Coarsening

the density of defects after a very slow quench

Leticia F. Cugliandolo

Université Pierre et Marie Curie – Paris VI

leticia@lpthe.jussieu.fr

www.lpthe.jussieu.fr/˜leticia/seminars

In collaboration with

G. Biroli (Saclay Paris) and A. Sicilia (Paris $\longrightarrow$ Cambridge, UK),

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Kanpur, India, February 2010

Problem

Predict the density of defects left over after traversing a 2nd order phase transition with a given speed.

Out of equilibrium physics :

the system does not have enough time to equilibrate to the continuously 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 expansion the universe cools down in the course of time, $E(t) \Rightarrow T_{micro}(t)$, and undergoes a number of **second order 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 ? (**cosmological strings**)

T. Kibble 76, W. Zurek 85

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**. (**vortices**)

Difficulties : Defects are hard to see ; only their possible consequences are. Many orders of magnitude in time should be explored. Sometimes it is not even clear which is the symmetry that is actually broken.

Summary in Les Houches winter school 99, T. Kibble, Phys. Today 07

Phenomenon

Statistical mechanics

This question can be posed on a well-known problem

Ordering dynamics following a quench through a phase transition

- between two **equilibrium phases** that are known on both sides of the transition ;
- with a well-understood **dynamic mechanism** at and below the critical point ;
- with easy to identify and count **topological defects**.

Plan of talk

Intended as a colloquium ; hopefully clear but not boring

- Paradigmatic equilibrium second-order phase transition :

  paramagnetic - ferromagnetic transition with scalar order-parameter,

  realized by e.g. the Ising model.

- **Stochastic dynamics** : temperature is the quenching parameter.

- Identification of a growing length and topological defects (**domain walls**).

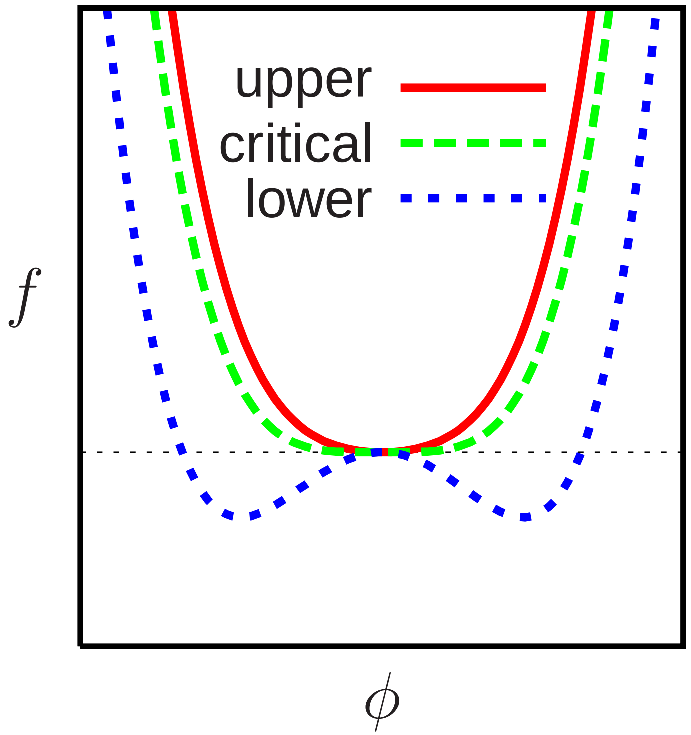
+ Dynamic scaling analysis :

  corrections to the Kibble-Zurek mechanism & new predictions.

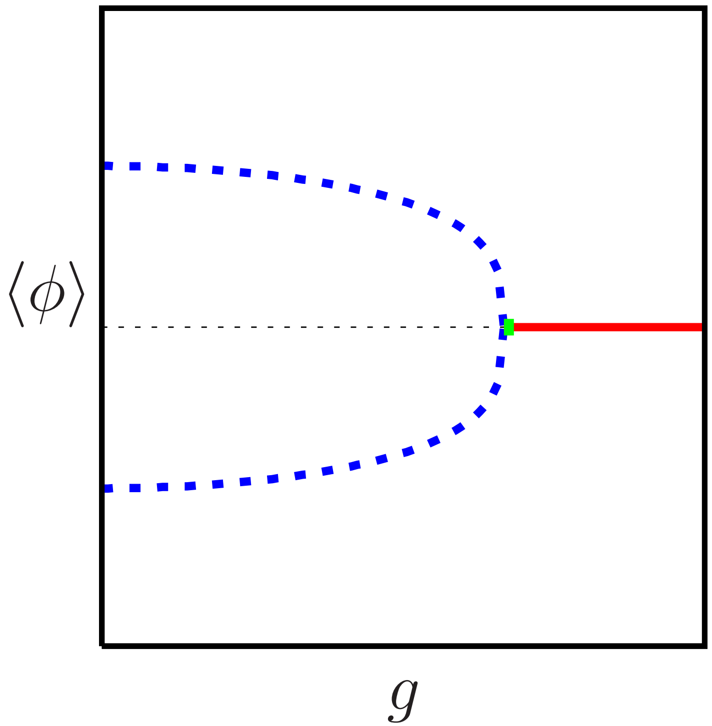
+ Numeric and analytic tests.

2nd order phase-transition

bi-valued equilibrium states related by symmetry, **e.g. Ising magnets**



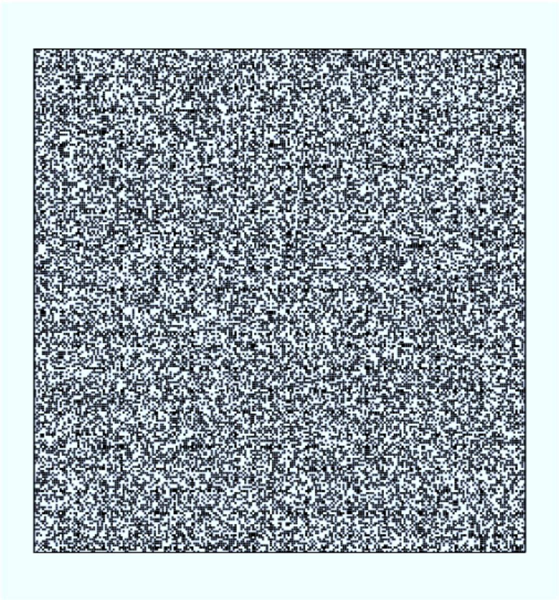
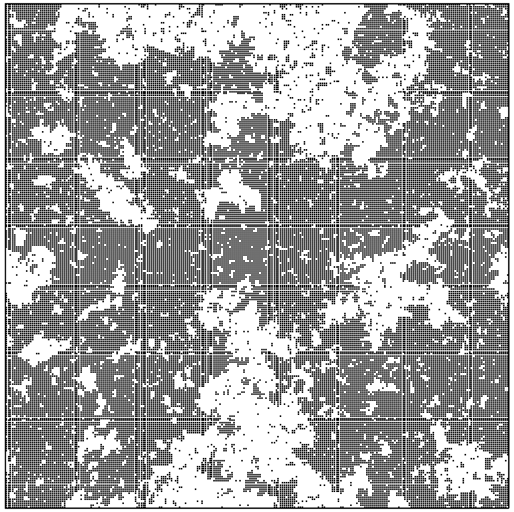
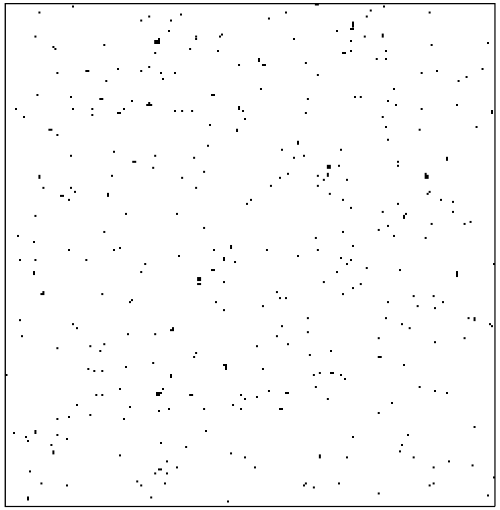
Ginzburg-Landau free-energy



