Quenches across phase transitions: the density of topological defects

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arXiv : 1012.0417 **J. Stat. Mech. P02032 (2011).**

In preparation

ENS March 2014

The problem

Predict the density of topological defects left over after traversing a phase transition with a given speed.

Out of equilibrium relaxation:

the system does not have enough time to equilibrate to new changing conditions.

Theoretical motivation

Cosmology

(Very coarse description, no intention to enter into the details, definitions given later in a simpler case.)

Scenario : Due to its expansion the universe cools down in the course of time, $R(t) \Rightarrow T_{micro}(t)$, and undergoes a number of **phase transitions**.

Modelization : Field-theory with **spontaneous symmetry-breaking** below a critical point.

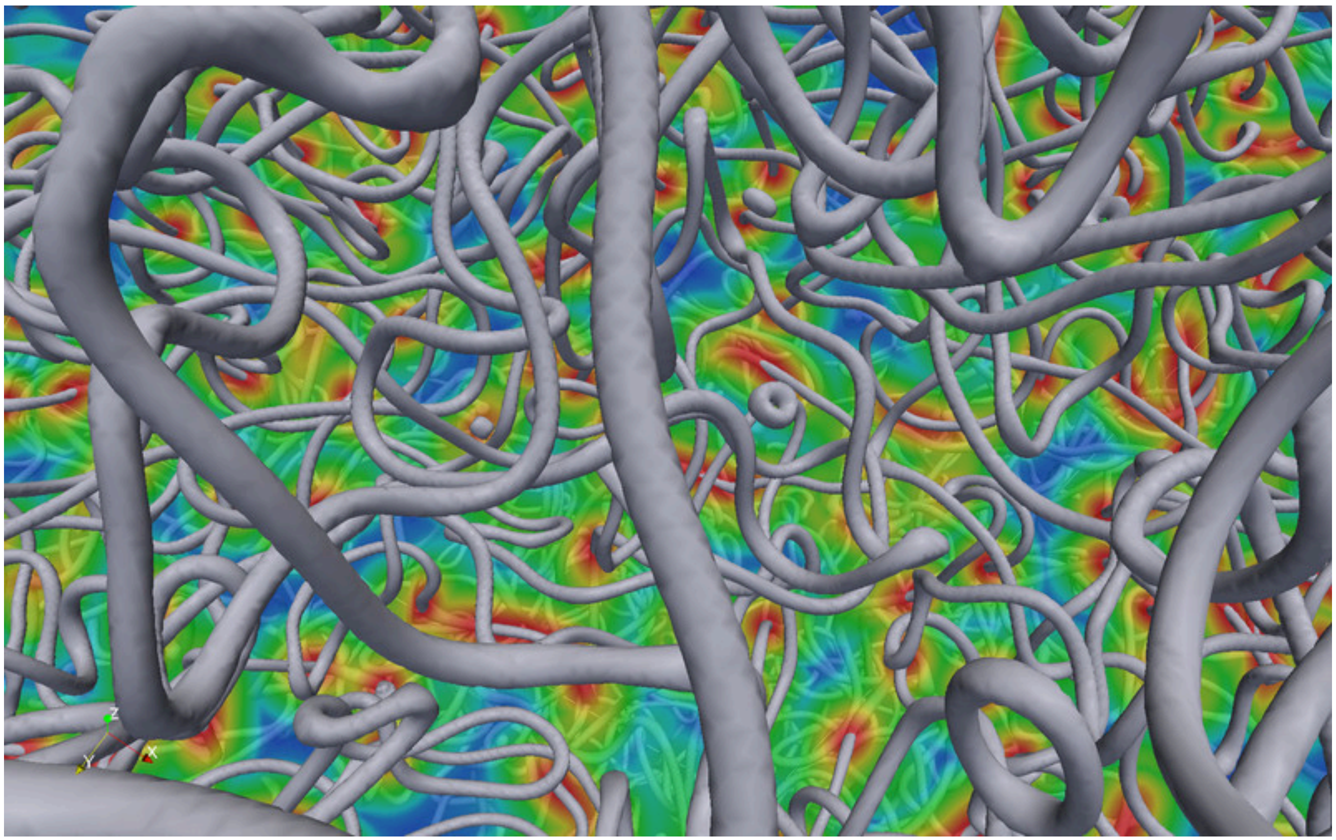
Consequence: The transition is crossed **out of equilibrium** and **topological defects** – depending on the broken symmetry – are left over.

Question: How many? (**network of cosmological strings**)

T. Kibble 76

Theoretical motivation

Network of cosmic strings



They should affect the Cosmic Microwave Background, double quasars, etc.

Picture from M. Kunz’s group (Université de Genève)

Experiments

Condensed matter

(Short summary, no intention to enter into the details either.)

Set-up: Choose a **material** that undergoes the desired **symmetry-breaking** (e.g. the one postulated in the standard cosmological models) and perform the quenching procedure.

Method : Measure, as directly as possible, the **density of topological defects**. (**could be strings**)

Difficulties : Defects are hard to see ; only their possible consequences are observable. Sometimes it is not even clear which is the symmetry that is broken. Only a few orders of magnitude in time can be explored.

W. Zurek 85 ; Les Houches winter school 99 ; T. Kibble Phys. Today 07

Density of topological defects

Kibble-Zurek mechanics for 2nd order phase transitions

The three basic assumptions

- Defects are created close to the critical point.
- Their density in the ordered phase is inherited from the value it takes when the system falls out of equilibrium on the symmetric side of the critical point. It is determined by

  Critical scaling above g_c

- The dynamics in the ordered phase is so slow that it can be neglected.

and one claim

- results are universal.

that we critically revisit within 'thermal' phase transitions

Plan of the talk

Intended as a colloquium ; hopefully clear but not boring

The problem's definition from the statistical physics perspective

- Canonical setting : system and environment.
- Paradigmatic phase transitions with a divergent correlation length :

  second-order paramagnetic – ferromagnetic transition realized by the $d > 1$ **Ising** or $d = 3$ **xy** models.

  Kosterlitz-Thouless disordered – quasi long-range ordered trans.

  realized by the $d = 2$ **xy model**.

- Stochastic dissipative dynamics : $g = T/J$ is the quench parameter.
- What are the topological defects to be counted ?

Plan of the talk

Intended as a colloquium ; hopefully clear but not boring

The analysis

- An instantaneous quench from the symmetric phase:
  - initial condition (a question of length scales) and evolution.
  - Critical dynamics and sub-critical coarsening.
  - Dynamic scaling and the typical ordering length.
- Relation between the growing length and the density of topological defects.
- A slow quench from from the symmetric phase:
  - Dynamic scaling, the typical ordering length, and the density of topological defects.

Correction to the KZ scaling

Open system

Equilibrium statistical mechanics

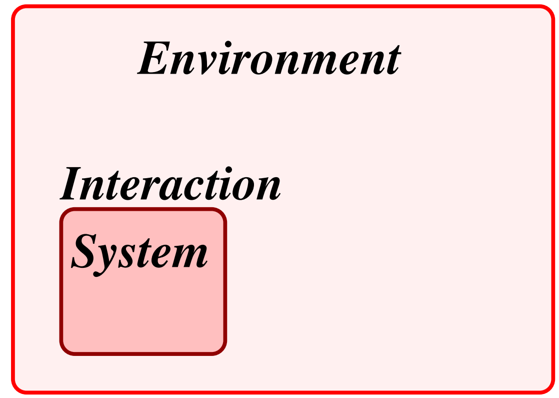
$\mathcal{E} = \mathcal{E}_{syst} + \mathcal{E}_{env} + \mathcal{E}_{int}$

Neglect $\mathcal{E}_{int}$ (short-range interact.)

