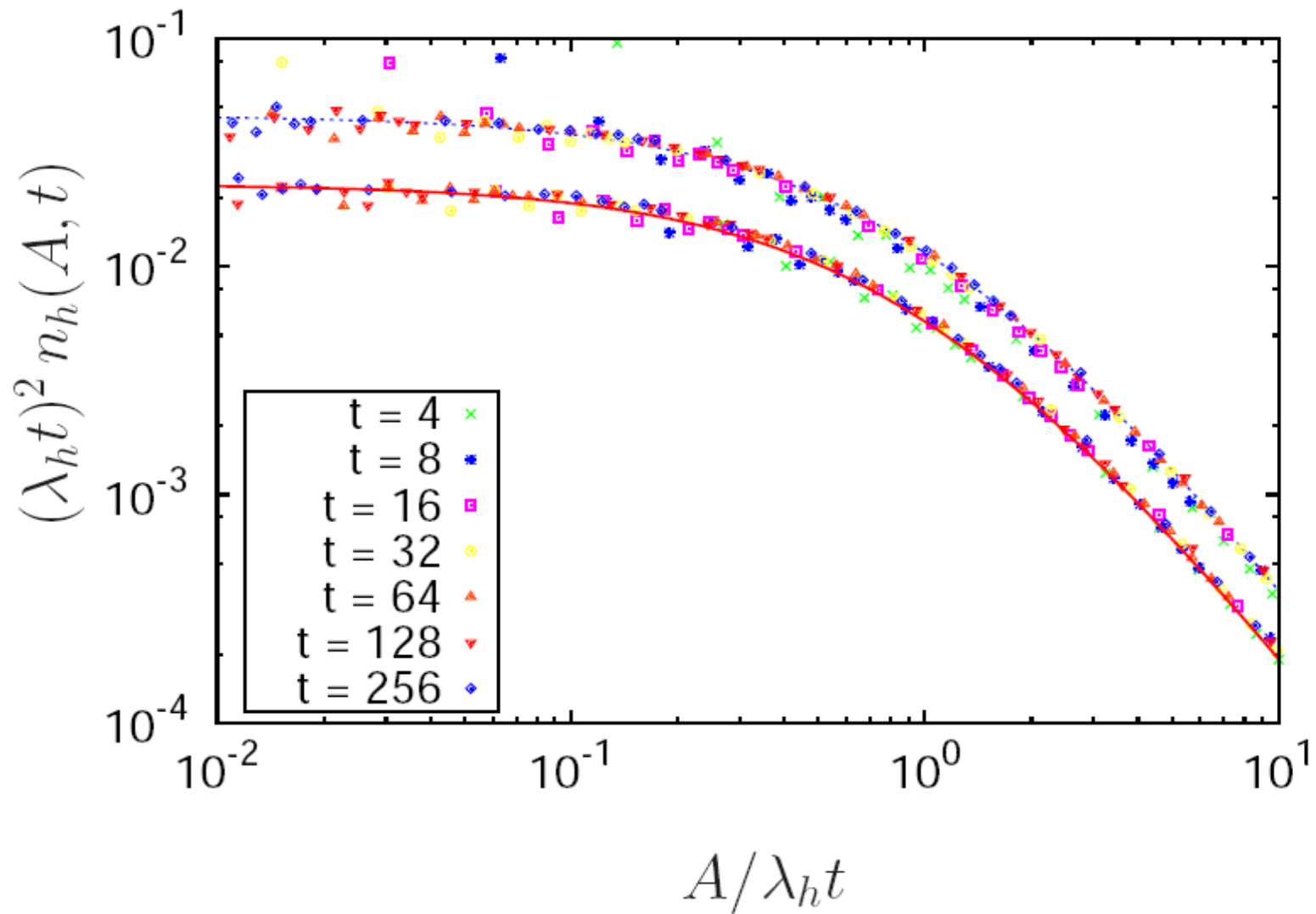
Numerical verification of our exact result



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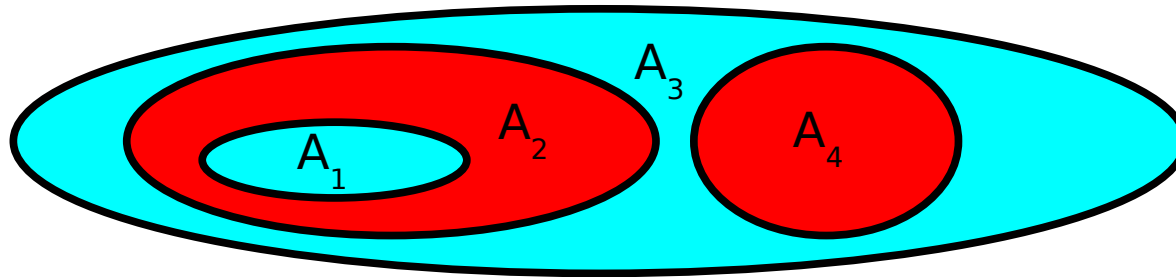


Numerical verification of our exact result



Geometrical Description of 2D Domain Growth

What happens for the domain areas?



- The evolution of a domain area will depend, in general on the movement of several walls.

For example, the evolution of A_3 :

$$\frac{dA_3}{dt} = -\lambda_h + \lambda_h + \lambda_h$$

In general :

$$\frac{dA_d(t)}{dt} = -\lambda_h [1 - \nu(t)]$$

Domain can grow/shrink/remain constant.

Distribution of areas in a quench to $T=0$

- Initial distributions are also known for domain areas.

$$n_d(A, 0) \sim \frac{2c_d A_0^{\tau'-2}}{A^{\tau'}} \quad \tau' = \frac{187}{91} \approx 2.055$$
$$n_d(A, 0) \sim \frac{c_d A_0^{\tau-2}}{A^{\tau}} \quad \tau = \frac{379}{187} \approx 2.027$$

- Taking advantage of the smallness of c_h one can (approximately) show:

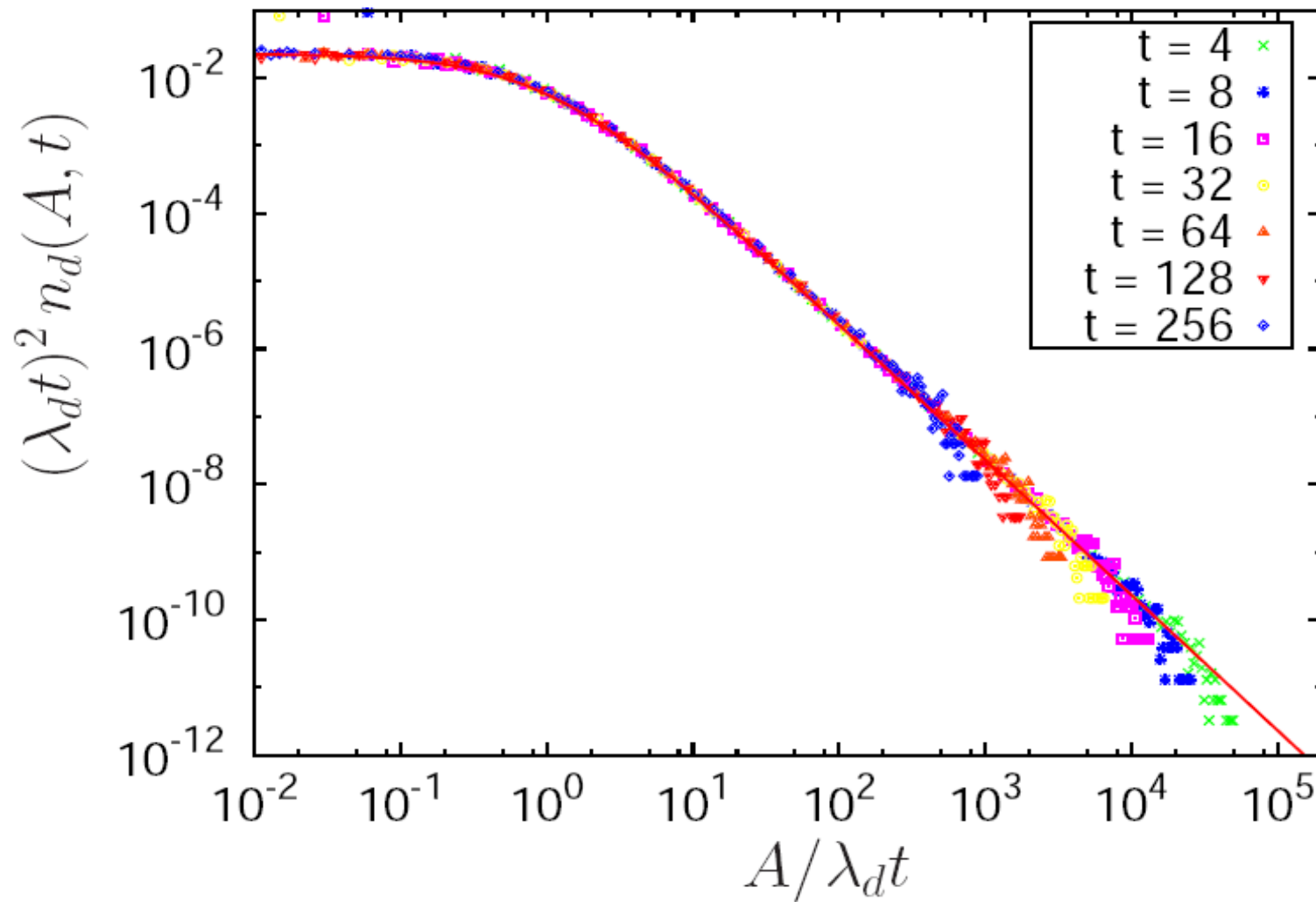
$$n_d(A, t) \sim \frac{2c[\lambda t]^{\tau-2}}{[A+\lambda t]^{\tau}}$$

- Two important sum rules:

$$N_d(t) \equiv \int_0^\infty dA n_d(A, t) = \int_0^\infty dA n_h(A, t) \equiv N_h(t)$$

$$\int_0^\infty dA A n_d(A, t) = 1$$

Distribution of areas in a quench to $T=0$

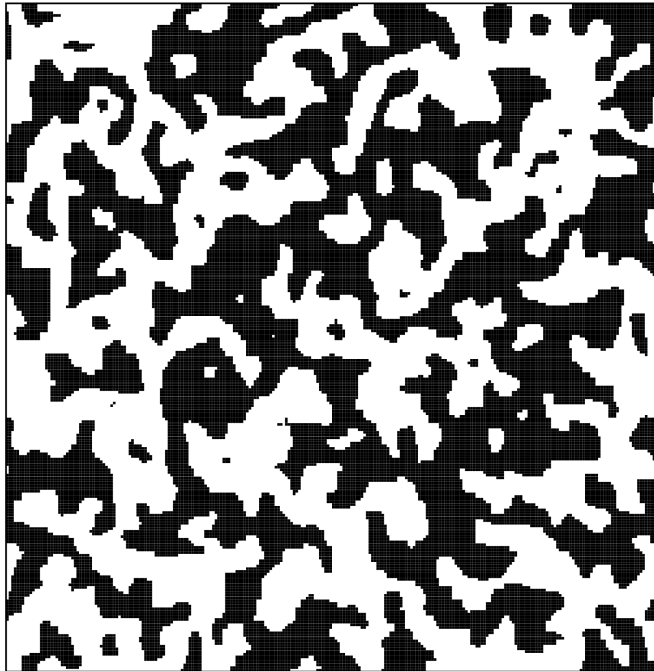


Effects of finite working temperature

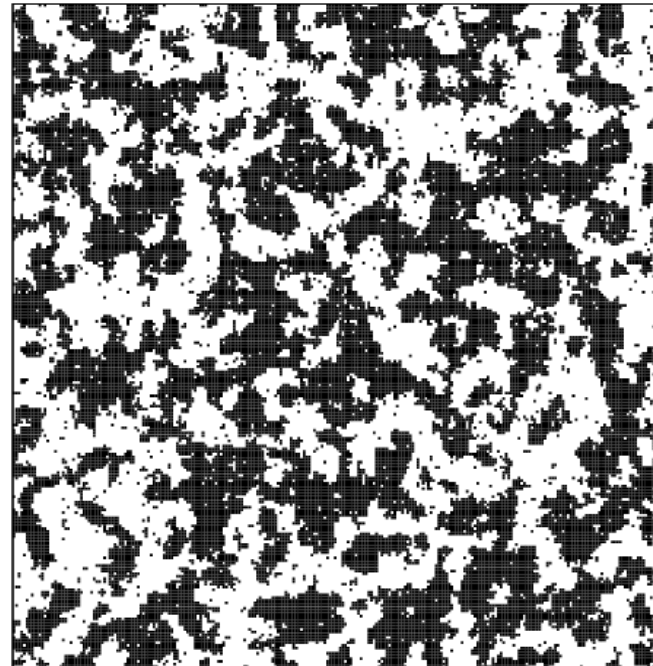
Domain area distributions during coarsening at $T \neq 0$