Scalar order parameter

Equilibrium configurations

e.g. up & down spins in a $2d$ Ising model (IM)

$g \to \infty$ $\qquad$ $g = g_c$ $\qquad$ $g < g_c$

In a canonical setting the control parameter is temperature, $g = T$.

Quantifying order

The spatial correlation of fluctuations

(In spin language)

$$C(r) \equiv \frac{1}{N} \sum_{i,j=1}^{N} \langle \delta s_i \delta s_j \rangle_{|\vec{r}_i - \vec{r}_j| = r}$$

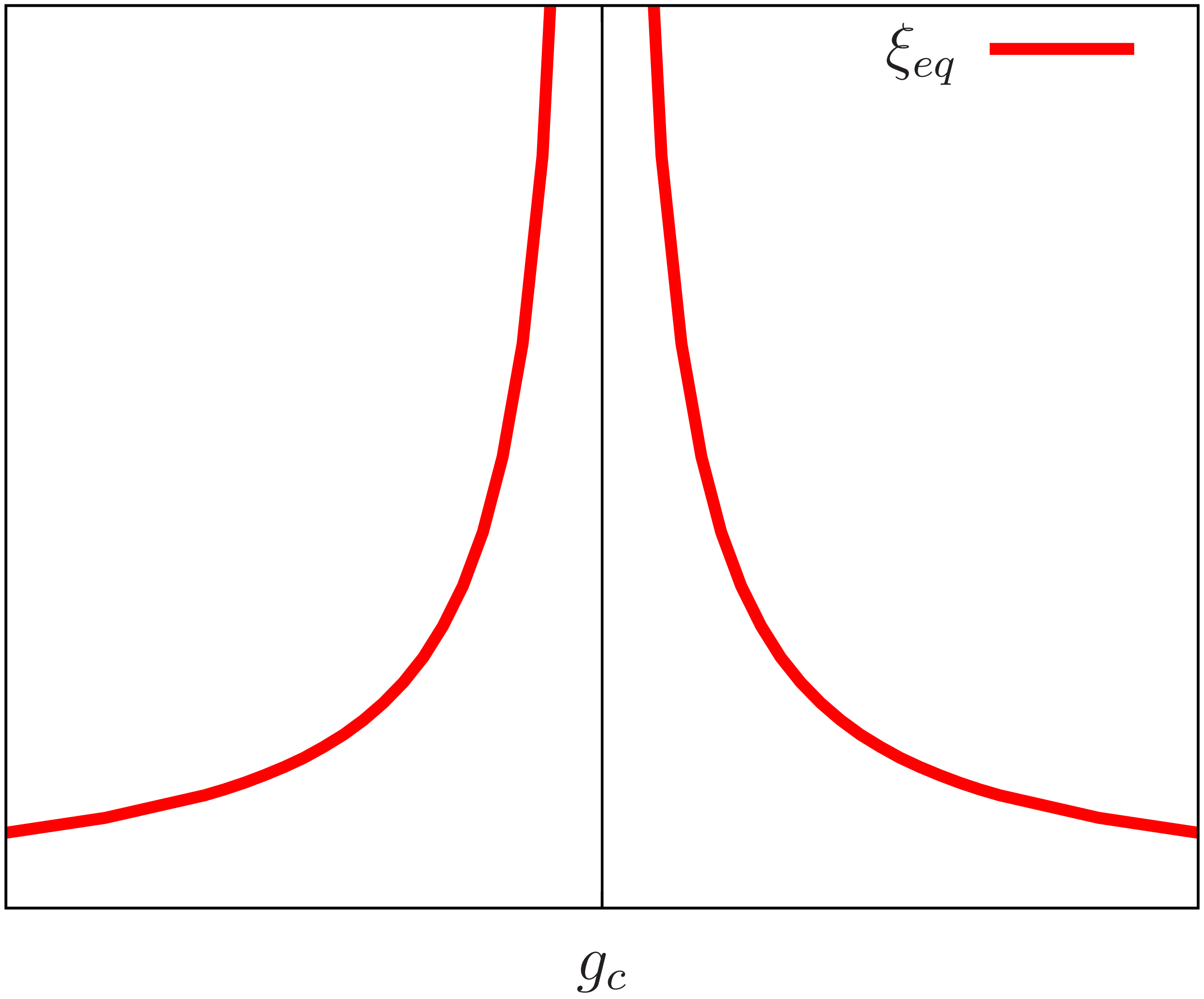
with $\delta s_i \equiv s_i - \langle s_i \rangle$, N the number of spins, and the average taken over different initial conditions and/or different runs.

In equilibrium

$$C_{eq}(r) \simeq r^{2-d-\eta} \; e^{-r/\xi_{eq}(g)}$$

with $\boxed{\xi_{eq}(g)}$ the **equilibrium correlation length**.