Much larger environment than system

$\mathcal{E}_{env} \gg \mathcal{E}_{syst}$

Canonical distribution

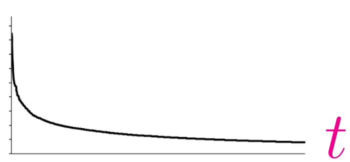


$$P(\{\vec{p}_i, \vec{x}_i\}) \propto e^{-\beta \mathcal{H}(\{\vec{p}_i, \vec{x}_i\})}$$

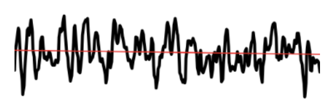
Dynamics

Energy exchange with the environment or thermal bath (dissipation) and thermal fluctuations (noise)

$\mathcal{E}_{syst}(t) \neq$ ct



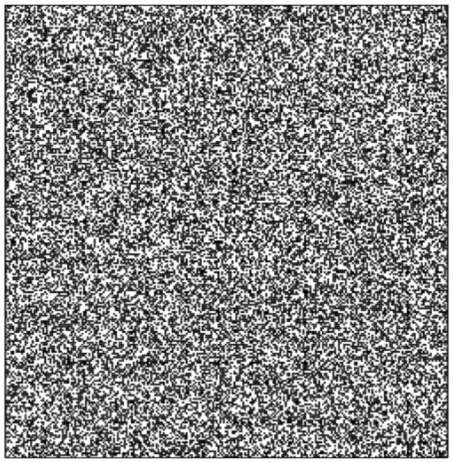
Zoom



Equilibrium configurations

up & down spins in a $2d$ Ising model in MC simulations

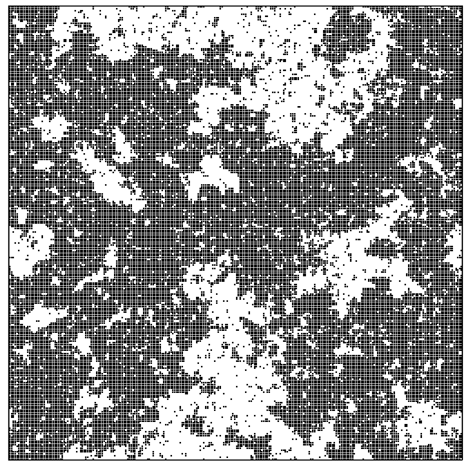
$g \to \infty$



$\langle s_i \rangle_{eq} = 0$

$\phi(\vec{r}) = 0$

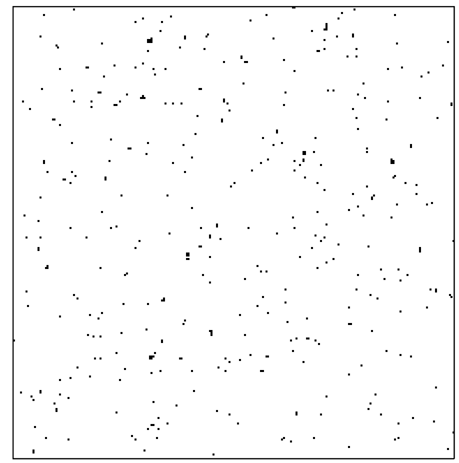
$g = g_c$



$\langle s_i \rangle_{eq} = 0$

$\phi(\vec{r}) = 0$

$g < g_c$



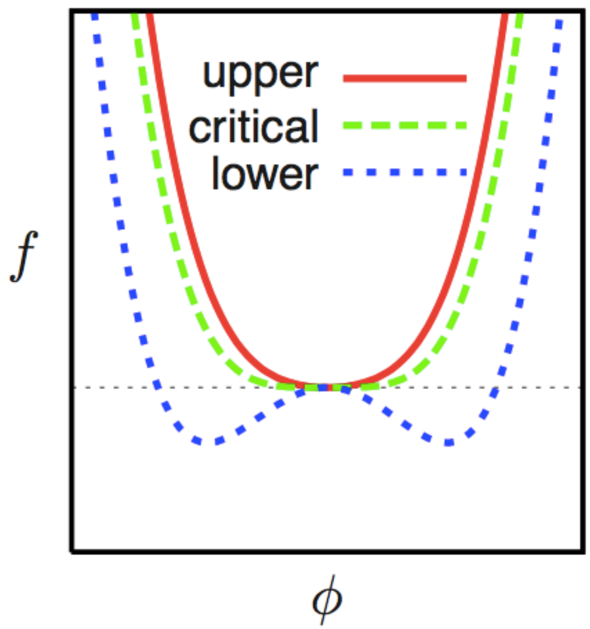
$\langle s_i \rangle_{eq^+} > 0$

$\phi(\vec{r}) > 0$

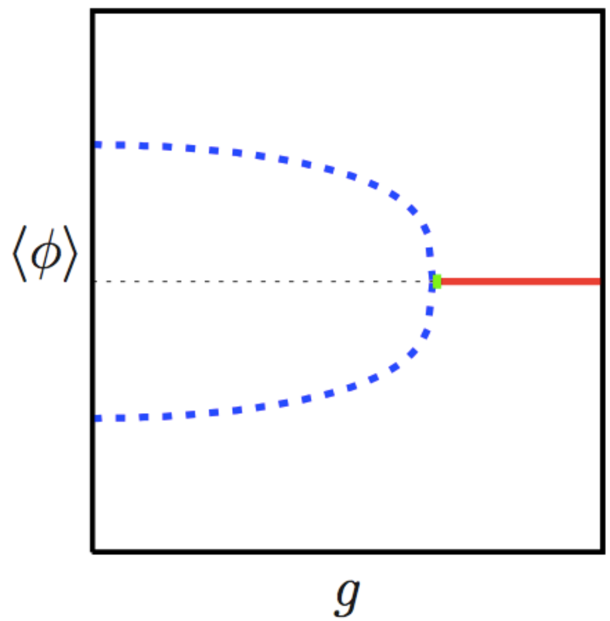
Coarse-grained scalar field $\phi(\vec{r}) \equiv \frac{1}{V_{\vec{r}}} \sum_{i \in V_{\vec{r}}} s_i$

2nd order phase-transition

Continuous phase trans. with spontaneous symmetry breaking



Ginzburg-Landau free-energy



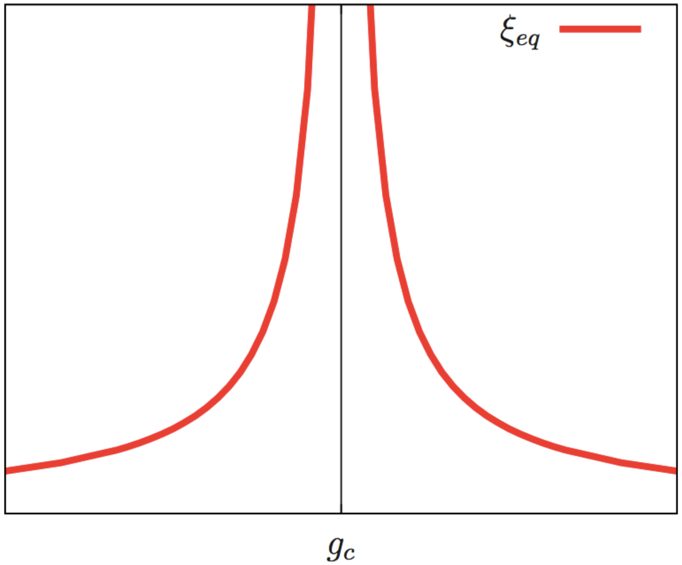
Scalar order parameter

e.g. $g = T/J$ is the control parameter

The correlation length

From the spatial correlations of equilibrium fluctuations

$$C(\vec{r}) = \langle \delta\phi(\vec{r})\delta\phi(\vec{0})\rangle_{eq} \simeq e^{-r/\xi_{eq}(g)}$$



$$\boxed{\xi_{eq}(g) \simeq |g - g_c|^{-\nu} = |\Delta g|^{-\nu}}$$

In KT transitions, ξ_{eq} diverges exponentially on the disordered and it is ∞ in the quasi long-range ordered sides of g_c, e..g. in the $2d$ xy model.

Stochastic dynamics

Open systems

- **Microscopic**: identify the 'smallest' relevant variables in the problem (e.g., the spins) and propose stochastic updates for them as the Monte Carlo or Glauber rules.

- **Coarse-grained**: write down a stochastic differential equation for the field, such as the effective (Markov) Langevin equation

$$\underbrace{m\ddot{\vec{\phi}}(\vec{r},t)}_{\text{Inertia}} + \underbrace{\gamma_0\dot{\vec{\phi}}(\vec{r},t)}_{\text{Dissipation}} = \underbrace{\vec{F}(\vec{\phi})}_{\text{Deterministic}} + \underbrace{\vec{\xi}(\vec{r},t)}_{\text{Noise}}$$

  with $\vec{F}(\vec{\phi}) = -\delta\mathcal{V}(\vec{\phi})/\delta\vec{\phi}$.

  e.g., time-dependent stochastic Ginzburg-Landau equation.

- Stochastic Gross-Pitaevskii equation.

Topological defects

Definition via one example

Exact, locally stable, solutions to non-linear field equations such as

$$\partial_t^2 \phi(\vec{r},t) - \nabla^2 \phi(\vec{r},t) = -\frac{\delta V[\phi(\vec{r},t)]}{\delta \phi(\vec{r},t)} = -r\phi(\vec{r},t) - \lambda \phi^3(\vec{r},t)$$

$r < 0$ with finite localized energy.