time = 32 MCS

$T = 0$



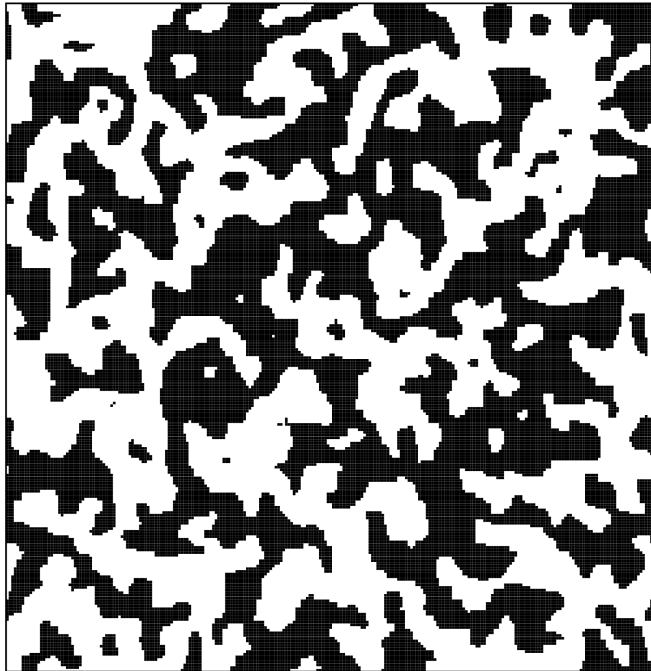
$T = 1.5$



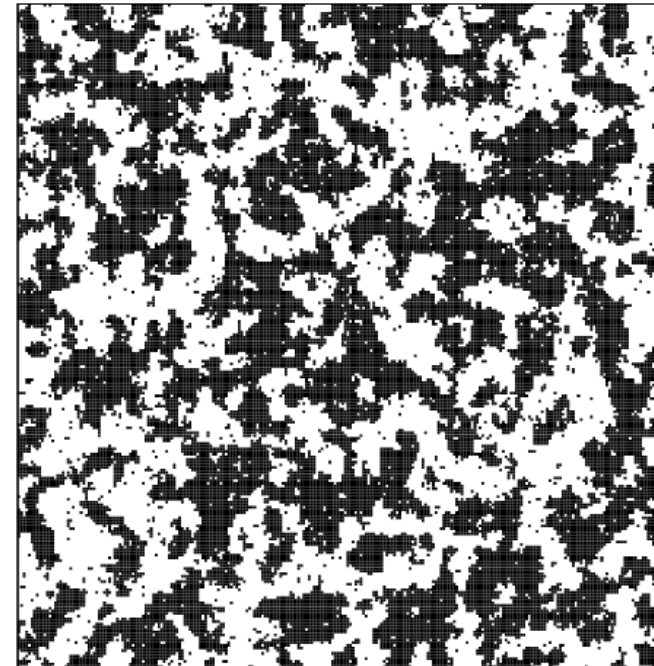
Domain area distributions during coarsening at $T \neq 0$

time = 32 MCS

$T = 0$



$T = 1.5$



EFFECTS OF TEMPERATURE:

- Roughens the domain walls.
- Generates 'thermal domains' (not formed by coarsening).

Domain area distributions during coarsening at $T \neq 0$

- Distribution of domains areas during coarsening at $T=0$.

$$n_d(A, t) \sim \frac{2c[\lambda t]^{\tau-2}}{[A+\lambda t]^\tau} \quad \text{where} \quad \tau = \frac{187}{91} \quad c = \frac{1}{8\pi\sqrt{3}}$$

$$\hookrightarrow \sqrt{A_{av}} \sim R(t) \sim [\lambda t]^{1/2}$$

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- Dynamical RG: dynamics at $T < T_c$ controlled by $T=0$ fixed point.
- Temperature dependence enters through prefactor $\lambda \rightarrow \lambda(T)$

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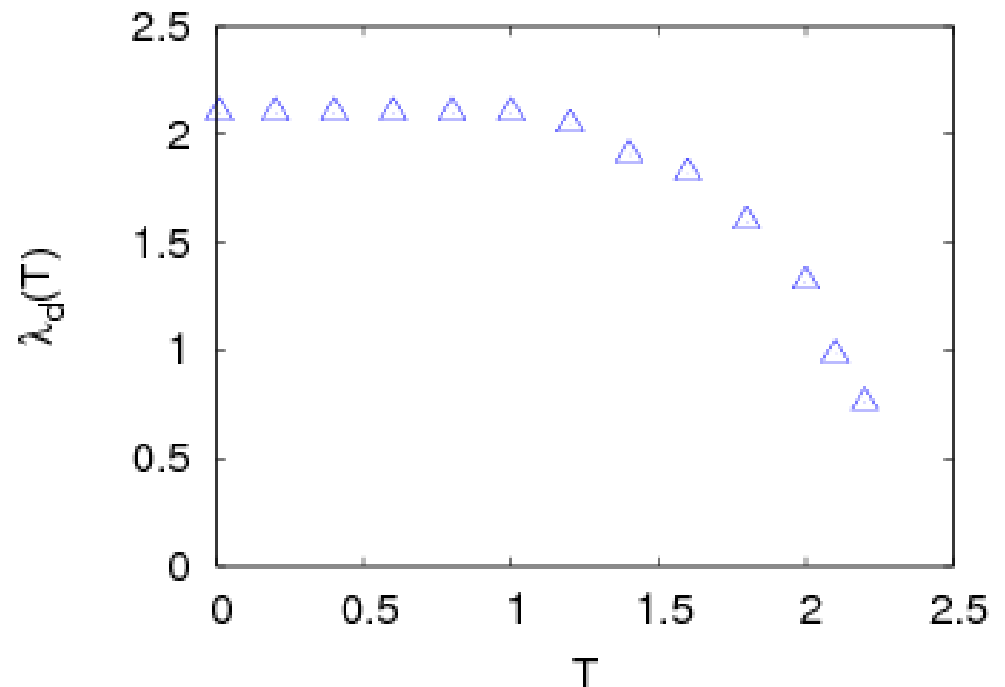
- Dynamical RG: dynamics at $T < T_c$ controlled by $T=0$ fixed point.
- Temperature dependence enters through prefactor $\lambda \rightarrow \lambda(T)$
- How to measure $\lambda(T)$?

From the spatial-correlation function

$$C(r, t) \equiv \frac{1}{N} \sum_{i=1}^N \langle s_i(t) s_{i+r}(t) \rangle$$

which scales with $R(t)$

$$C(r, t) \sim m^2(T) f\left(\frac{r}{R(t)}\right)$$



Domain area distributions during coarsening at $T \neq 0$

- Let us test our prediction:

$$n_d(A, t) \sim \frac{2c[\lambda(T)t]^{\tau-2}}{[A+\lambda(T)t]^\tau} \quad \text{where} \quad \tau = \frac{187}{91} \quad c = \frac{1}{8\pi\sqrt{3}}$$

- Simulations in the 2d Ising Model.

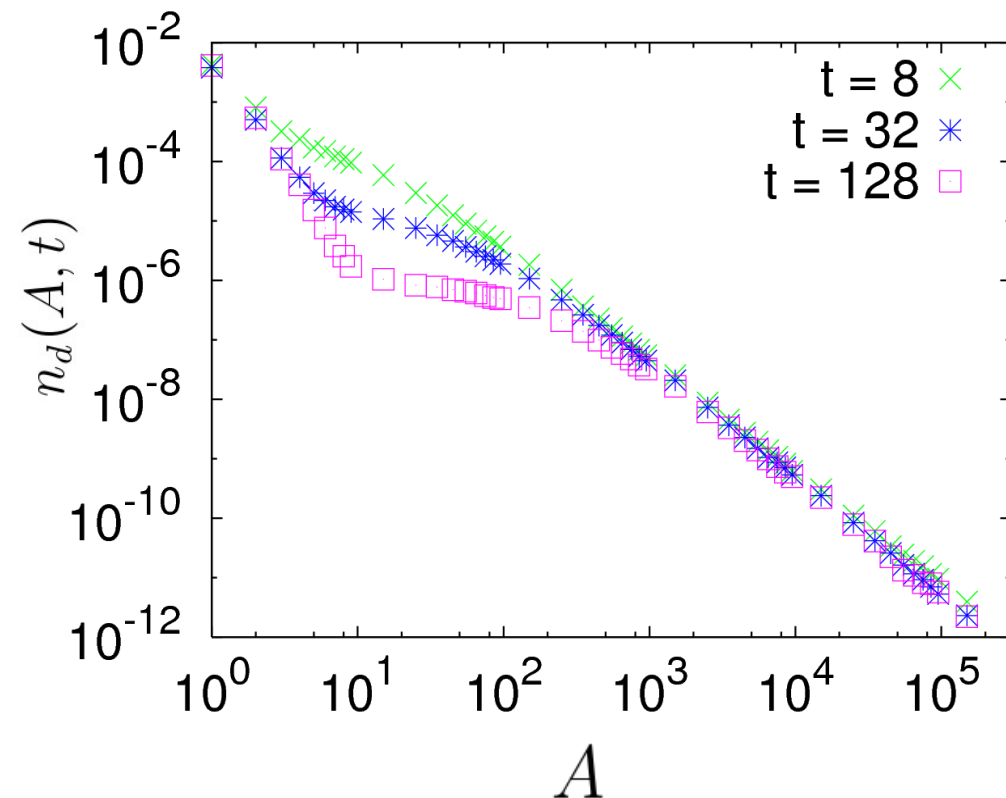
Domain area distributions during coarsening at $T \neq 0$

- Let us test our prediction:

$$n_d(A, t) \sim \frac{2c[\lambda(T)t]^{\tau-2}}{[A+\lambda(T)t]^{\tau}}$$

where $\tau = \frac{187}{91}$ $c = \frac{1}{8\pi\sqrt{3}}$

- Simulations in the 2d Ising Model.

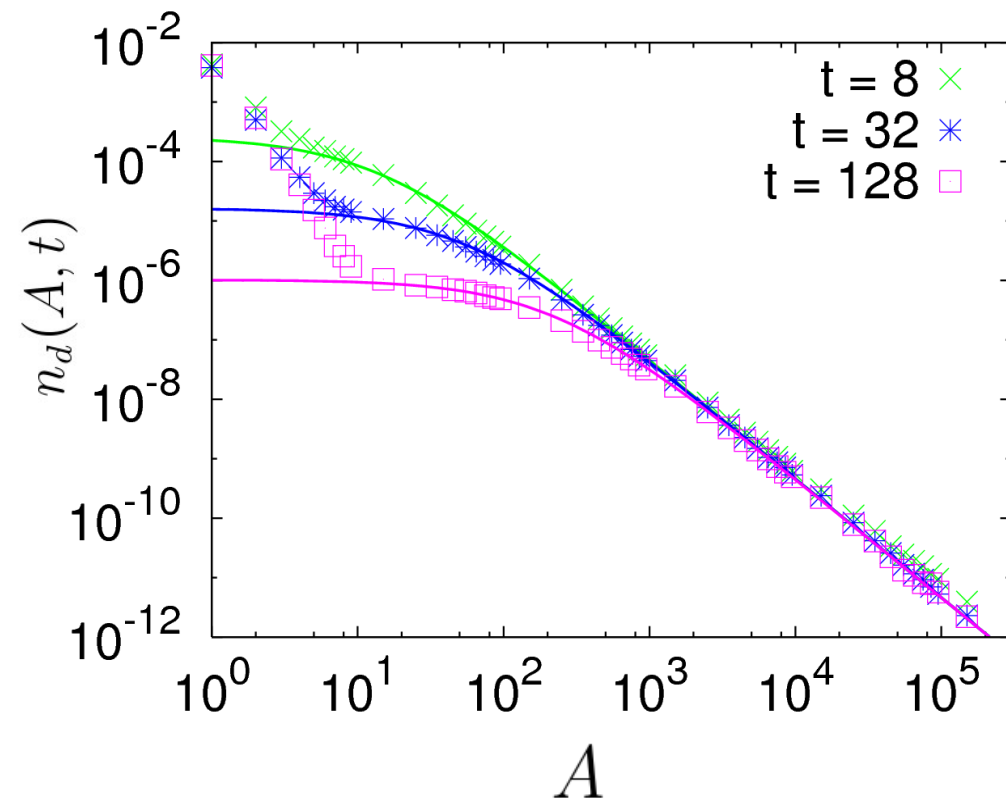


Domain area distributions during coarsening at $T \neq 0$

- Let us test our prediction:

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- Simulations in the 2d Ising Model.