The equil. correlation length



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

Dynamics

Contact with a thermal bath : **Thermal agitation**

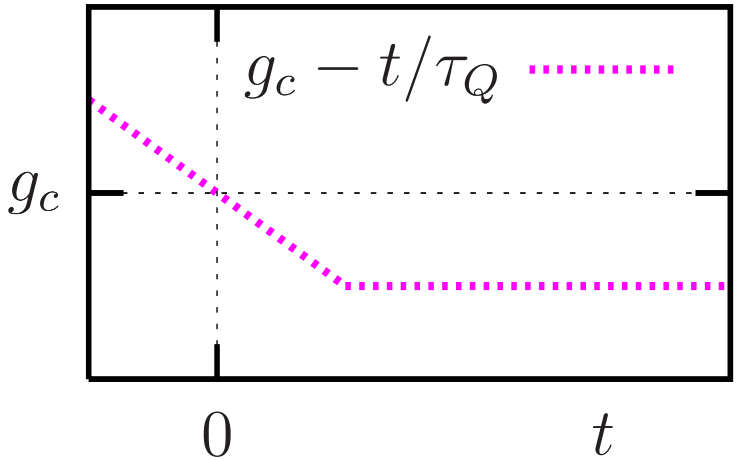
- **Microscopic** : identify the 'smallest' relevant variables in the problem (**e.g. spins or particles**) ;

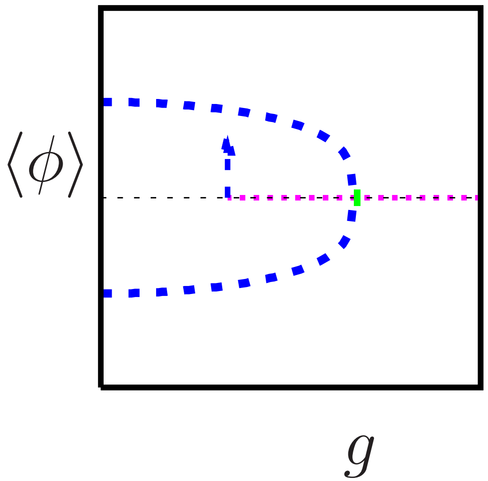
  propose stochastic updates for them (**e.g. Monte Carlo**).

- **Coarse-grained** : average the microscopic variables over a coarse-graining length to construct a field ;

  propose a differential equation for its dynamics (**e.g. Langevin or time-dependent $\lambda\phi^4$ Ginzburg-Landau with noise & friction**).

A quench





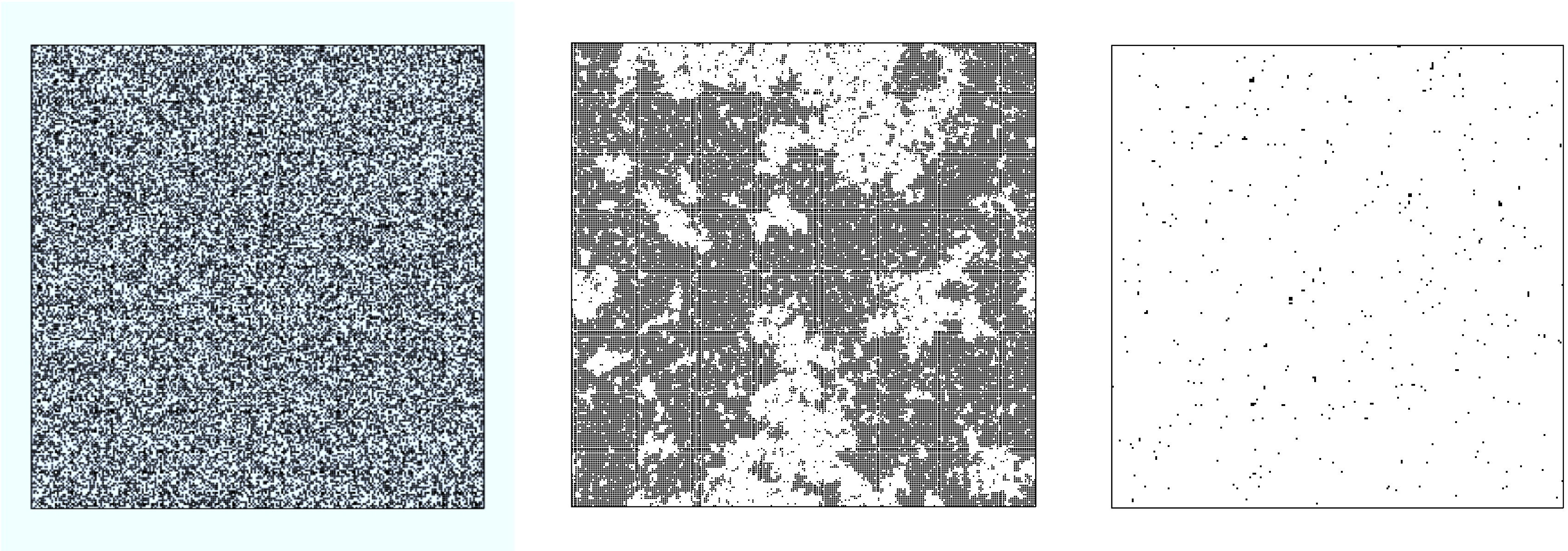
$\langle \phi \rangle(t, g) \neq$ **ct** : **Non-conserved order parameter**

e.g. development of magnetization in a ferromagnet after a quench.

Focus on $E(t) \neq$ **ct** : **due to dissipation the energy is not conserved either**

The problem

e.g. up & down spins in a $2d$ Ising model (IM)



$g \to \infty$ $\qquad$ $g = g_c$ $\qquad$ $g < g_c$

Question : starting from equilibrium at g_i and changing g to g_f with some protocol, how is equilibrium at g_f approached ?

∞ rapid quench

- At $g_f = g_c$ the system needs to grow structures of all sizes.

  Critical coarsening.

- At $g_f < g_c$: the system tries to order locally in one of the two competing equilibrium states at the new conditions.

  Sub-critical coarsening.

In both cases one extracts from $\boxed{C(r,t)}$ a **linear size of equilibrated patches** $\boxed{\mathcal{R}(t)}$ that **increases in time**.

The growing length

The space-time correlation

(In spin language)

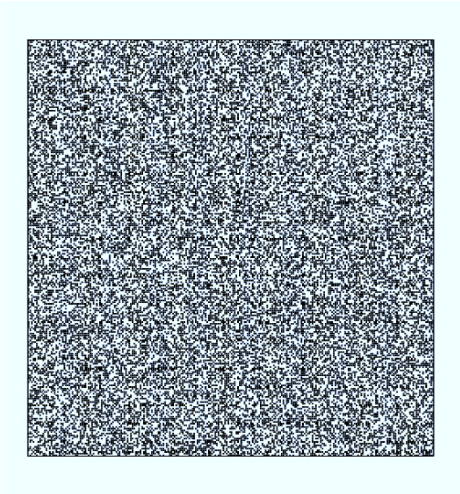
$$C(r,t) \equiv \frac{1}{N} \sum_{i,j=1}^{N} \langle \delta s_i(t) \delta s_j(t) \rangle_{|\vec{r}_i - \vec{r}_j| = r}$$

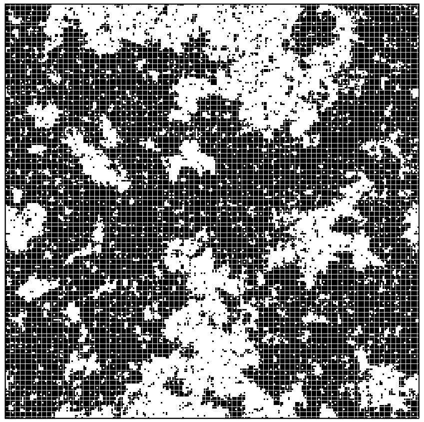
with $\delta s_i(t) \equiv s_i(t) - \langle s_i(t) \rangle$, N the number of spins, and the average taken over different initial conditions and/or different runs.