$d = 1$ **domain wall**

$$\phi(x,0) \propto \sqrt{\frac{-r}{\lambda}} \tanh\left(\sqrt{\frac{-r}{\lambda}}\, x\right)$$

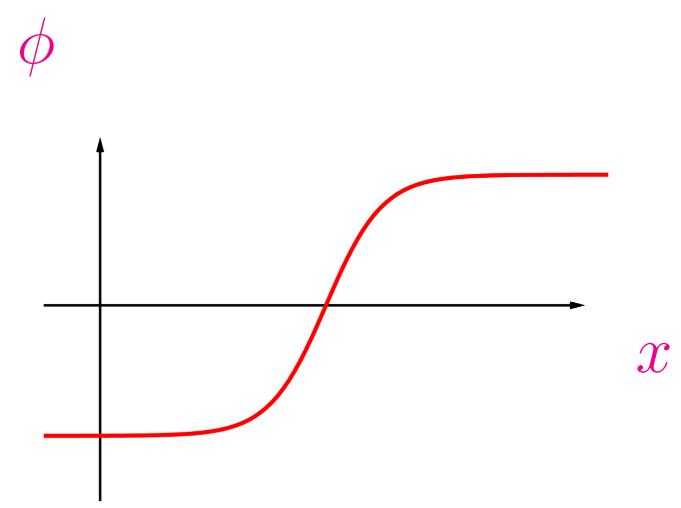
Interface between oppositely ordered

FM regions

Boundary conditions

$$\phi(x \to \infty, 0) = -\phi(x \to -\infty, 0)$$

The field vanishes at the center of the wall



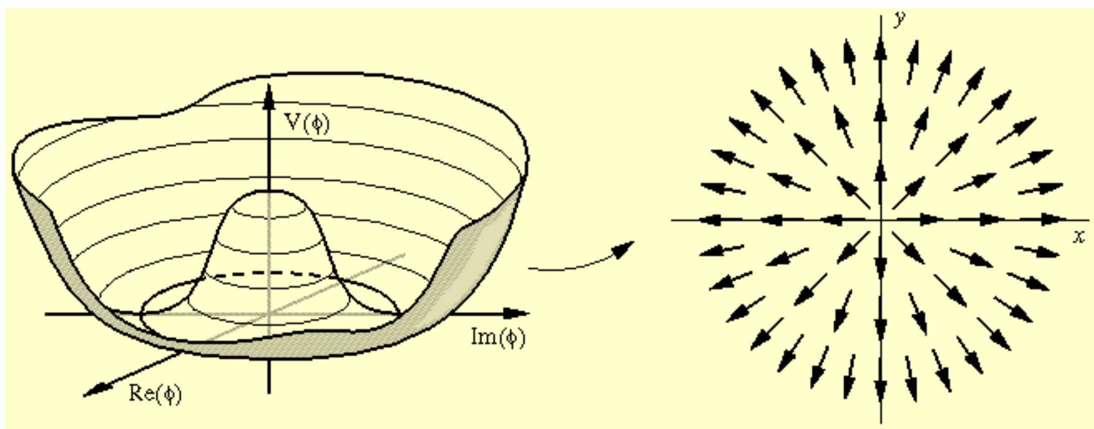
Topological defects

Definition via another example

A vector field

$$\partial_t^2 \vec{\phi}(\vec{r},t) - \nabla^2 \vec{\phi}(\vec{r},t) = -\frac{\delta V[\vec{\phi}(\vec{r},t)]}{\delta \vec{\phi}(\vec{r},t)} = -r\vec{\phi}(\vec{r},t) - \lambda \vec{\phi}(\vec{r},t)\, \phi^2(\vec{r},t)$$

leads to a two or a three dimensional **vortex**

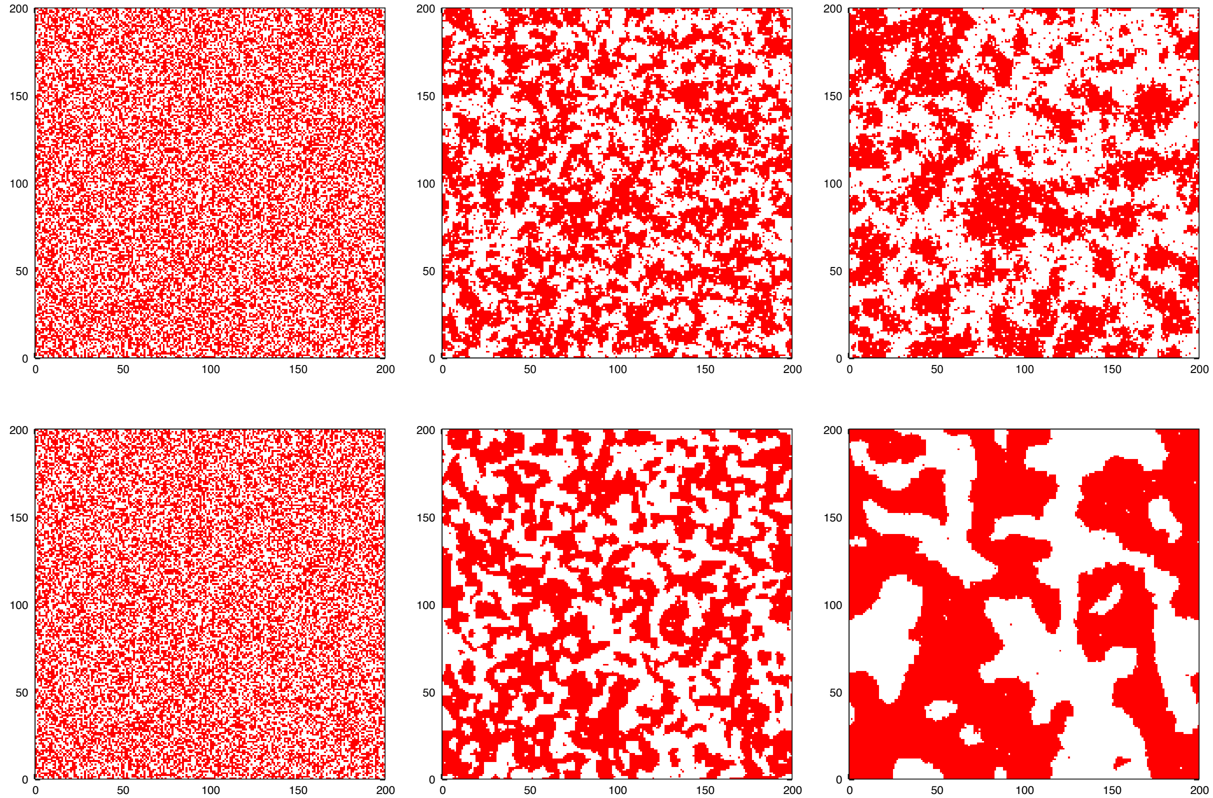


Picture from the Cambridge Cosmology Group webpage

The two-component field turns around a point where it vanishes

$2d$ **Ising model**

Snapshots after an instantaneous quench at $t = 0$



$g_f = g_c$

$g_f < g_c$

At $g_f = g_c$ **critical dynamics** At $g_f < g_c$ **coarsening**.

A certain number of interfaces or domain walls in the last snapshot.

Vortex dynamics

Instantaneously quenched 3d xy model

M. Kobayashi & LFC

Instantaneous quench

Dynamic scaling

very early MC simulations **Lebowitz et al 70s** & experiments

One identifies a **growing linear size of equilibrated patches**

$$\boxed{\mathcal{R}(t,g)}$$

If this is the only length governing the dynamics, the **space-time correlation functions** should scale with $\mathcal{R}(t,g)$ according to