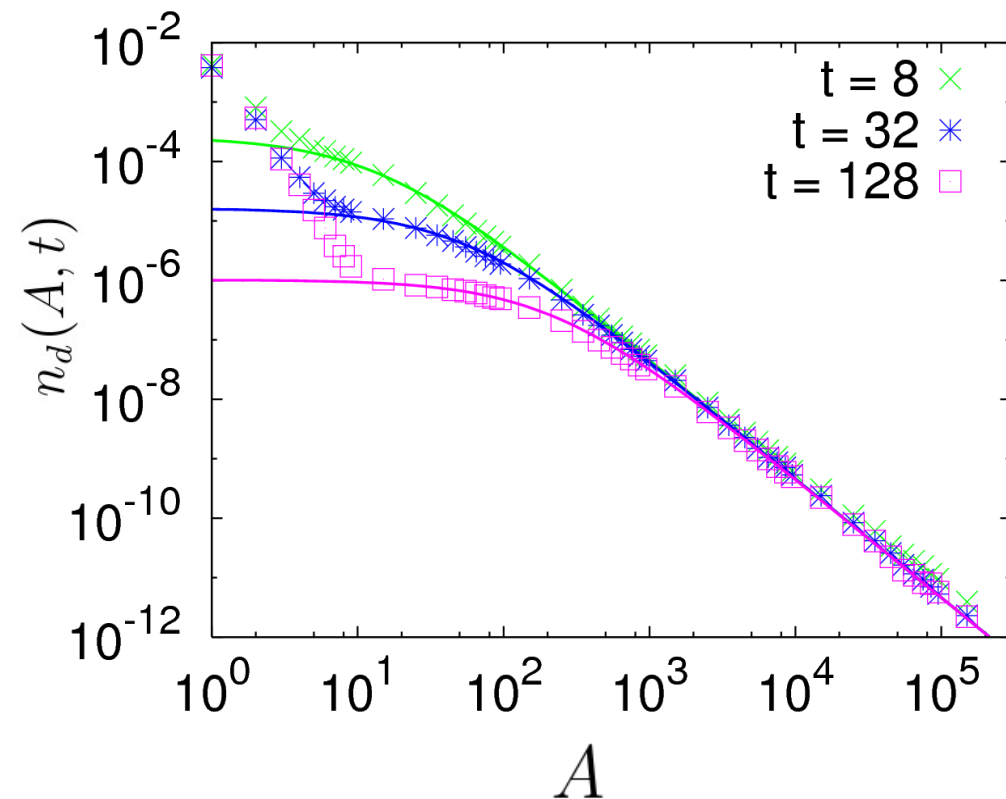
Domain area distributions during coarsening at $T \neq 0$

- Let us test our prediction:

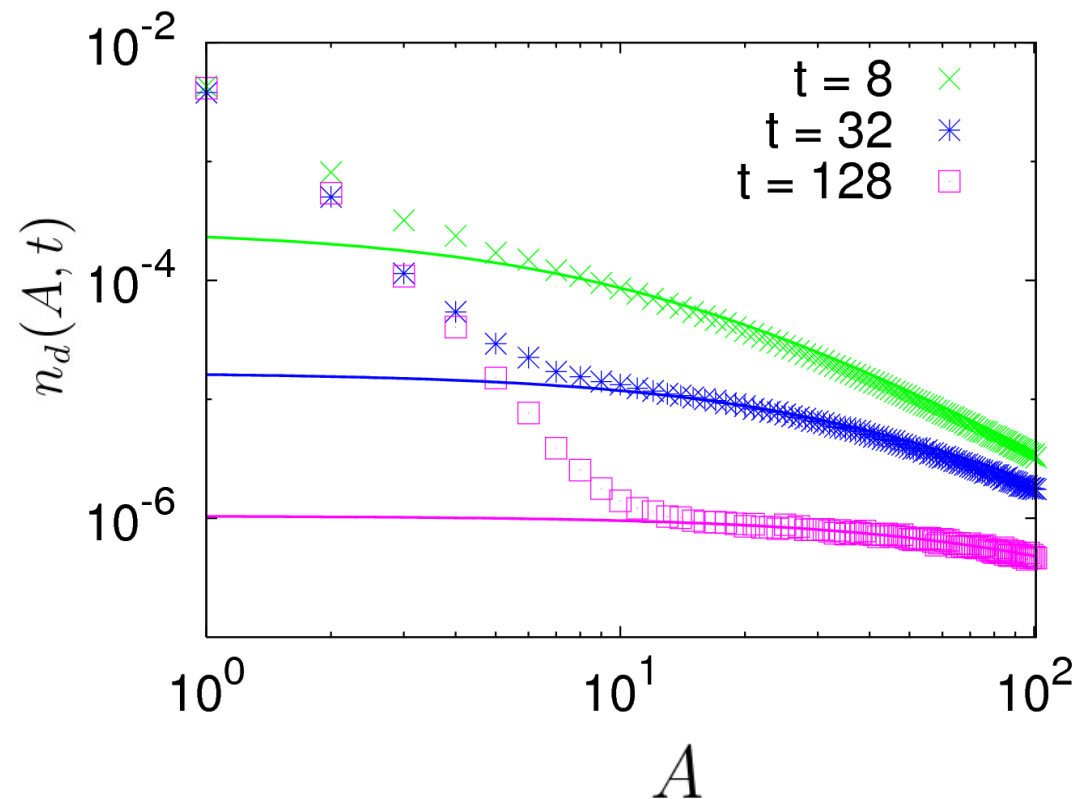
$$n_d(A, t) \sim \frac{2c[\lambda(T)t]^{\tau-2}}{[A + \lambda(T)t]^{\tau}}$$

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- Simulations in the 2d Ising Model.



Zoom on the small domain region:



Crossing a phase transition out of equilibrium

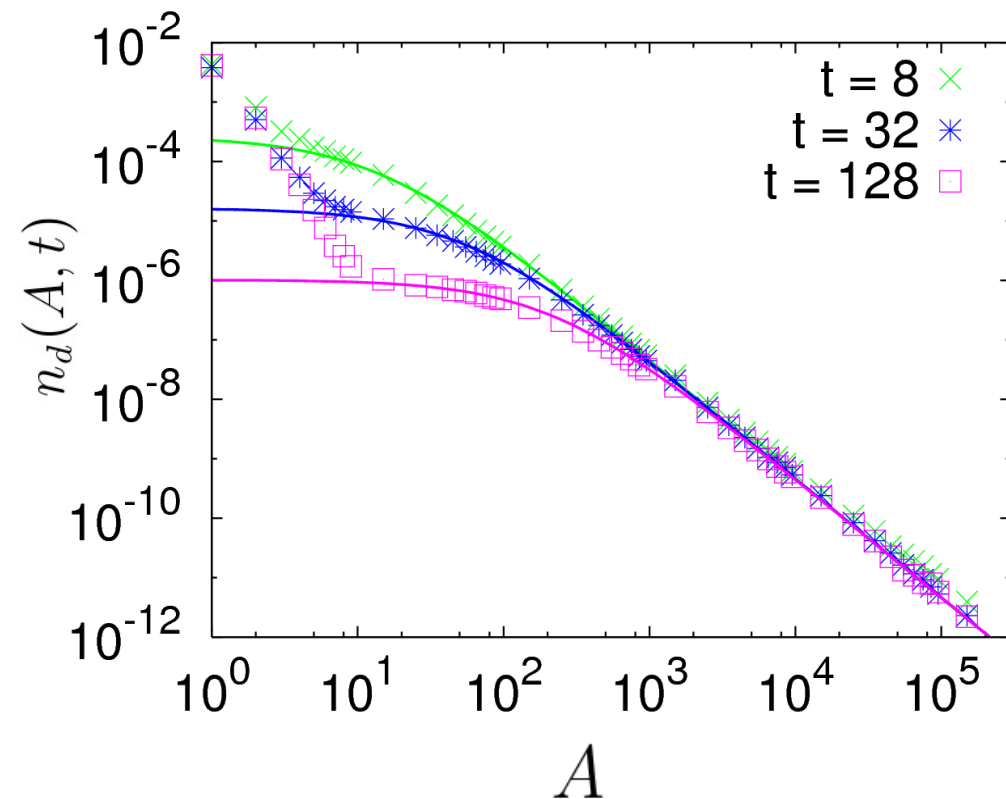
Domain area distributions during coarsening at $T \neq 0$

- Let us test our prediction:

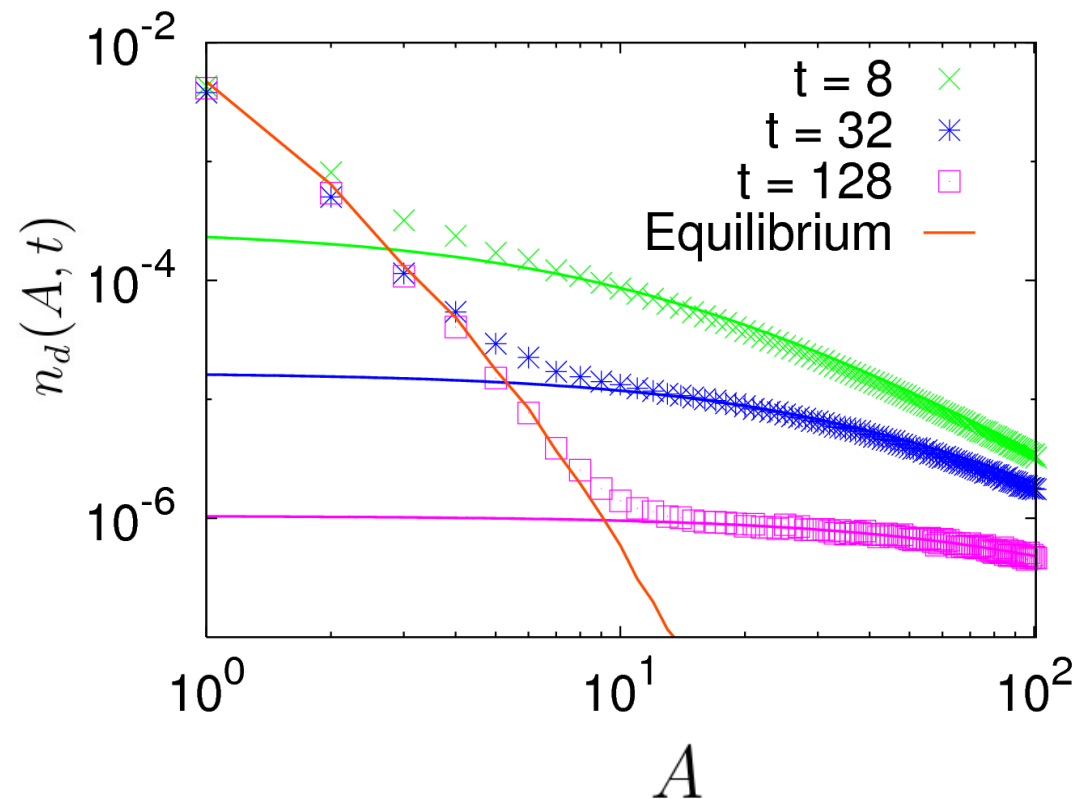
$$n_d(A, t) \sim \frac{2c[\lambda(T)t]^{\tau-2}}{[A + \lambda(T)t]^{\tau}}$$

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- Simulations in the 2d Ising Model.