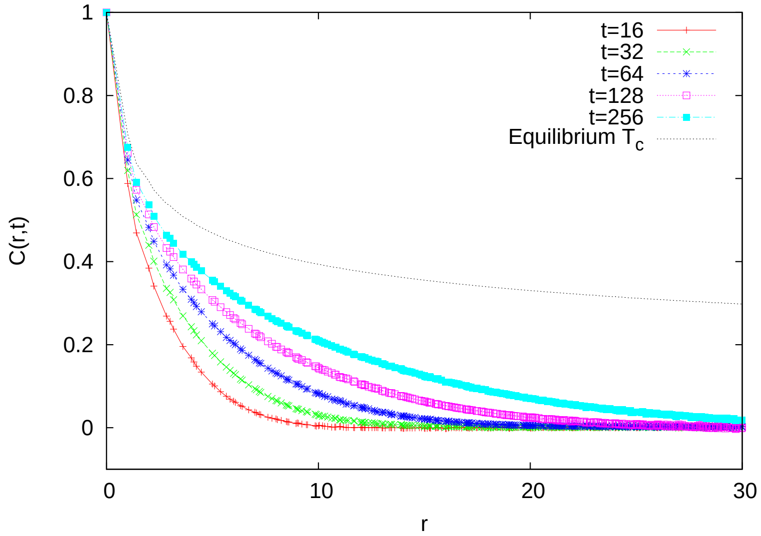
- $C(\mathcal{R}(t), t) = 1/e$
- $\mathcal{R}(t) = [\int d^d r\, r^\alpha\, C(r,t) / \int d^d r\, C(r,t)]^{1/\alpha}$
- Dynamic scaling. *(Explained later.)*

Critical growth

∞ rapid quench to T_c : $T(t<0) = T_i$ **and** $T(t>0) = T_c$





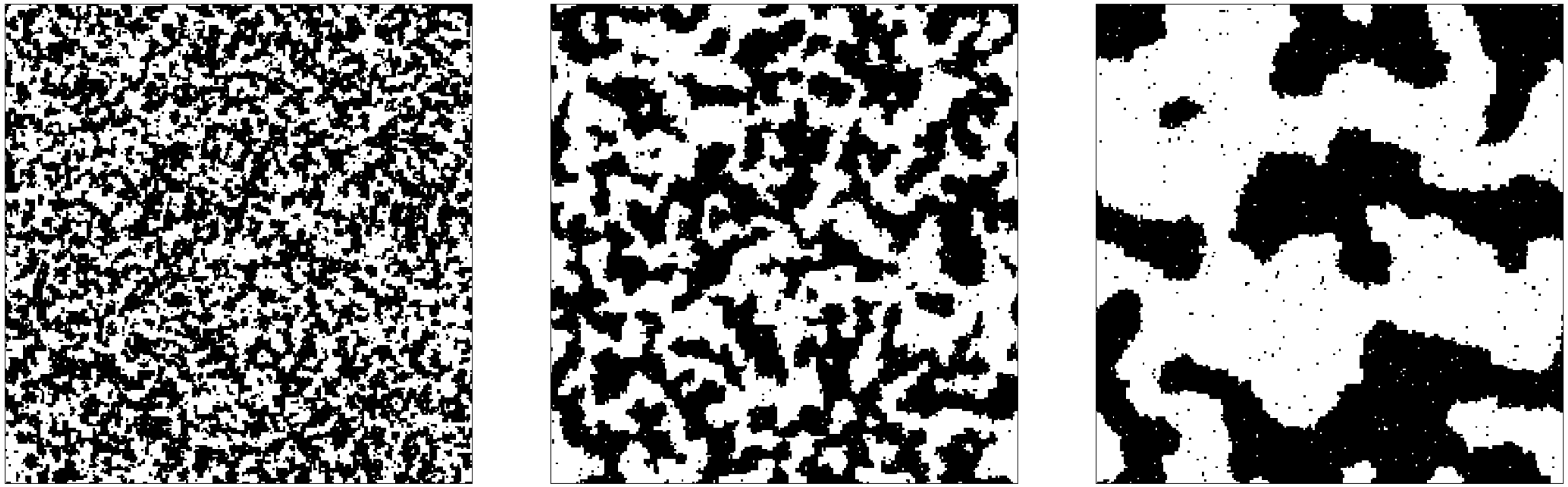


- Black curve : **equilibrium power-law decay** $C_{eq}(r) \simeq r^{2-d-\eta}$.
- Coloured curves are $C(r,t)$ for different times after the quench and they slowly approach $C_{eq}(r)$.
- The **growing length** is $\boxed{\mathcal{R}_c(t) \simeq t^{1/z_{eq}}}$ with $\boxed{z_{eq} \simeq 2.17}$