At $g_f = g_c$ $\quad C(r,t) \simeq C_{eq}(r)\ f_c(\frac{r}{\mathcal{R}_c(t)})$

At $g_f < g_c$ $\quad C(r,t) \simeq C_{eq}(r) + f(\frac{r}{\mathcal{R}(t,g)})$

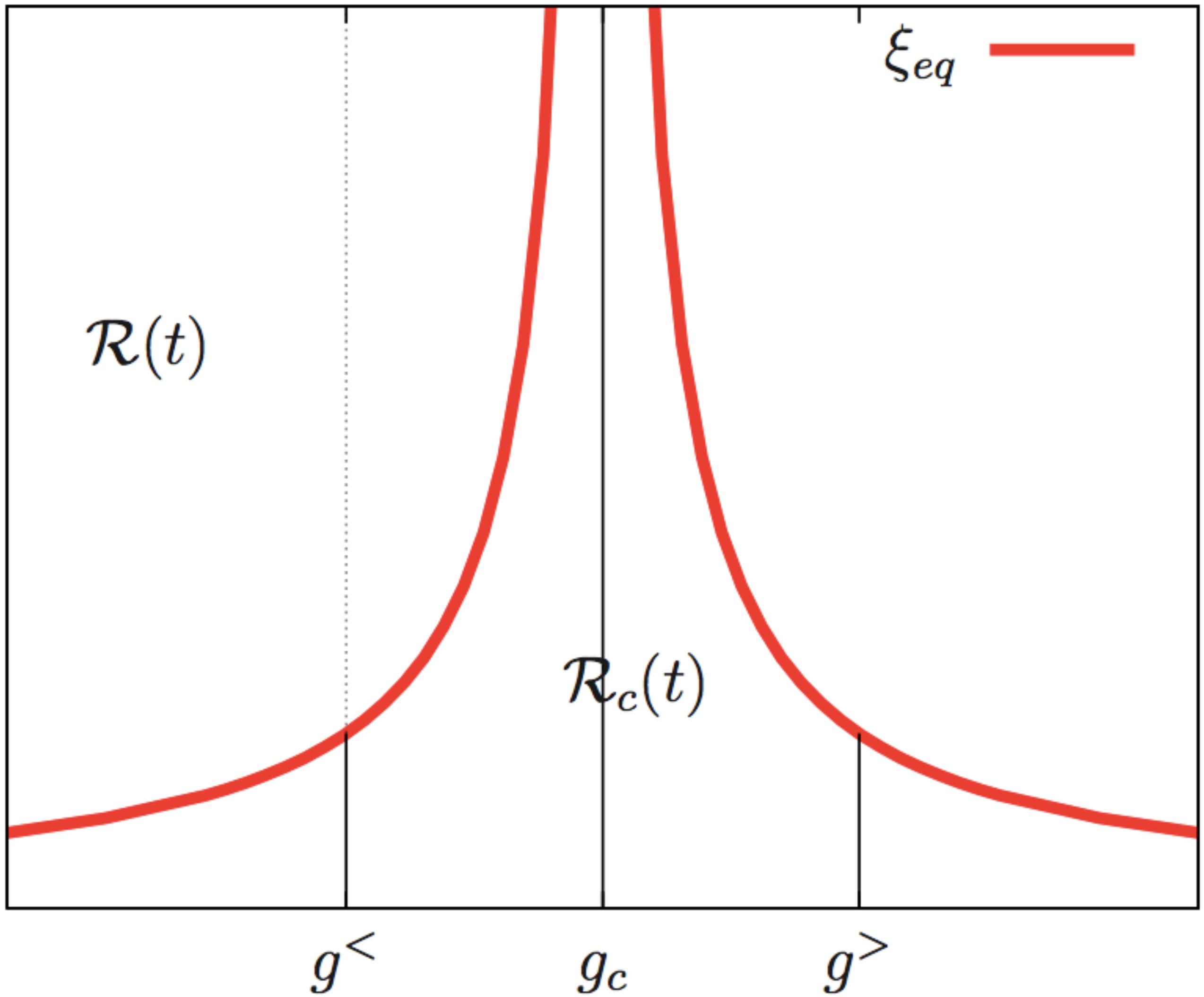
and the number density of topological defects at $g_f < g_c$ as

$$\boxed{n_{inst}(t,g) = \#(t,g)/L^d \simeq [\mathcal{R}(t,g)]^{-d}}$$

Review **Bray 94**

Instantaneous quench

Control of cross-overs



Instantaneous quench to $g_c + \epsilon$

Growth and saturation

The **length** grows and saturates

$$\mathcal{R}(t,g) \simeq \begin{cases} t^{1/z_c} & t \ll \tau_{eq}(g) \\ \xi_{eq}(g) & t \gg \tau_{eq}(g) \end{cases}$$

with $\tau_{eq}(g) \simeq \xi_{eq}^{z_c}(g) \simeq |g - g_c|^{-\nu z_c}$ the equilibrium relaxation time.

Saturation at $t \simeq \tau_{eq}(g)$ when $\boxed{\mathcal{R}(\tau_{eq}(g), g) \simeq \xi_{eq}(g)}$.

z_c is the exponent linking times and lengths in **critical coarsening and equilibrium dynamics** ; e.g. $z_c \simeq 2.17$ **for the 2dIM with NCOP**.

Dynamic RG calculations **Bausch, Schmittmann & Jenssen 80s**.

Instantaneous quench to $g_c - \epsilon$

Control of cross-overs

The **length** grows with different laws

$$\mathcal{R}(t,g) \simeq \begin{cases} t^{1/z_c} & t \ll \tau_{eq} \\ \lambda(g)\, t^{1/z_d} \approx \xi_{eq}^{1-z_c/z_d}(g)\, t^{1/z_d} & t \gg \tau_{eq} \end{cases}$$

with ξ_{eq} and τ_{eq} the equilibrium correlation length and relaxation time.

Crossover at $t \simeq \tau_{eq}(g)$ when $\boxed{\mathcal{R}(\tau_{eq}(g), g) \simeq \xi_{eq}(g)}$

Arenzon, Bray, LFC & Sicilia 08

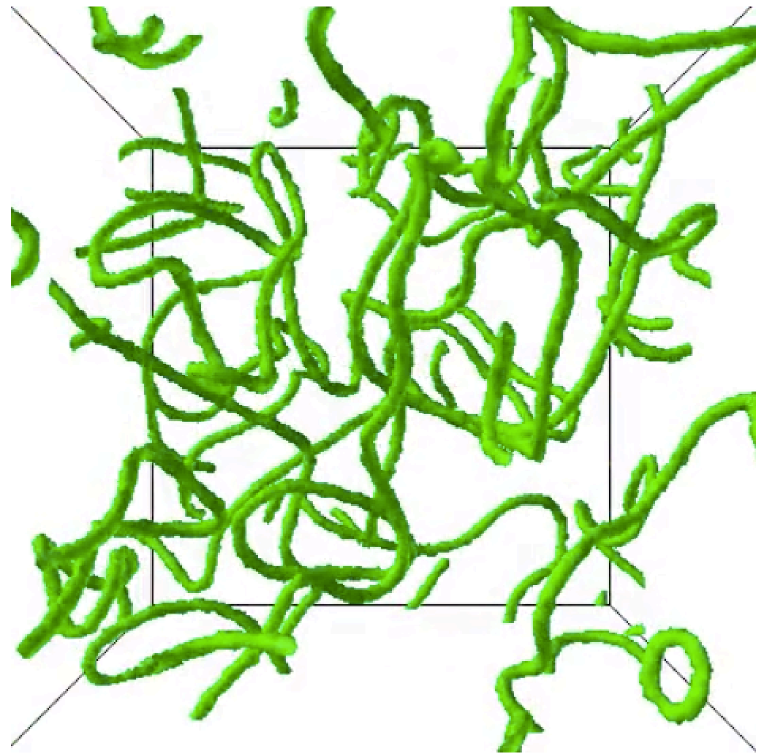
Note that $z_c \geq z_d$

e.g. $z_c \simeq 2.17$ **and** $z_d = 2$ **for the 2dIM with NCOP**

$z_c \simeq 2.13$ **and** $z_d = 2$ **for the 3d xy with NCOP**

Topological defects

instantaneous configurations

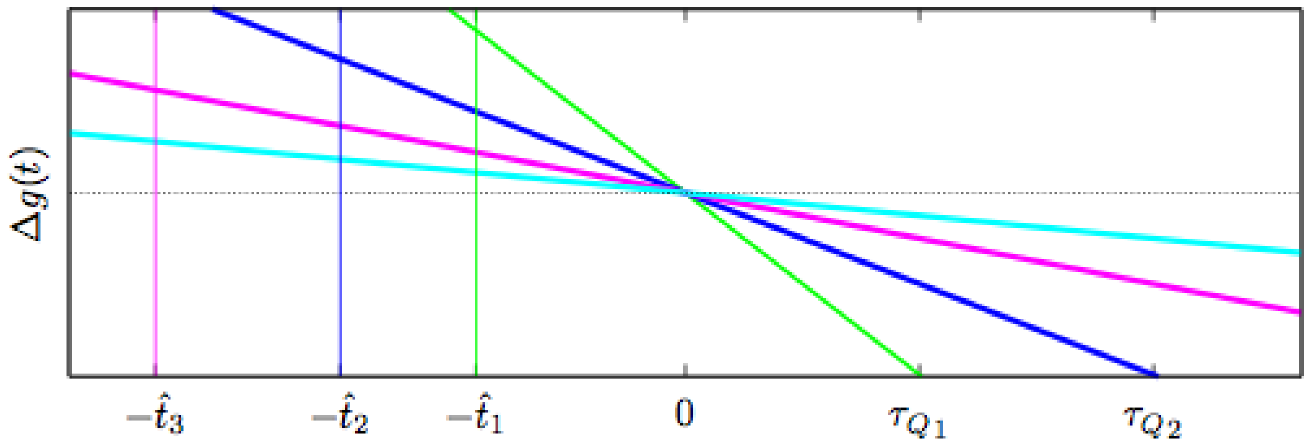


$$\boxed{n_{inst}(t) \simeq [\mathcal{R}(t,g)]^{-d} \simeq [\lambda(g)]^{-d}\, t^{-d/z_d}}$$

Remember the initial ($g \to \infty$) configuration: already there !