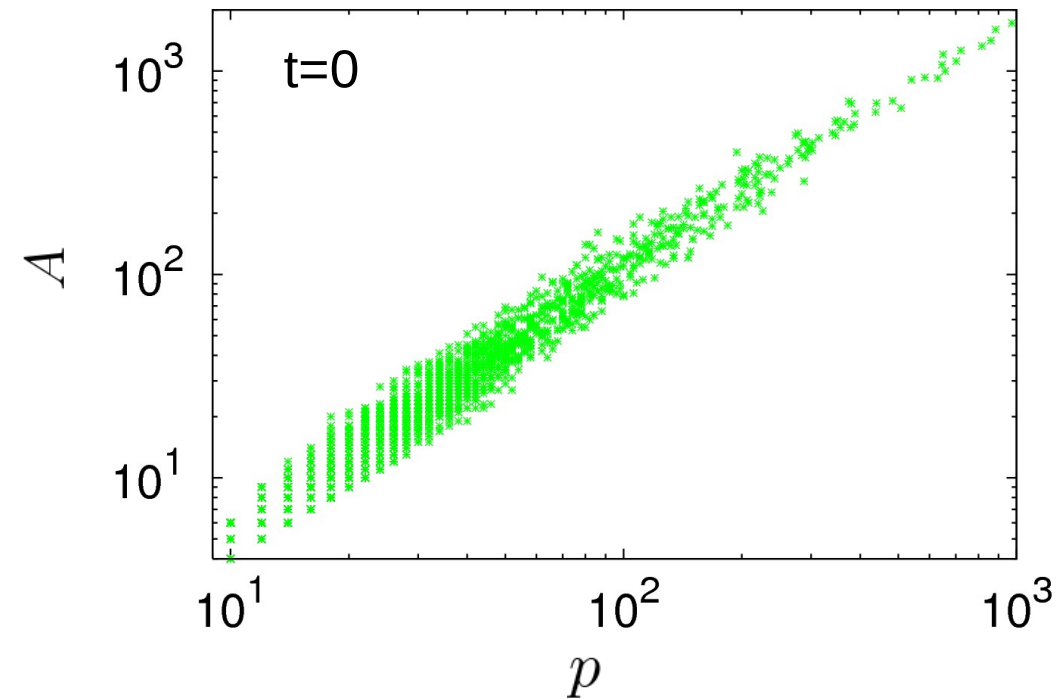
Zoom on the small domain region:



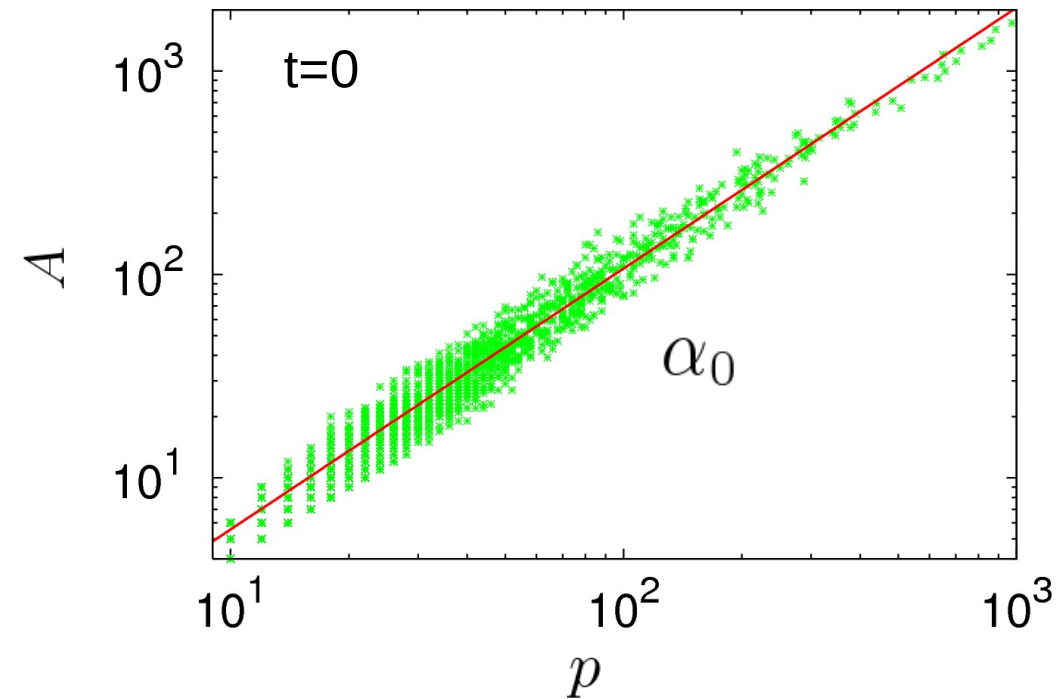
Crossing a phase transition out of equilibrium

Fractal structure of the domains

Domain growth morphology: area vs. perimeter.



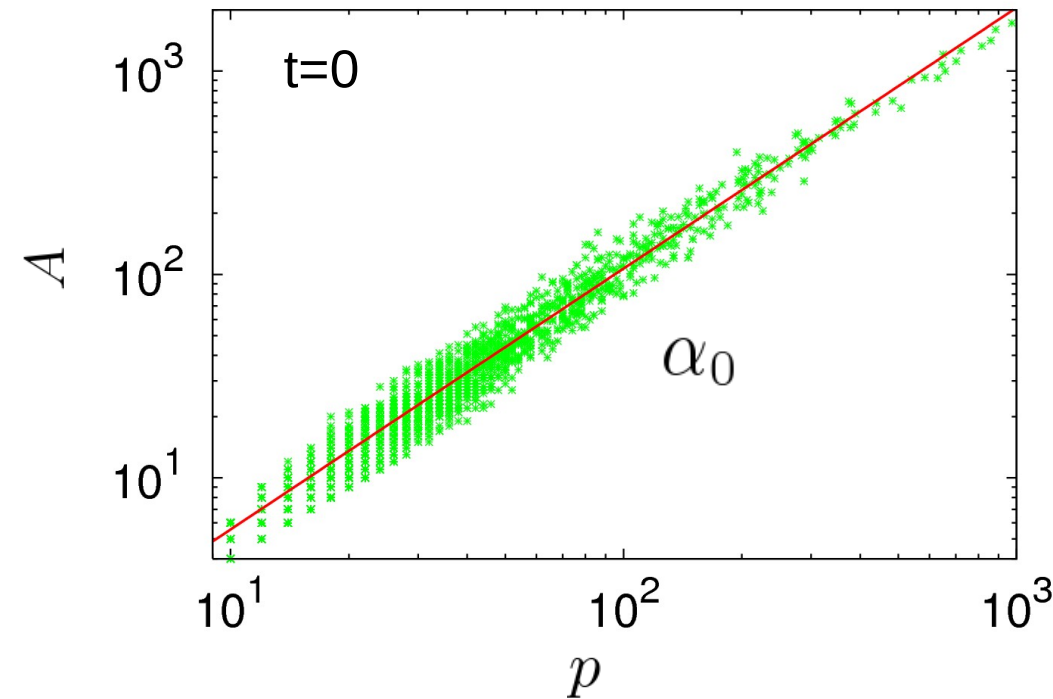
Domain growth morphology: area vs. perimeter.



$$A = c_0 p^{\alpha_0}$$

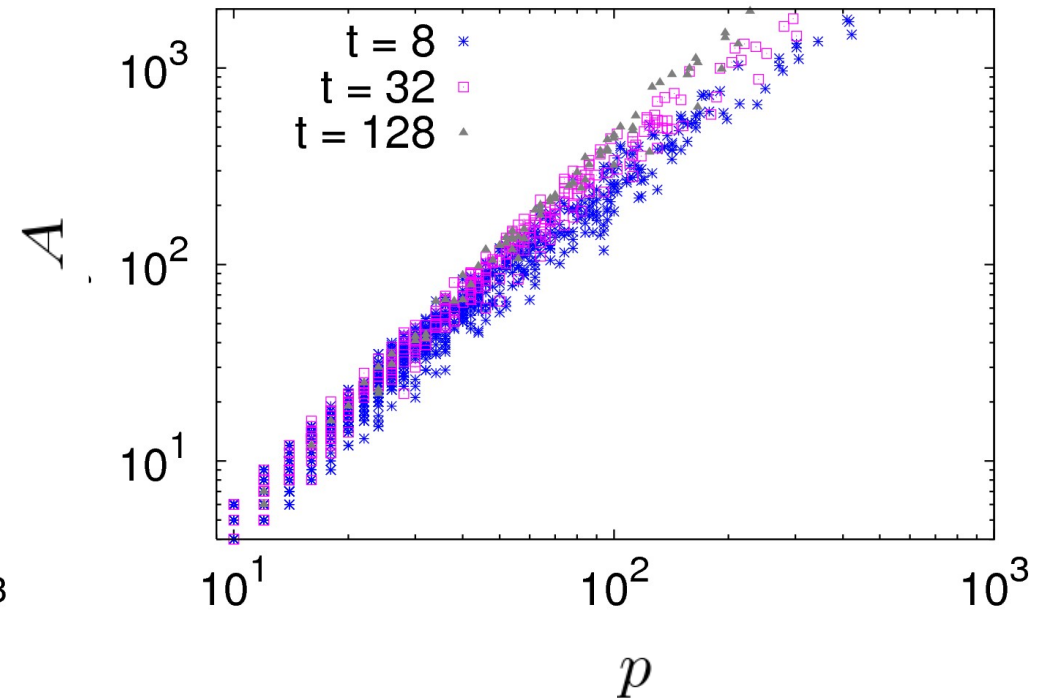
$$\alpha_0 = 1.4$$

Domain growth morphology: area vs. perimeter.