Subcritical domain growth

∞ **rapid quench to** T_c **:** $T(t<0) = T_i$ **and** $T(t>0) \ll T_c$

Domains of up & down spins in a $2d$**IM quenched to** $\boxed{T_f < T_c}$



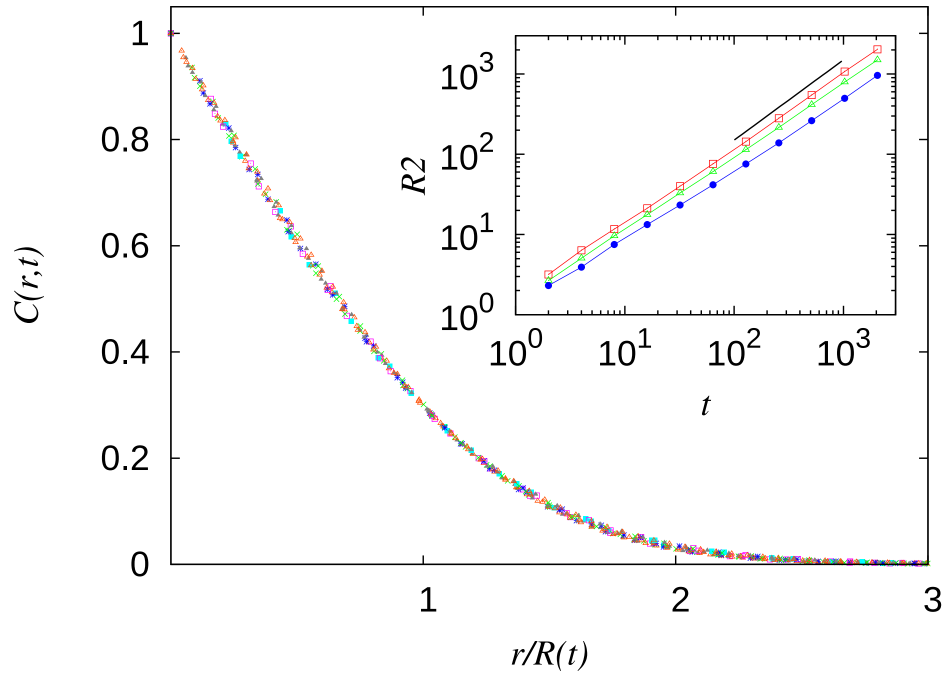
$0 < t_1$ $< t_2$ $< t_3$

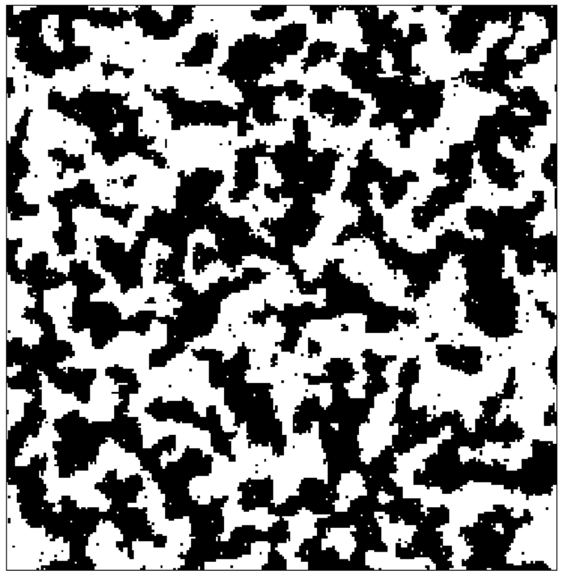
Space-time correlation

In the regime $a \ll r \ll L$, $r/\mathcal{R}(t,T) \approx$ finite,

one finds **dynamic scaling** $C(r,t) \simeq m_{eq}^2(T)\, f_c\left(\frac{r}{\mathcal{R}(t,T)}\right)$

with $\mathcal{R}(t,T) \simeq \lambda(T)\, t^{1/z_d}$ and $z_d = 2$





∞ rapid quench to $g = g_c + \epsilon$

Control of crossover

The **'typical length'** scales as

$$\boxed{\mathcal{R}(t,g) \simeq \xi_{eq}(g)\, f\left(\frac{t}{\tau_{eq}(g)}\right)}$$

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

$$f(x) \simeq \begin{cases} x^{1/z_{eq}} & x \ll 1 \\ \textbf{ct} & x \gg 1 \end{cases} \qquad \mathcal{R}(t,g) \simeq \begin{cases} t^{1/z_{eq}} & t \ll \tau_{eq} \\ \xi_{eq}(g) & t \gg \tau_{eq} \end{cases}$$

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

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

∞ rapid quench to $g = g_c - \epsilon$

Control of crossover

The **'typical length'** scales as

$$\mathcal{R}(t,g) \simeq \xi_{eq}(g)\, f\left(\frac{t}{\tau_{eq}(g)}\right)$$

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

$$f(x) \simeq \begin{cases} x^{1/z_{eq}} & x \ll 1 \\ x^{1/z_d} & x \gg 1 \end{cases} \qquad \mathcal{R}(t,g) \simeq \begin{cases} t^{1/z_{eq}} \\ \xi_{eq}^{1-z_{eq}/z_d}(g)\, t^{1/z_d} \end{cases}$$

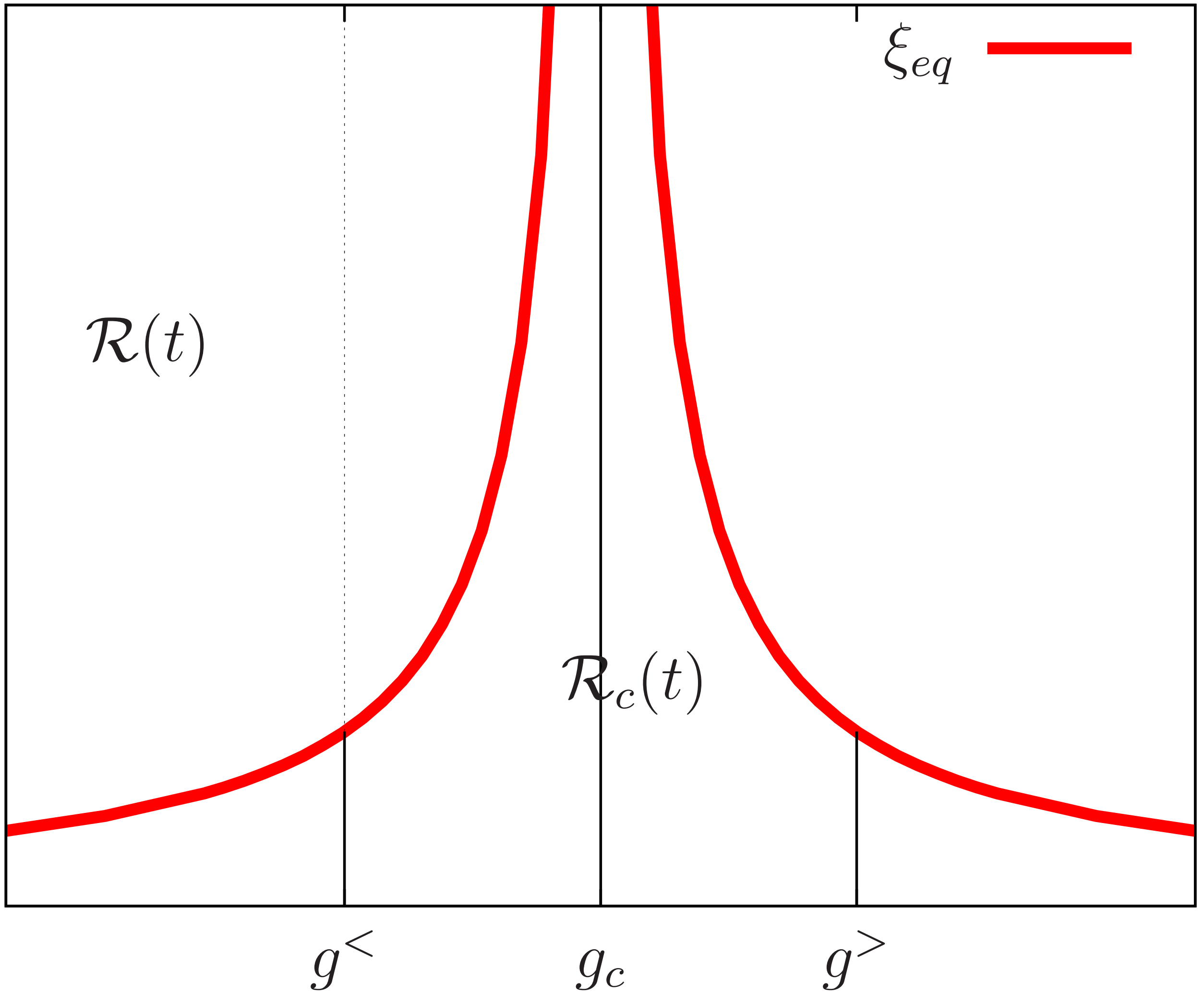
Crossover at $t \simeq \tau_{eq}(g)$ when $\mathcal{R}(\tau_{eq}(g)) \simeq \xi_{eq}(g)$

Arenzon, Bray, LFC, Sicilia 08

Note that z_d **(**$\neq z_{eq}$**)** ; e.g. $z_d = 2$ **for 2dIM with NCOP**.