Finite rate quenching protocol

How is the scaling modified for a very slow quenching rate ?



$\Delta g \equiv g(t) - g_c = -t/\tau_Q$ with $\tau_{Q_1} < \tau_{Q_2} < \tau_{Q_3} < \tau_{Q_4}$

Standard time parametrization $\boxed{g(t) = g_c - t/\tau_Q}$

Simplicity argument: linear cooling could be thought of as an approximation of any cooling procedure close to g_c.

Zurek's argument

Slow quench from equilibrium well above g_c

The system follows the pace imposed by the changing conditions, $\Delta g(t) = -t/\tau_Q$, until a time $-\hat{t} < 0$ (or value of the control parameter $\hat{g} > g_c$) at which its dynamics are too slow to accommodate to the new rules. The system **falls out of equilibrium**.

$-\hat{t}$ is estimated as the moment when the relaxation time, τ_{eq}, is of the order of the typical time-scale over which the control parameter, g, changes :

$$\tau_{eq}(g) \simeq \left. \frac{\Delta g}{d_t \Delta g} \right|_{-\hat{t}} \simeq \hat{t} \qquad \Rightarrow \qquad \boxed{\hat{t} \simeq \tau_Q^{\nu z_c/(1+\nu z_c)}}$$

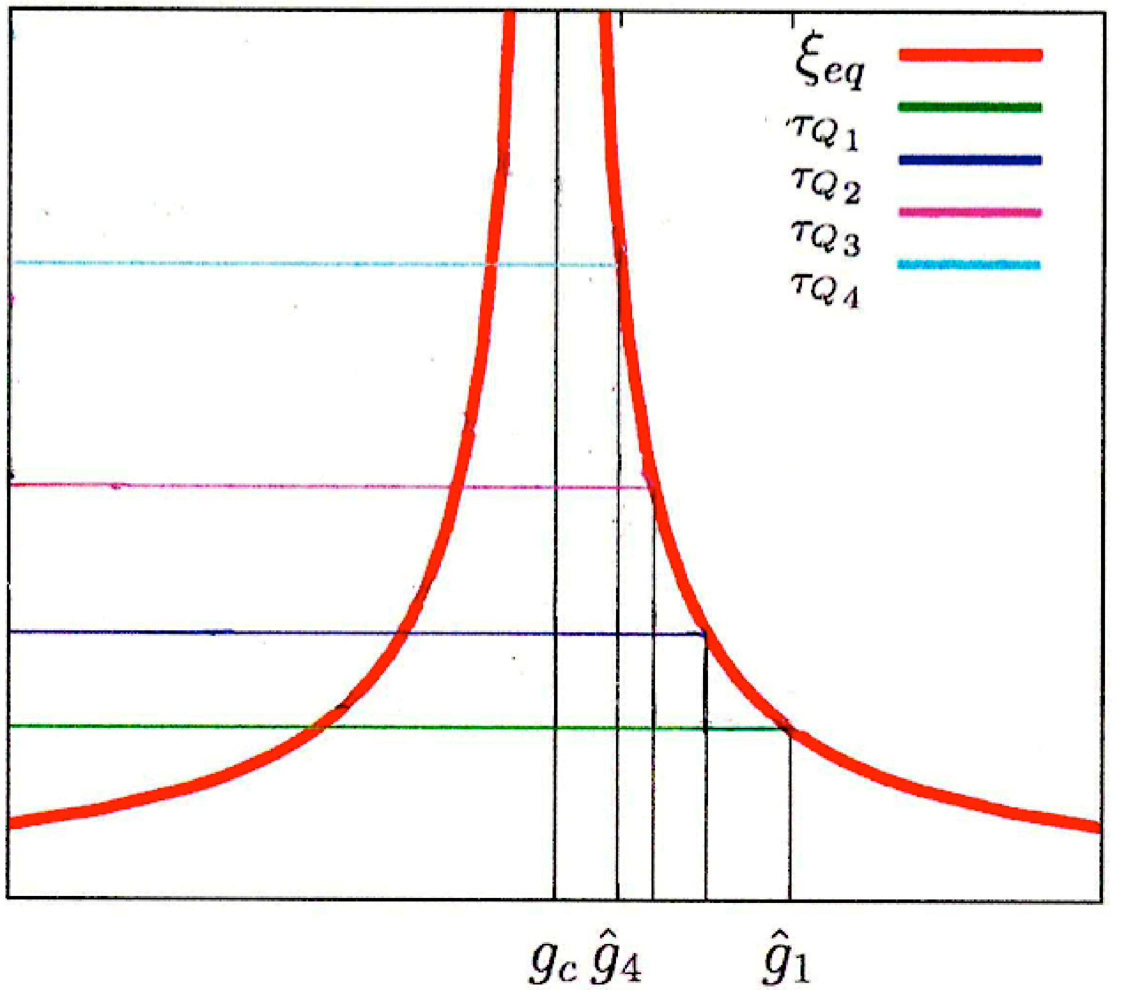
The density of defects is $\boxed{\hat{n}_{KZ} \simeq \xi_{eq}^{-d}(\hat{g}) \simeq (\Delta\hat{g})^{\nu d} \simeq \tau_Q^{-\nu d/(1+\nu z_c)}}$

*** and gets blocked at this value ever after ***

Zurek 85

Finite rate quench

Sketch of Zurek's proposal for R_{τ_Q}



Finite rate quench

Critical coarsening out of equilibrium

In the critical region the system coarsens through critical dynamics and these dynamics operate until a time $t^* > 0$ at which the growing length is again of the order of the equilibrium correlation length, $\mathcal{R}^* \simeq \xi_{eq}(g^*)$.

For a linear cooling rate a simple calculation yields

$$\boxed{\mathcal{R}(g^*) \simeq \zeta\, \mathcal{R}(\hat{g}) \simeq \zeta\, \xi_{eq}(\hat{g})}$$

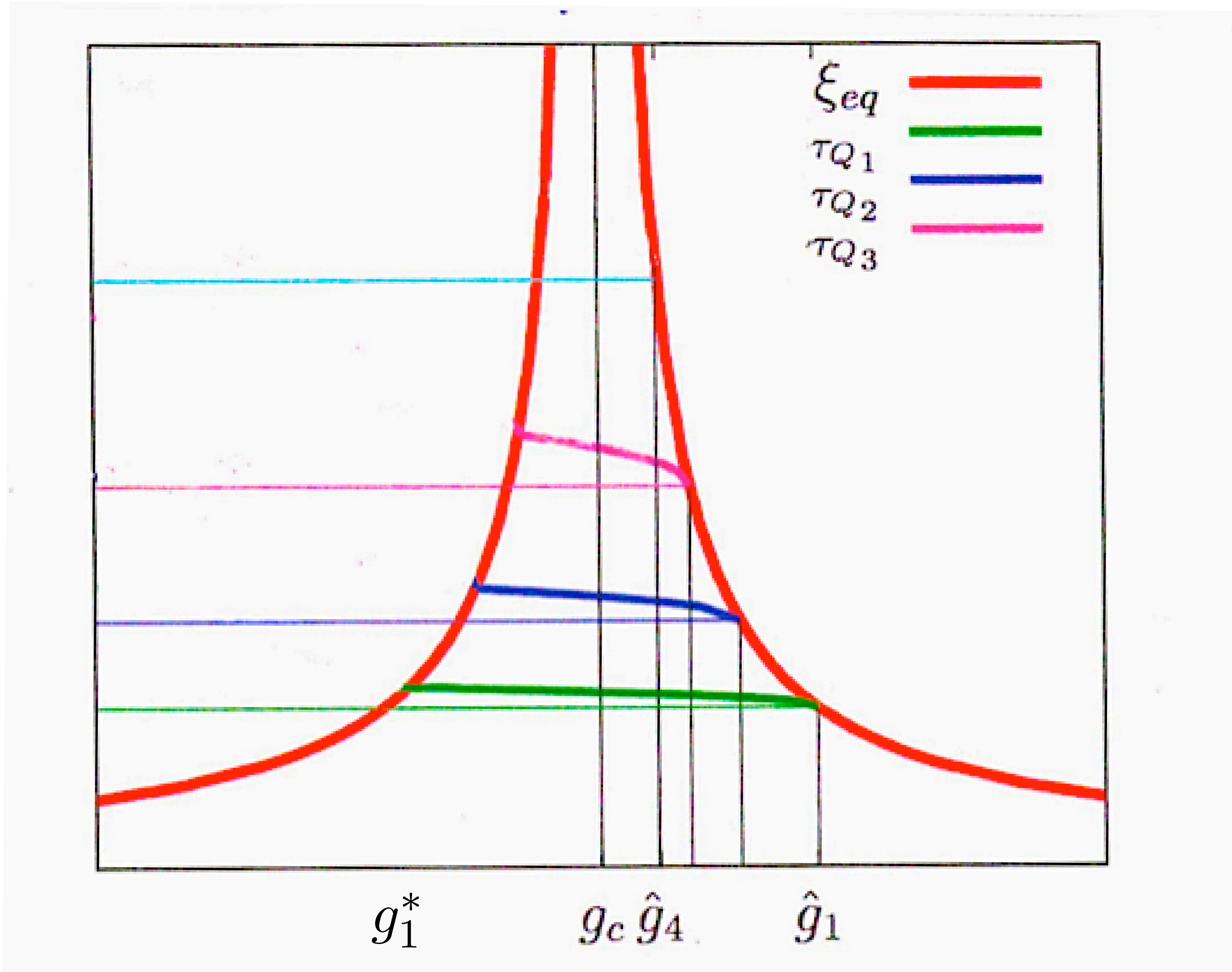
(if the scaling for an infinitely rapid critical quench, $\Delta\mathcal{R}(\Delta t) \simeq \Delta t^{1/z_c}$, with Δt the time spent since entering the critical region, still holds).