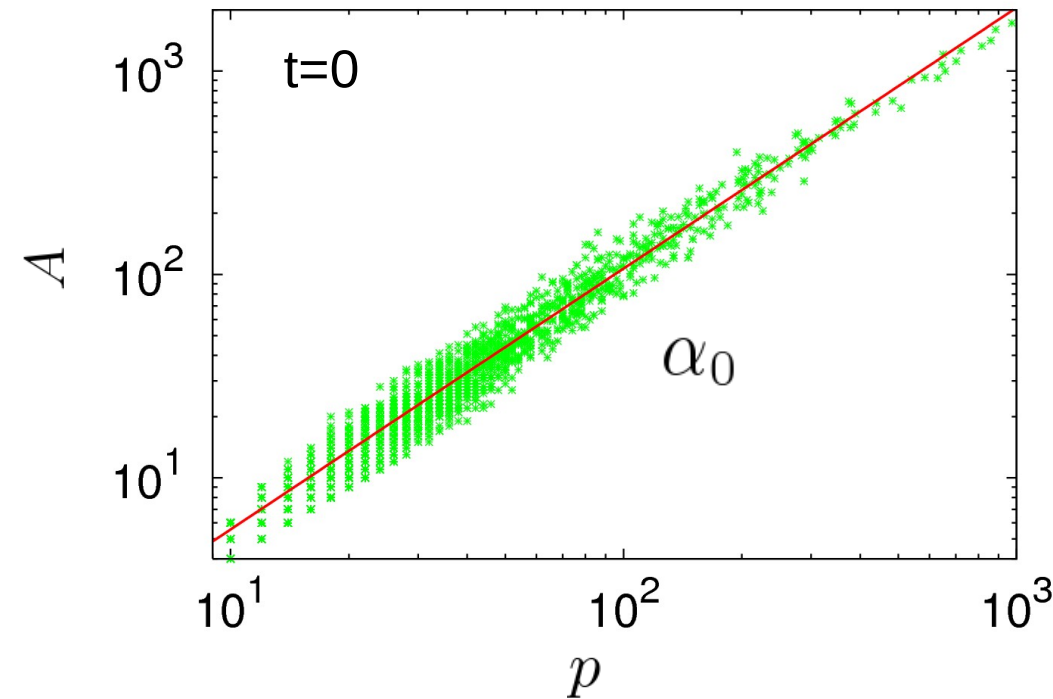


$$A = c_0 p^{\alpha_0}$$

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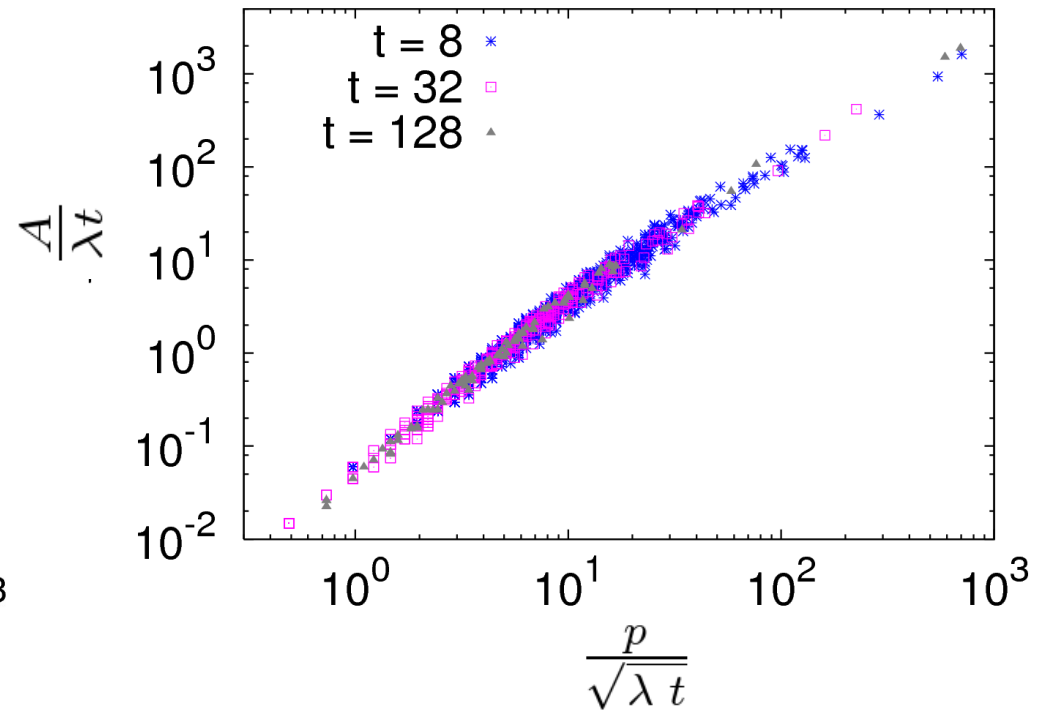


Domain growth morphology: area vs. perimeter.

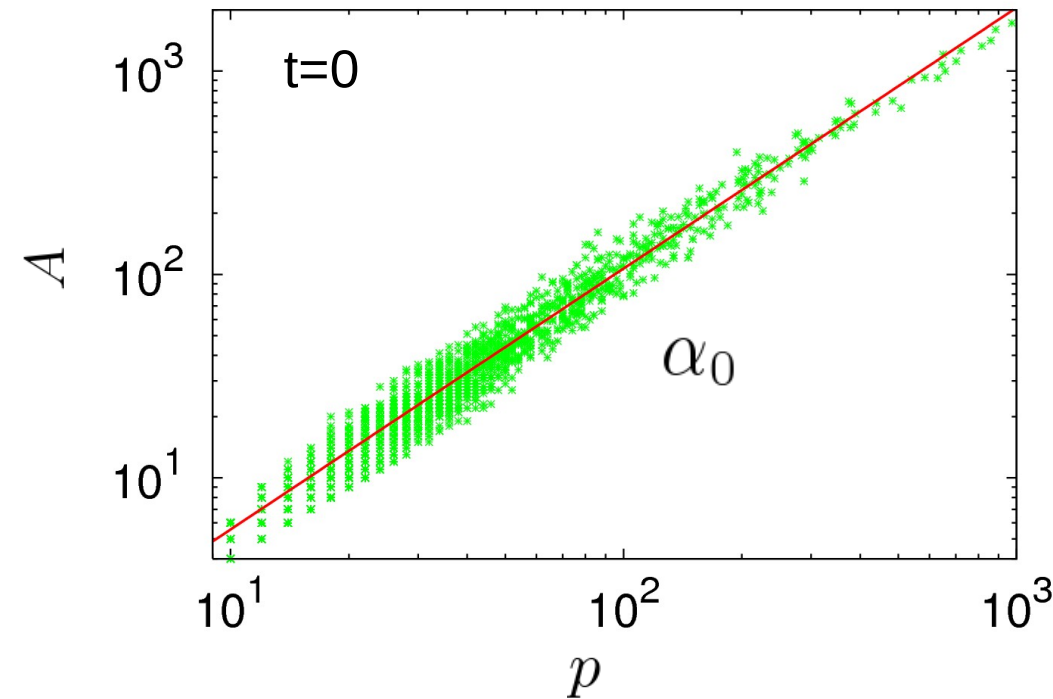


$$A = c_0 p^{\alpha_0}$$

$$\alpha_0 = 1.4$$

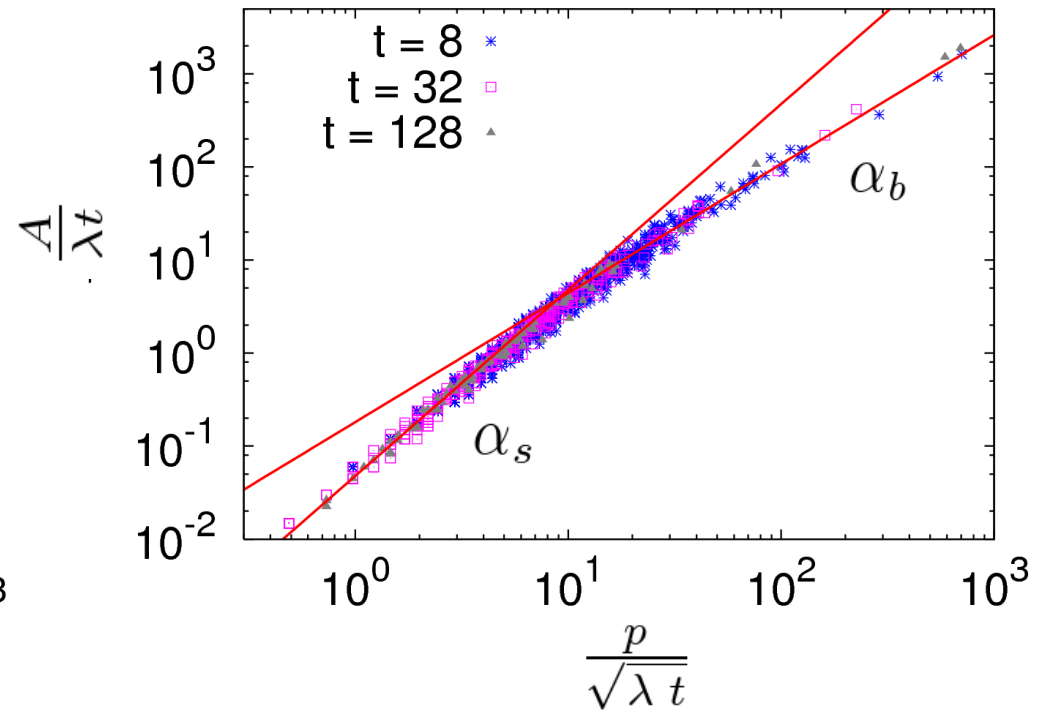


Domain growth morphology: area vs. perimeter.

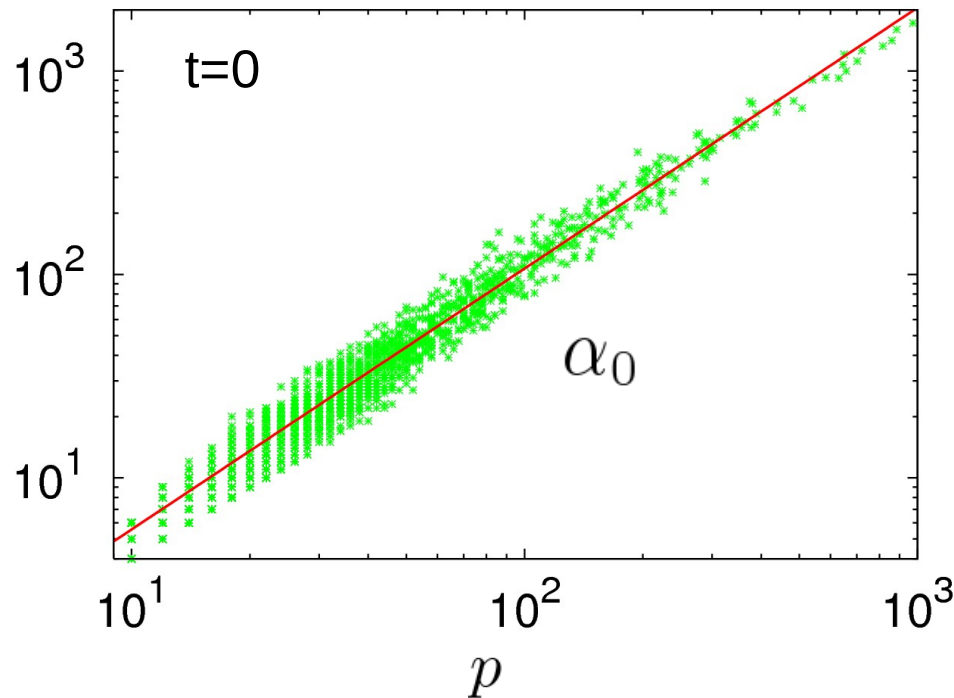


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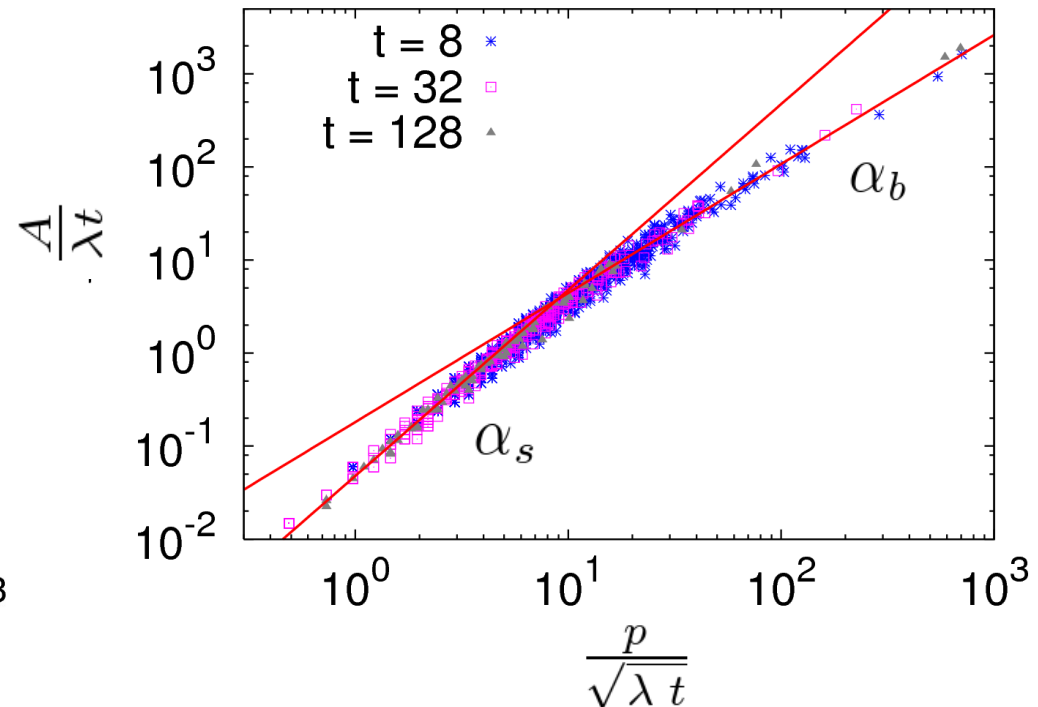


Domain growth morphology: area vs. perimeter.



$$A = c_0 p^{\alpha_0}$$

$$\alpha_0 = 1.4$$



$$\frac{A}{\lambda t} = c_s \left(\frac{p}{\sqrt{\lambda t}} \right)^{\alpha_s} \quad A < A^* \sim \lambda t$$

$$\frac{A}{\lambda t} = c_b \left(\frac{p}{\sqrt{\lambda t}} \right)^{\alpha_b} \quad A > A^* \sim \lambda t$$

$$\alpha_s = 2.0$$

$$\alpha_b = \alpha_0 = 1.4$$

➤ **Regular**

➤ **Fractal** as the initial state

UNROUGHENING TRANSITION!