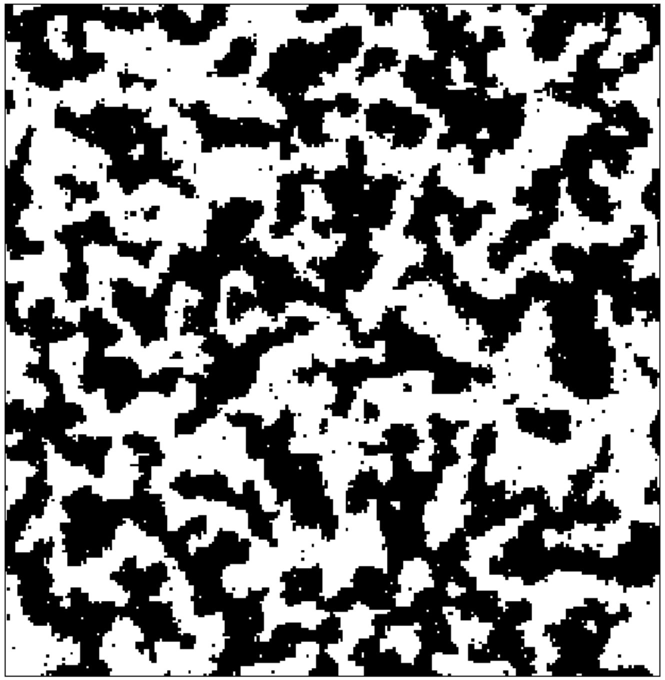
∞ rapid quenches

Summary

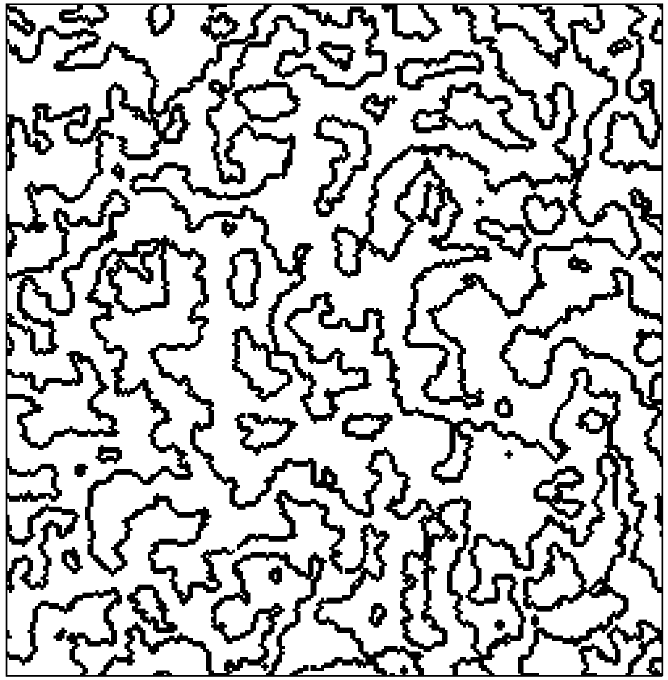


Topological defects : walls

An instantaneous configuration at $t = 32$ **MCs**, $T = 1.5$



Domains



Walls

Dynamic scaling

At late times there is a single length-scale, the typical radius of the domains $\mathcal{R}(t,g)$, such that the domain structure is (in statistical sense) independent of time when lengths are scaled by $\mathcal{R}(t,g)$, e.g.

$$C(r,t) \equiv \langle\, s_i(t) s_j(t)\,\rangle|_{|\vec{x}_i-\vec{x}_j|=r} \sim \langle\phi\rangle^2_{eq}(g)\; f\left(\frac{r}{\mathcal{R}(t,g)}\right),$$

$$C(t,t_w) \equiv \langle\, s_i(t) s_i(t_w)\,\rangle \sim \langle\phi\rangle^2_{eq}(g)\; f_c\left(\frac{\mathcal{R}(t,g)}{\mathcal{R}(t_w,g)}\right),$$

etc. when $r \gg \xi(g)$, $t, t_w \gg t_0$ and $C < \langle\phi\rangle^2_{eq}(g)$.

Suggested by experiments and numerical simulations. Proved for

- **Ising chain with Glauber dynamics**.
- **Langevin dynamics of the $O(N)$ model with $N \to \infty$, and the spherical ferromagnet.**

Review Bray 94.

Dynamic scaling

Consequence

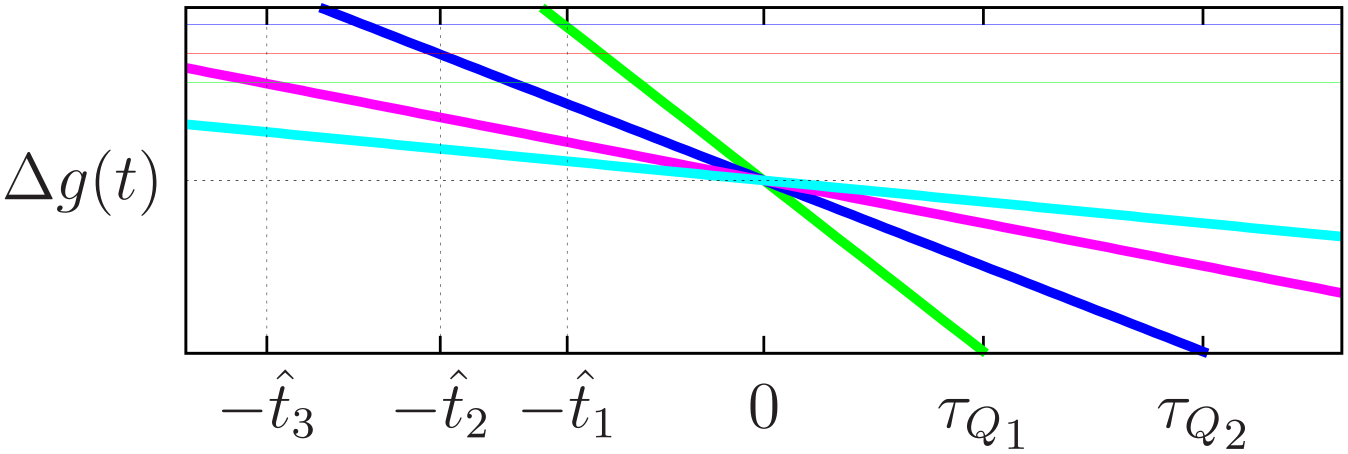
If there is only one length governing the dynamics, the **density of topological defects** *should also be determined by* $\mathcal{R}(t,g)$.