No change in leading scaling with τ_Q although there is a gain in length through the prefactor ζ.

(This argument is different from the one in **Zurek 85**.)

Finite rate quench

Contribution from critical relaxation, $R_{\tau_Q} \simeq \zeta\, \xi_{eq}(\hat{g})$



Finite rate quench

Far from the critical region, in the coarsening regime

In the 'ordered' phase usual coarsening takes over. The correlation length $\mathcal{R}$ continues to evolve and its growth cannot be neglected.

Working assumption for the slow quench

$$\boxed{\mathcal{R}(\Delta t, g) \qquad \to \qquad \mathcal{R}(\Delta t, g(\Delta t))}$$

with Δt the time spent since entering the sub-critical region at $\mathcal{R}(g^*)$.

∞-**rapid** quench with	$\to$	**finite-rate** quench with
$g = g_f$ held constant		g slowly varying.

Finite rate quench

The two cross-overs

One needs to match the three regimes :

equilibrium, critical and sub-critical growth.

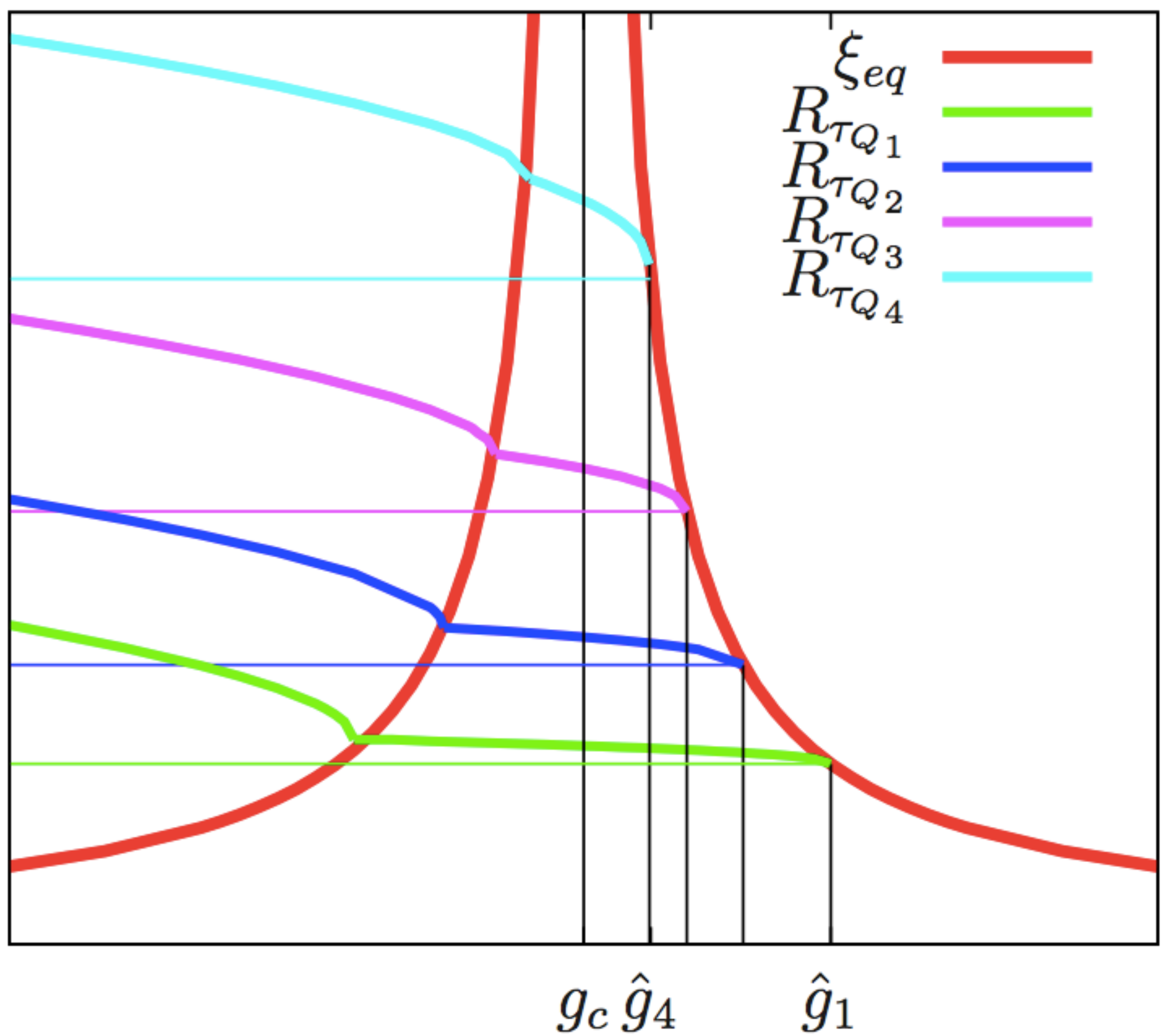
New **scaling assumption** for a linear cooling $|\Delta g(t)| = t/\tau_Q$:

$$\boxed{\mathcal{R}(t, g(t)) \simeq \begin{cases} |\Delta g(t)|^{-\nu} & t \ll -\hat{t} \quad \text{in eq.} \\ |\Delta g(t)|^{-\nu(1-z_c/z_d)}\; t^{1/z_d} & t \gg t^* \quad \text{out of eq.} \end{cases}}$$

Scaling on both sides of the critical (finally uninteresting) region.