Crossing a phase transition out of equilibrium

Distributions of domain perimeters

We know

- Distributions of areas
- Relation area - perimeter

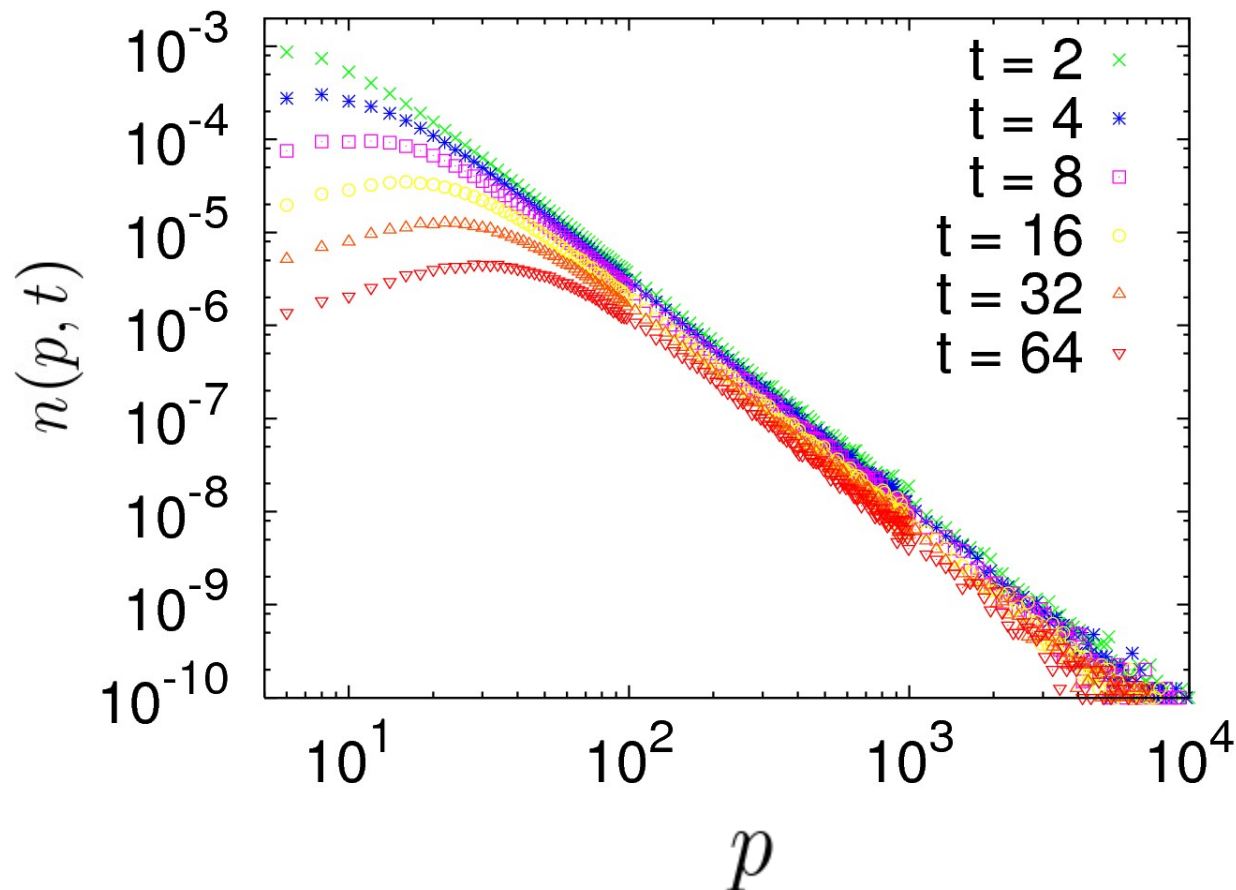
➔ **Distributions of perimeters**

Distributions of domain perimeters

We know

- Distributions of areas
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➔ **Distributions of perimeters**



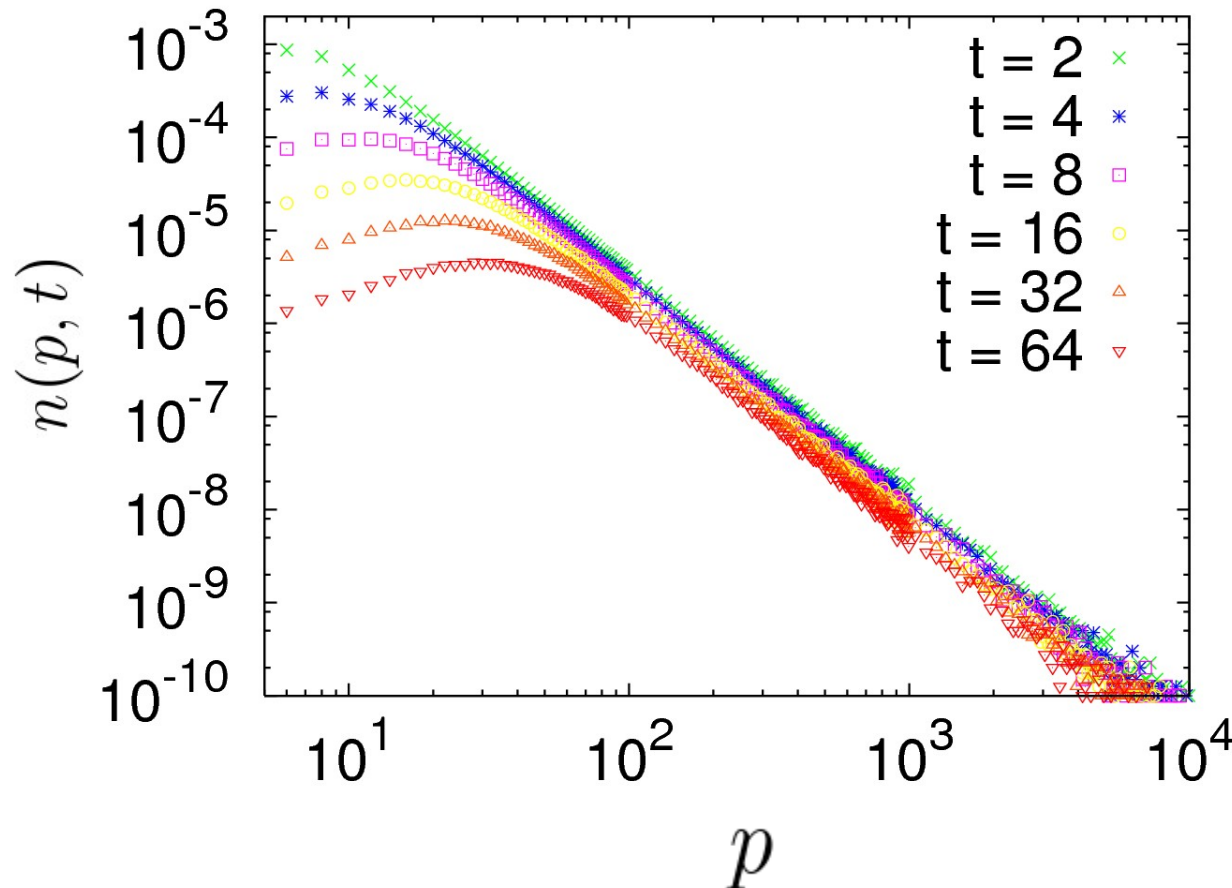
Distributions of domain perimeters

We know

- Distributions of areas
- Relation area - perimeter

➔ **Distributions of perimeters**

$$(\lambda t)^{3/2} n(p, t) = f\left(\frac{p}{\sqrt{\lambda t}}\right)$$

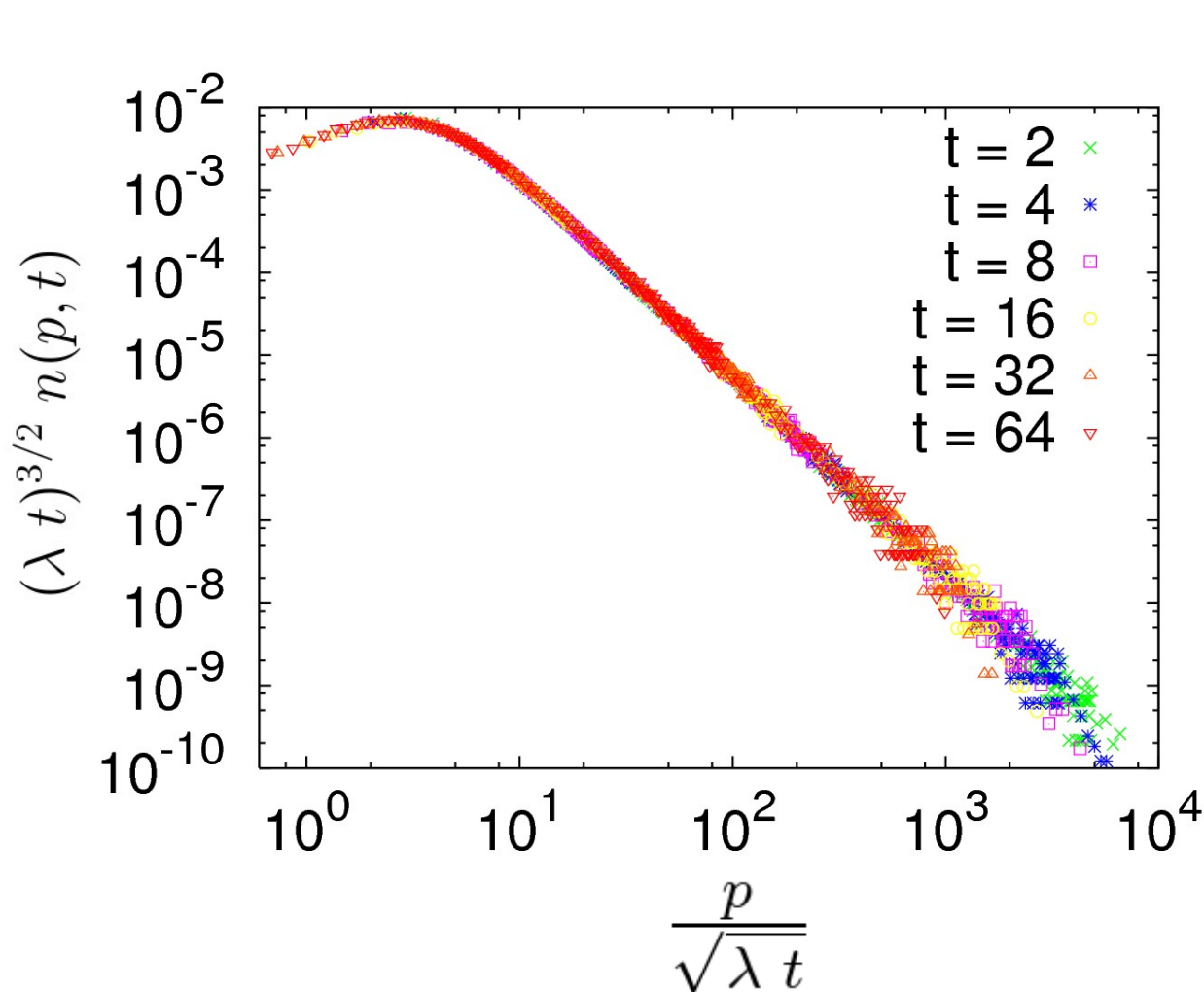


Distributions of domain perimeters

We know

- Distributions of areas
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➔ **Distributions of perimeters**