Then one has

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

where n is the searched density, or number of topological defects per unit system size.

Annealing or finite τ_Q quenches



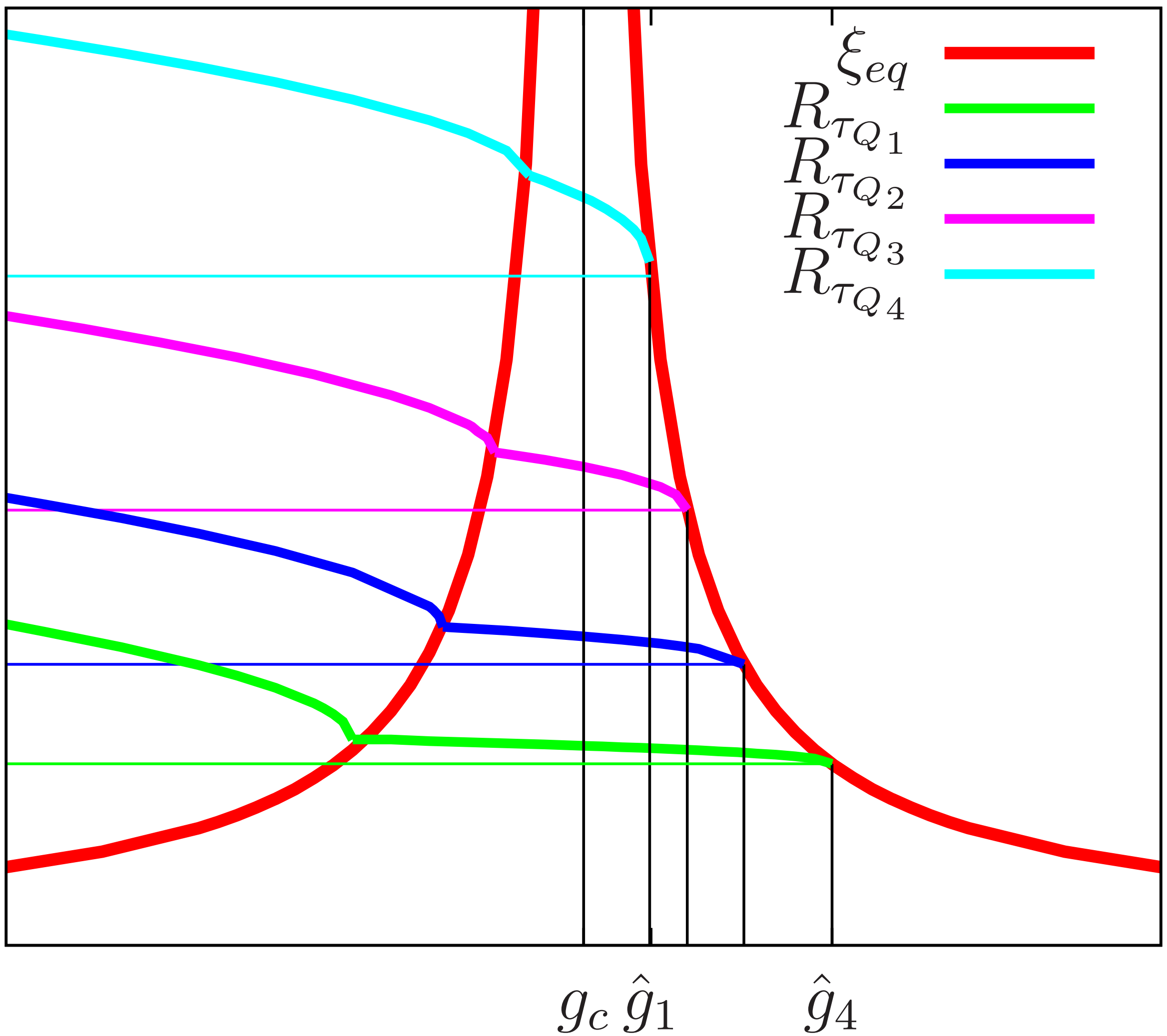
$\Delta g \equiv g(t) - g_c$

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

Linear cooling could be thought of as an approximation close to g_c.

Annealing

What is the effect of a finite cooling rate on $\mathcal{R}(t, g)$?



Annealing

In equilibrium

The system follows the pace imposed by the changing conditions, $g(t)$*, until a time* $-\hat{t} < 0$ *(or value of the control parameter* $\hat{g} > g_c$*) at which its dynamics is too slow to accomodate 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 changes.

For a linear cooling rate :

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

and $$\boxed{\Delta \hat{g} \simeq \tau_Q^{-1/(1+\nu z_{eq})}}$$

Zurek 85

Annealing

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, $\mathcal{R}(\Delta t) \simeq \Delta t^{1/z_{eq}}$, still holds.

No change in 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**.)

Annealing out of equilibrium

Far from the critical region

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

Working assumption

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

∞ rapid quench with $g = g_f$ $\quad\to\quad$ finite rate quench with g

held constant $\qquad\qquad$ slowly varying.

Annealing

Crossover

One needs to match the three regimes : equilibrium, critical and sub-critical growth.

New **scaling assumption** for the convention $g(t=0)=g_c$:

$$\mathcal{R}(t) \simeq \xi_{eq}\, \mathcal{F}\left(\frac{t}{\tau_{eq}}\right)$$

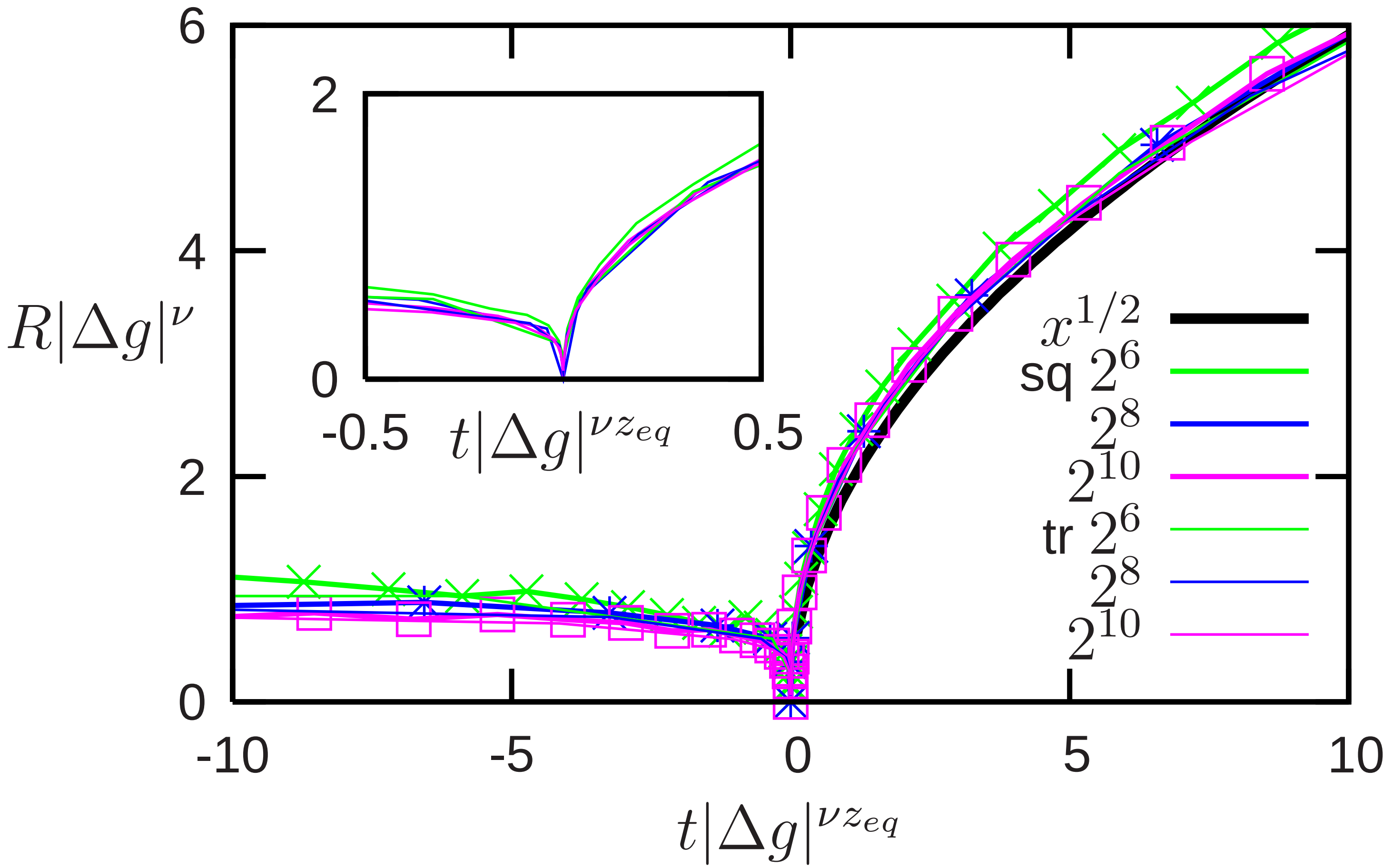
with the limits

$$\mathcal{F}(x) \simeq \begin{cases} \textbf{ct} \\ x^{1/z_d} \end{cases} \qquad \mathcal{R}(t) \simeq \begin{cases} \xi_{eq} & t \ll -\hat{t} \\ |\Delta g(t)|^{-\nu(1-z_{eq}/z_d)}\, t^{1/z_d} & t \gg t^* \end{cases}$$

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

Simulations

Test of universal scaling in the 2dIM with NCOP dynamics



$z_{eq} \simeq 2.17$ 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 topological defects

Dynamic scaling implies

$$N(t,\tau_Q) \simeq \mathcal{R}^{-d}(t,\tau_Q)$$

with d the dimension of space

Therefore

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

depends on *both* times t and τ_Q.

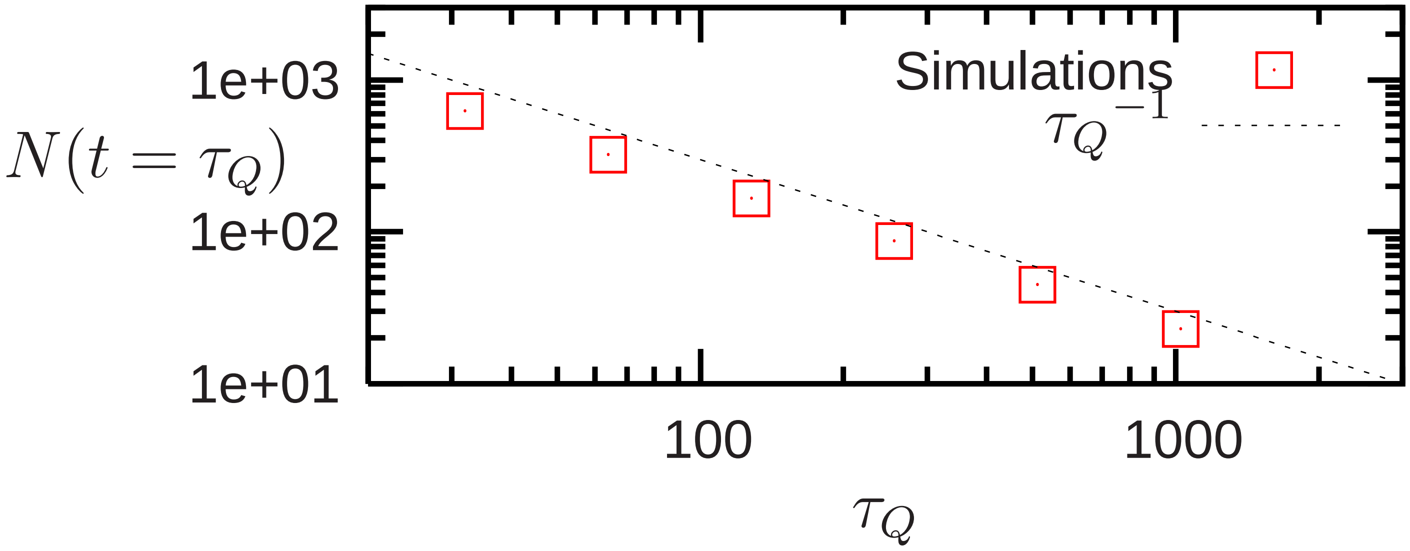
NB t can be much longer than t^* ; in particular t can be of order τ_Q while t^* scales as τ_Q^{α} with $\alpha < 1$.

Since z_{eq} is larger than z_d this quantity grows with τ_Q at fixed t.

Density of topological defects

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

$$N(t \simeq \tau_Q, \tau_Q) \simeq \tau_Q^{-1}$$



while the KZ mechanism yields $N_{KZ} \simeq \tau_Q^{-\nu/(1+\nu z_e q)} \simeq \tau_Q^{-1/3.17}$.

Biroli, LFC, Sicilia, arXiv : 1001.0693

Conclusions

- Since 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 that 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, e.g. **xy models (vortices)**.
- **Microcanonical quenches.**

Related work **P. Krapivsky, arXiv : 1001**, on the Glauber Ising chain, thanks for discussions.

Conclusions

There is still much to learn from these “simple” problems.