Finite rate quench

Sketch of the effect of τ_Q on $\mathcal{R}(t,g)$

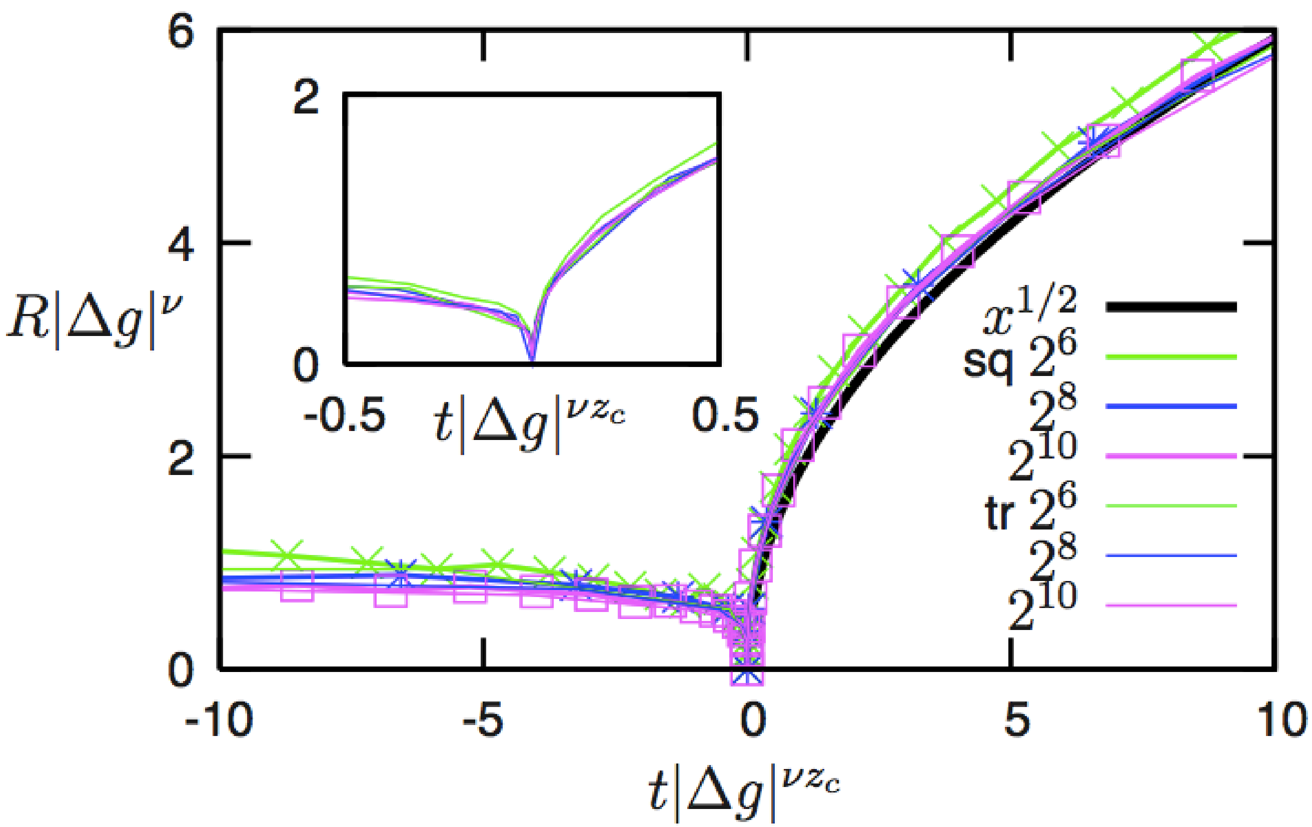


cfr. constant thin lines, **Zurek 85**

Simulations

Test of universal scaling in the 2dIM with NCOP dynamics

$\mathcal{R}\ |\Delta g|^{\nu}$ cst $(|\Delta g|^{\nu z_c} t)^{1/z_d}$



$z_c \simeq 2.17$ and $\nu \simeq 1$; the square root ($z_d = 2$) is in black

Also checked (analytically) in the $O(N)$ model in the large N limit.

Density of domain walls

Test of universal scaling in the 2dIM with NCOP dynamics

Dynamic scaling implies

$$n(t, \tau_Q) \simeq [\mathcal{R}(t, \tau_Q)]^{-d}$$

with d the dimension of space

Therefore

$$\boxed{n(t, \tau_Q) \simeq \tau_Q^{d\nu(z_c - z_d)/z_d} \; t^{-d[1+\nu(z_c - z_d)]/z_d}}$$

depends on *both* times t and τ_Q.

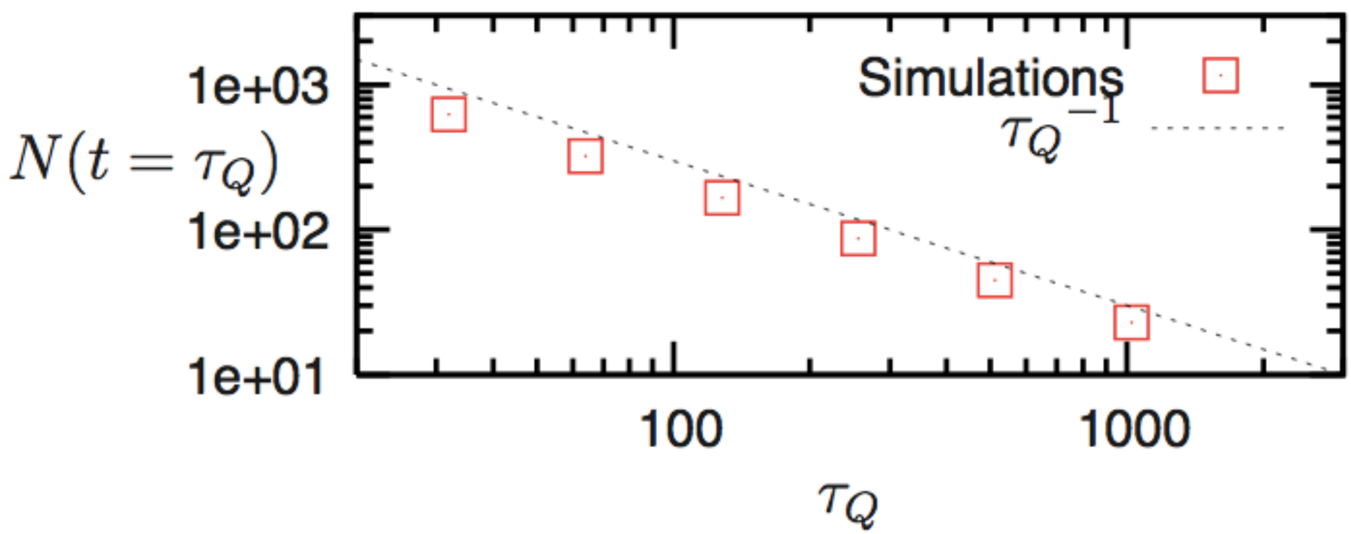
NB t can be much longer than t^* (time for starting sub-critical coarsening) ; in particular t can be of order τ_Q while t^* scales as τ_Q^α with $\alpha < 1$.

Since z_c is larger than z_d this quantity grows with τ_Q at fixed t.

Density of domain walls

At $t \simeq \tau_Q$ in the 2dIM with NCOP dynamics

$$\boxed{N(t \simeq \tau_Q, \tau_Q) = n(t \simeq \tau_Q, \tau_Q) L^2 \simeq \tau_Q^{-1}}$$



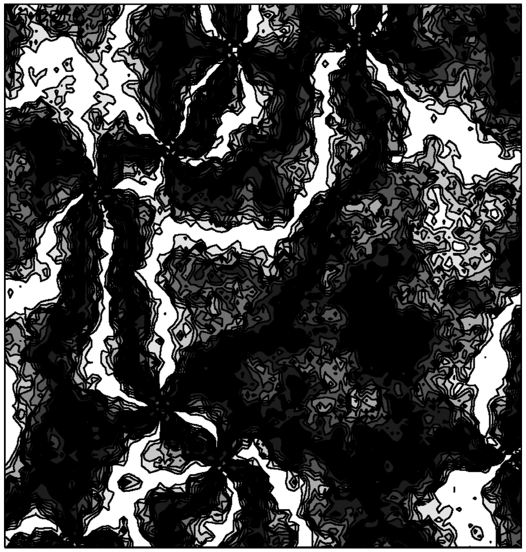
while the KZ mechanism yields $N_{KZ} \simeq \tau_Q^{-\nu/(1+\nu z_c)} \simeq \tau_Q^{-0.31}$.

Biroli, LFC, Sicilia, Phys. Rev. E 81, 050101(R) (2010)

Dynamics in the $2d$ XY model

Vortices : planar spins turn around points

Schrielen pattern : gray scale according to $\sin^2 2\theta_i(t)$



After a quench vortices annihilate and tend to bind in pairs

$$\boxed{\mathcal{R}(t,g) \simeq \lambda(g)\{t/\ln[t/t_0(g)]\}^{1/2}}$$

Pargellis ***et al*** **92, Yurke** ***et al*** **93, Bray & Rutenberg 94**

Dynamics in the $2d$ XY model

KT phase transition & coarsening

- The high T phase is plagued with vortices. These should bind in pairs (with finite density) in the low T quasi long-range ordered phase.