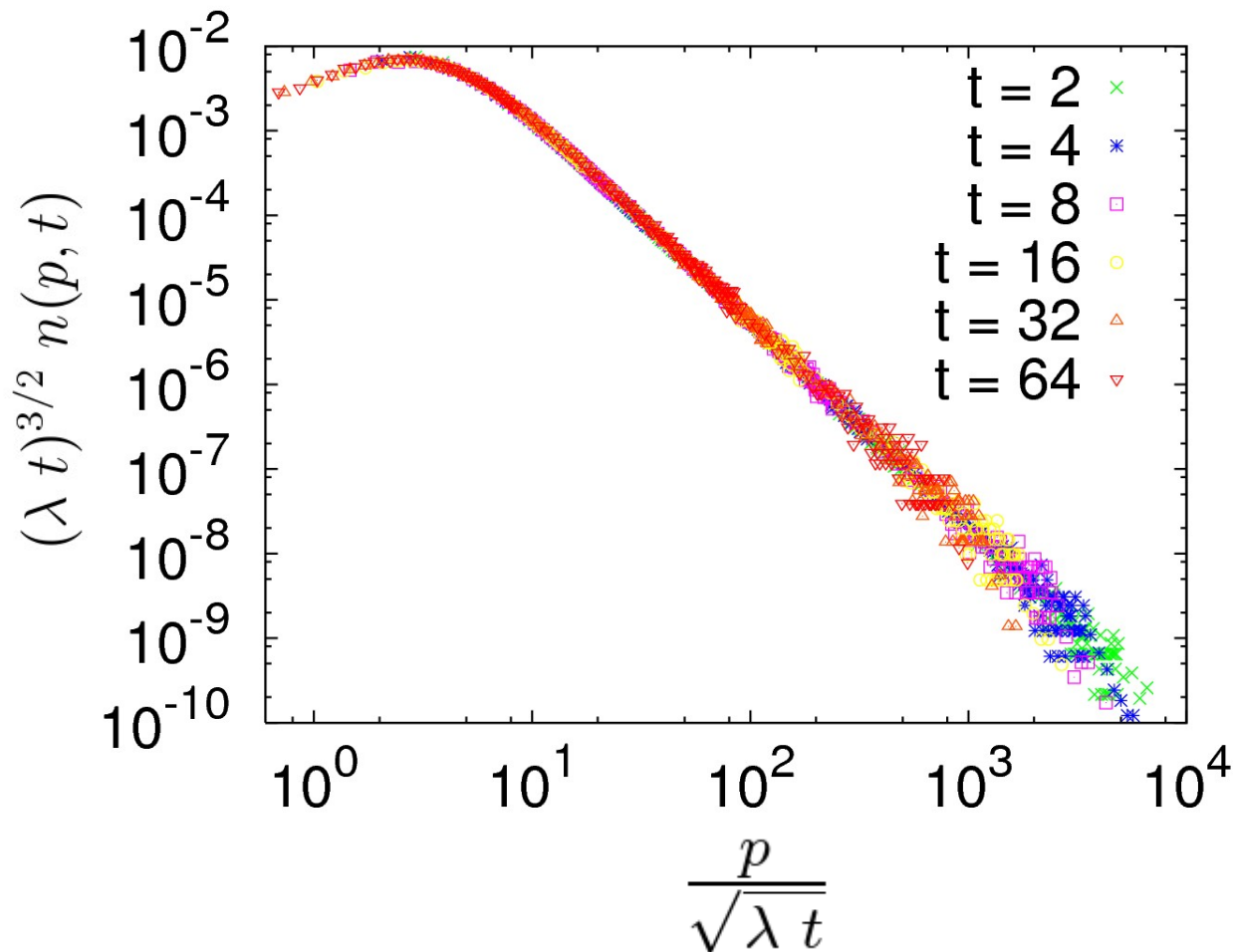
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Distributions of domain perimeters

We know

- Distributions of areas
- Relation area - perimeter

➔ **Distributions of perimeters**



$$(\lambda t)^{3/2} n(p, t) = f\left(\frac{p}{\sqrt{\lambda t}}\right)$$

if $A < A^* \sim \lambda t$

$$f(x) = \frac{\alpha_s c_s c x^{(\alpha_s-1)}}{[1 + c_s x^{\alpha_s}]^\tau}$$

if $A > A^* \sim \lambda t$

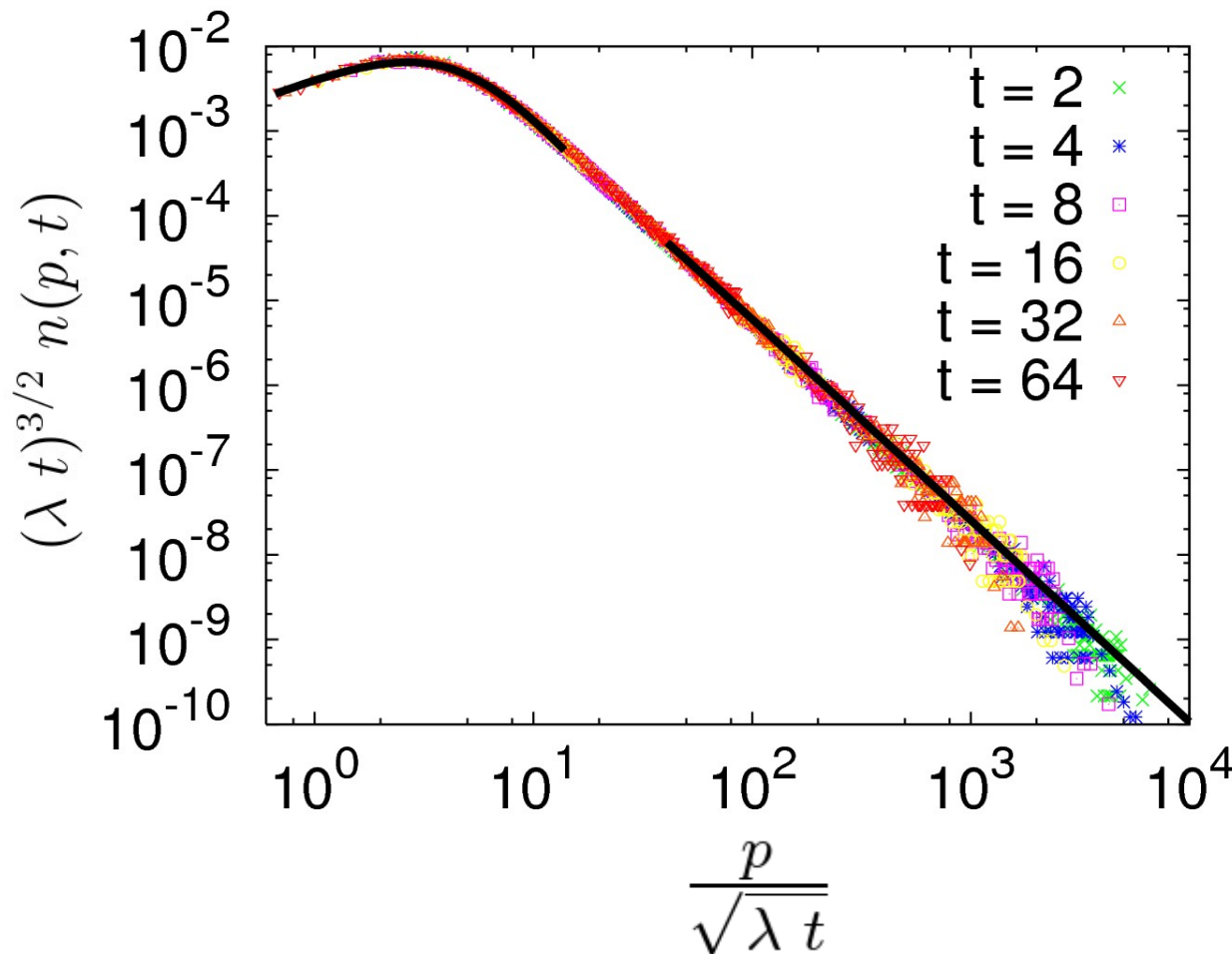
$$f(x) = \frac{\alpha_b c_b c x^{(\alpha_b-1)}}{[1 + c_b x^{\alpha_b}]^\tau}$$

Distributions of domain perimeters

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➔ **Distributions of perimeters**



$$(\lambda t)^{3/2} n(p, t) = f\left(\frac{p}{\sqrt{\lambda t}}\right)$$

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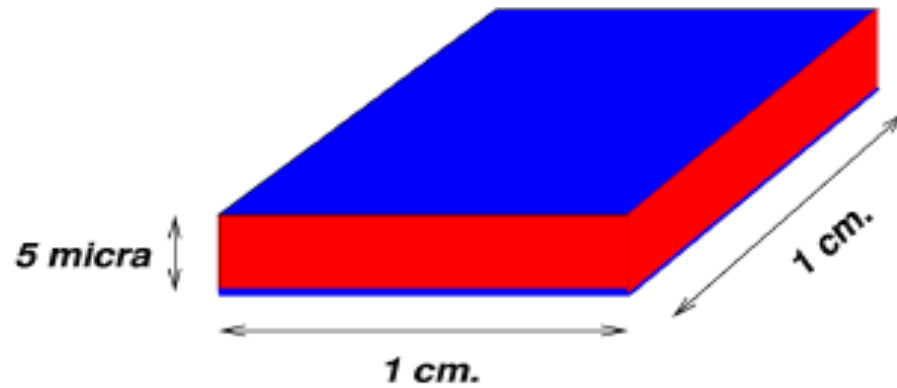
if $A > A^* \sim \lambda t$

$$f(x) = \frac{\alpha_b c_b c x^{(\alpha_b-1)}}{[1 + c_b x^{\alpha_b}]^\tau}$$

Experiments in liquid crystals

Experimental application of our result

- “bent core” liquid crystals.
- Quasi 2-d cell filled with the liquid crystal

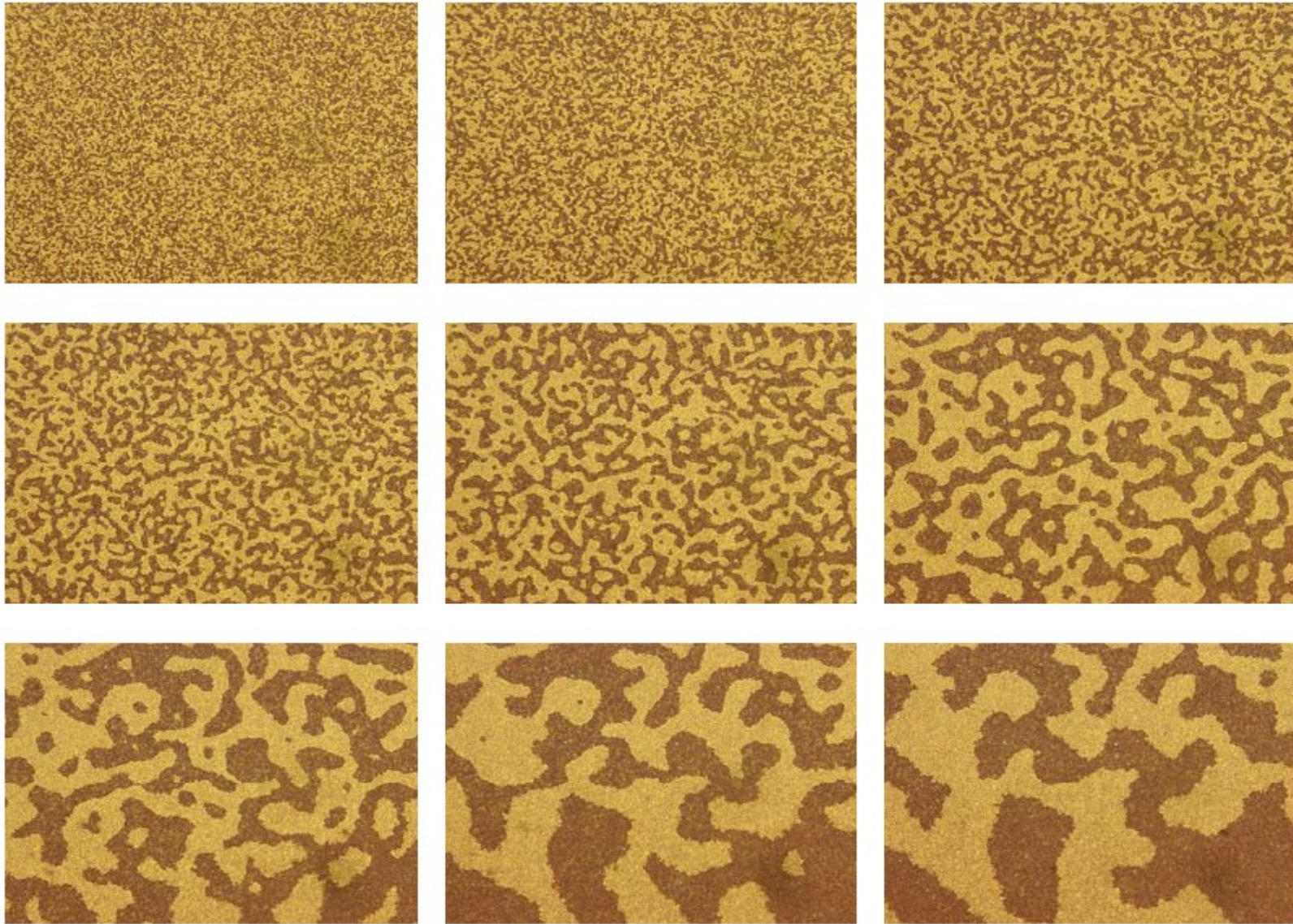


- Application of an electric field $\Rightarrow$ Growth of chiral domains

Right handed domains

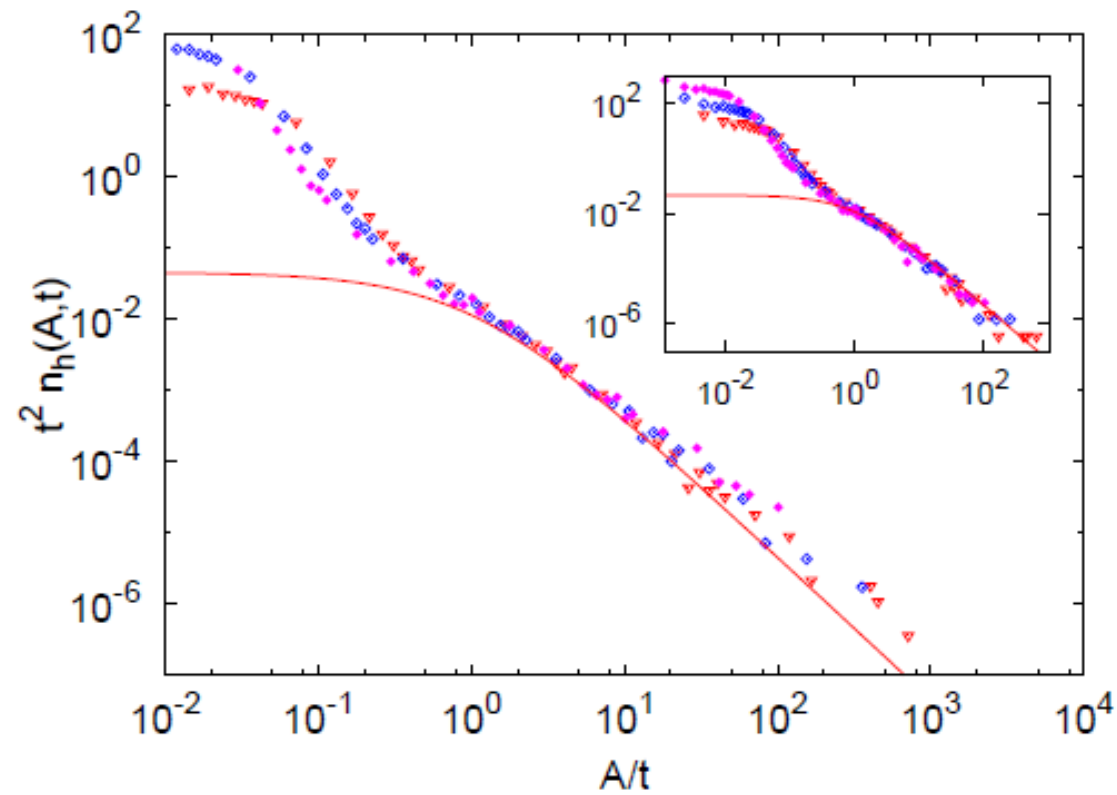
Left handed domains

Experimental application of our result



Crossing a phase transition out of equilibrium

Experimental application of our result



CONCLUSIONS

Conclusions and Future Work

- Proof of Dynamical Scaling Hypothesis in 2D.
- Analytic, Numerical and Experimental results.
- Role played by different initial conditions.
- Role played by the working temperature.
- Geometrical Picture of 2D Coarsening.
- Refs. for the results presented today:
**98, 145701 (2007), PRE 76, 061116 (2007),
82, 10001 (2008), PRL 101, 197801 (2008).**

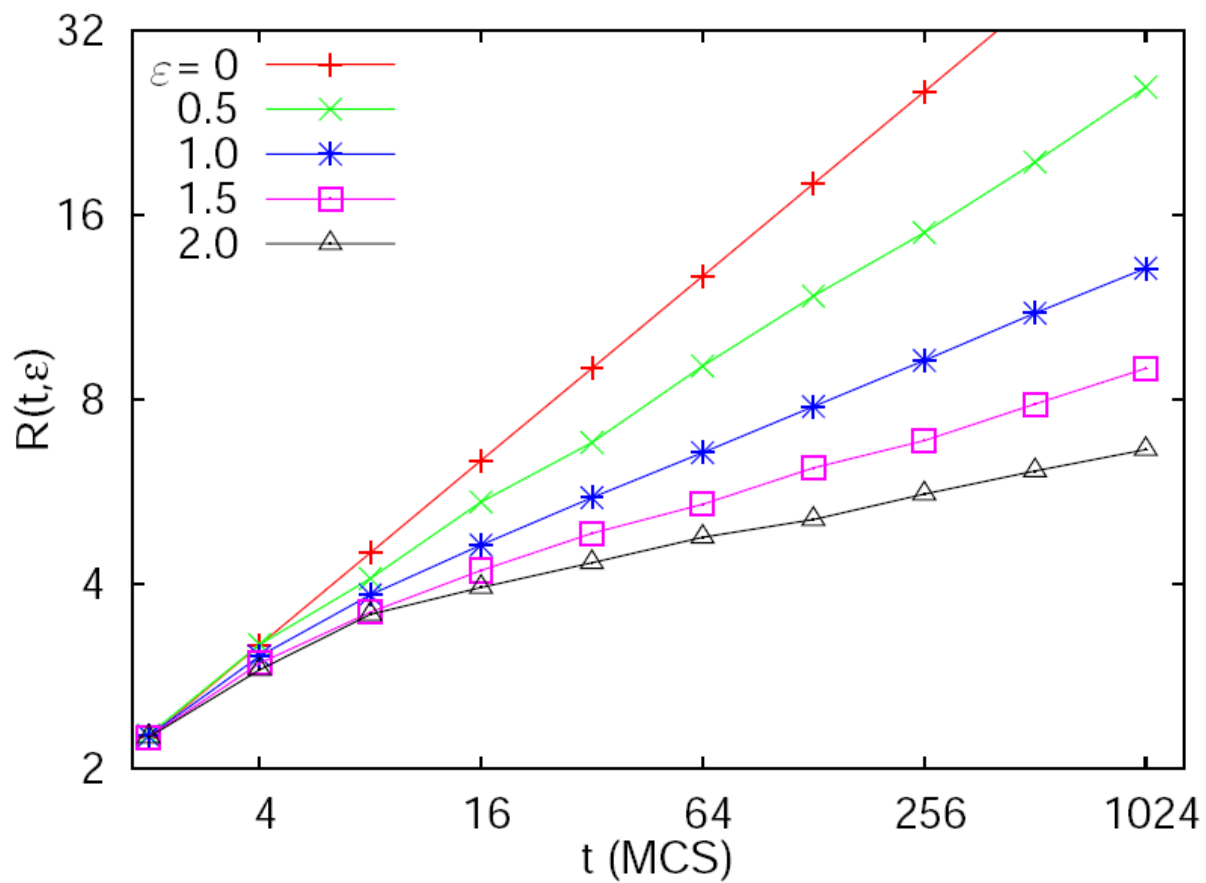
**PRL
EPL**

Effects of weak quenched disorder

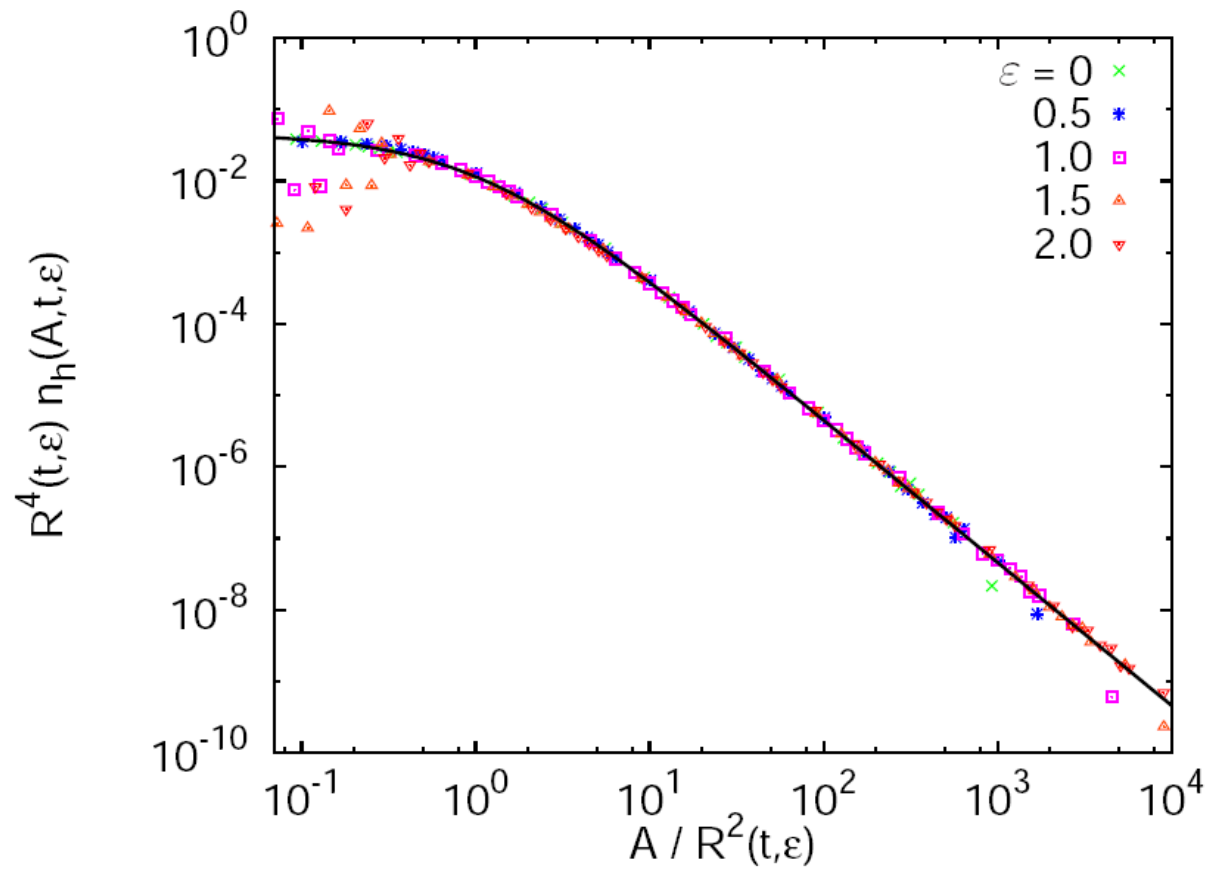
Effects of the disorder

Effects of the disorder

$$J_{ij} = \text{ran} \left[1 - \frac{\epsilon}{2}, 1 + \frac{\epsilon}{2} \right]$$



DISTRIBUTION OF DOMAIN SIZES



DISTRIBUTION OF DOMAIN PERIMETERS