- Exponential divergence of the equilibrium correlation length above T_{KT}

$$\boxed{\xi_{eq} \simeq a_\xi e^{b_\xi [(T-T_{KT})/T_{KT}]^{-\nu}}} \qquad \text{with} \qquad \nu = 1/2.$$

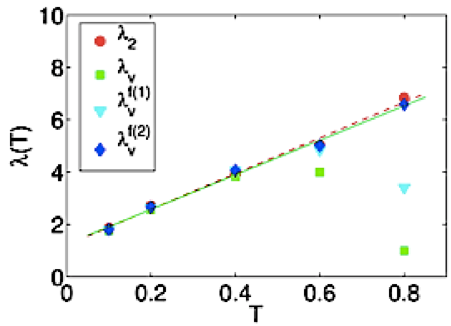
- Zurek's argument for falling out of equilibrium in the disordered phase

$$\boxed{\hat{\xi}_{eq} \simeq (\tau_Q/\ln^3(\tau_Q/t_0))^{1/z_c}} \qquad \text{with } z_c = 2 \text{ for NCOP.}$$

- Logarithmic corrections to the sub-critical growing length

$$\boxed{\mathcal{R}(t,T) \simeq \lambda(T) \left[\frac{t}{\ln(t/t_0)}\right]^{1/z_d}}$$

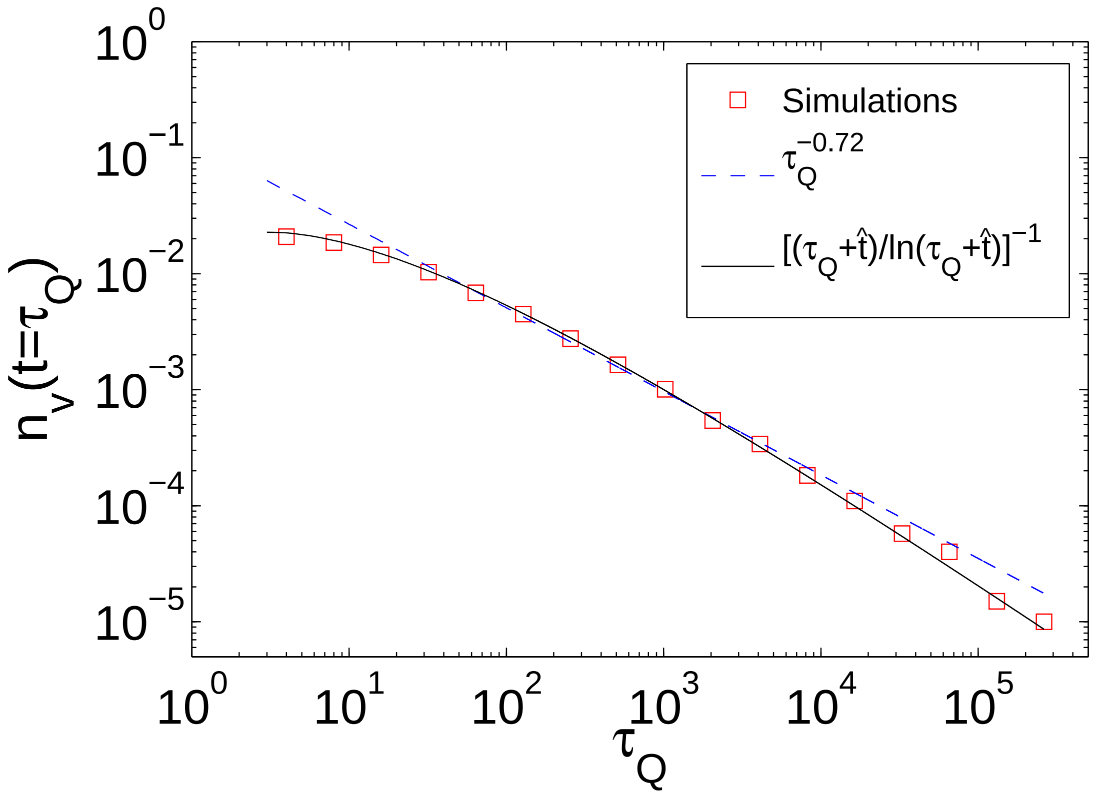
with $z_d = 2$ for NCOP



Dynamics in the $2d$ XY model

KT phase transition & coarsening

$$\boxed{n_v(t \simeq \tau_Q, \tau_Q) \simeq \ln[\tau_Q/\ln^2\tau_Q + \tau_Q]/(\tau_Q/\ln^2\tau_Q + \tau_Q)}$$



Large τ_Q

$$n_v \simeq \frac{\ln \tau_Q}{\tau_Q}$$

while

$$n_{KZ} \simeq \frac{\ln^3 \tau_Q}{\tau_Q}$$

A. Jelić and LFC, J. Stat. Mech. P02032 (2011).

Work in progress

Quench rate dependencies in the dynamics of the

$3d\; O(2)$ relativistic field theory

$$\partial_t^2 \psi(\vec{r},t) = \nabla^2 \psi(\vec{r},t) - (|\psi|^2 - 1)\psi(\vec{r},t) - \gamma_0 \partial_t \psi(\vec{r},t) + \xi(\vec{r},t)$$

its non-relativistic limit

$$-i\partial_t \psi(\vec{r},t) = \nabla^2 \psi(\vec{r},t) - (|\psi|^2 - 1)\psi(\vec{r},t) - \gamma_0 \partial_t \psi(\vec{r},t) + \xi(\vec{r},t)$$

the stochastic Gross-Pitaevskii equation

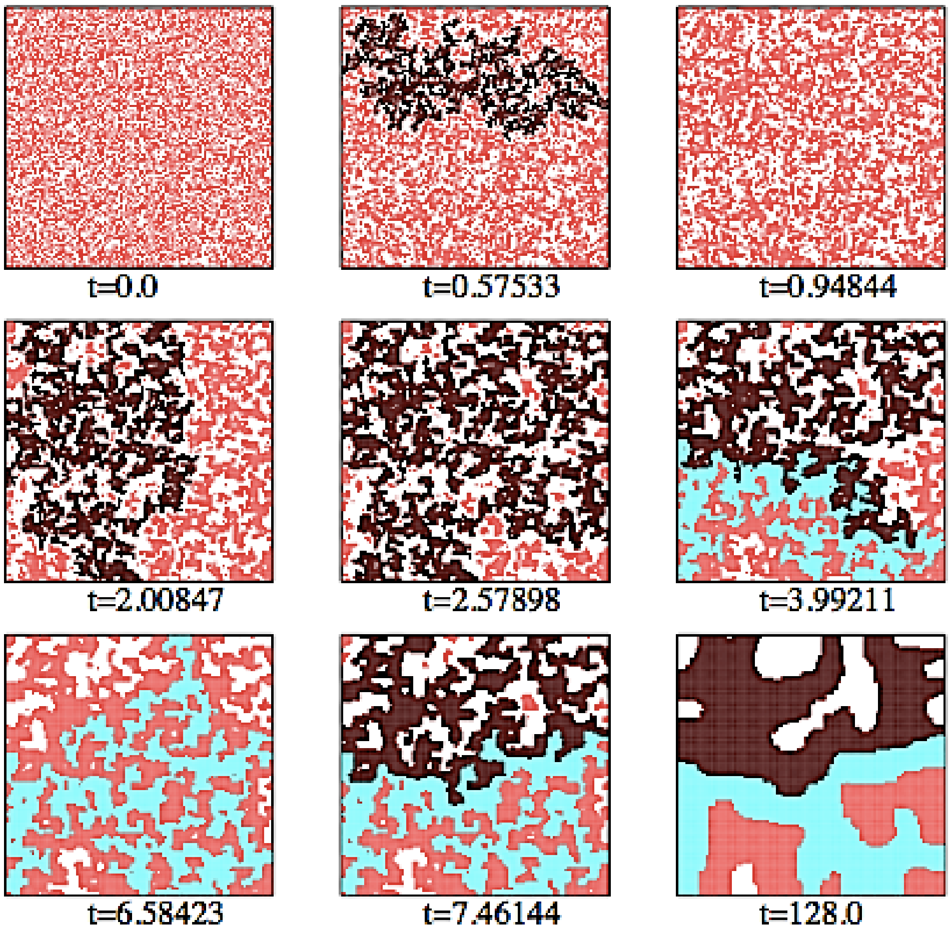
$$-i\partial_t \psi(\vec{r},t) = (1 - i\gamma_0)\left[\nabla^2 - (|\psi|^2 - 1)\right] \psi(\vec{r},t) + \xi(\vec{r},t)$$

$(\psi(\vec{r},t) \in \mathbb{C})$

Study of **vortex lines**.

Kobayashi & LFC

Work in progress



$2d$ IM

Short-time dynamics.

Blanchard, Corberi

LFC & Picco

Conclusions

- The criterium to find the time when the system falls out of equilibrium above the phase transition ($-\hat{t}$) is correct ; exact results in the $1d$ Glauber Ising chain **P. Krapivsky, J. Stat. Mech. P02014 (2010).**
- However, defects continue to annihilate during the ordering dynamics ; their density at times of the order of the cooling rate, $t \simeq \tau_Q$, is **significantly lower** than the one predicted in **Zurek 85**.
- Experiments should be revisited in view of this claim (with the proviso that defects should be measured as directly as possible).
- Some future projects : annealing in systems with **other type of phase transitions and topological defects**.
- **Microcanonical quenches.**