Coarsening

the density of defects after a very slow quench

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arXiv : 1001.0693 **Phys. Rev. E 81, 050101(R) (2010).**

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

Bari, Italia,, 2011

The problem

Predict the density of defects left over after traversing a 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, $R(t) \Rightarrow T_{micro}(t)$, 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

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 vortices**)

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

KZ for 2nd order phase trans.

3 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 above the critical point.

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

that we critically revisited.

Focus on $$n = \frac{\text{\# of walls, vortices, etc.}}{L^d}$$

Plan of the talk

Intended as a colloquium ; hopefully clear but not boring

- Paradigmatic phase transitions :

  second-order : **paramagnetic – ferromagnetic transition with scalar order-parameter**, realized by the $d > 1$ **Ising model**.

  Kosterlitz-Thouless : **disordered – quasi long-range ordered transition with vector order parameter**, realized by the $2d$ **xy model**.

- **Stochastic dissipative dynamics** : T/J is the quench parameter.
- Identification of a growing length and the topological defects.

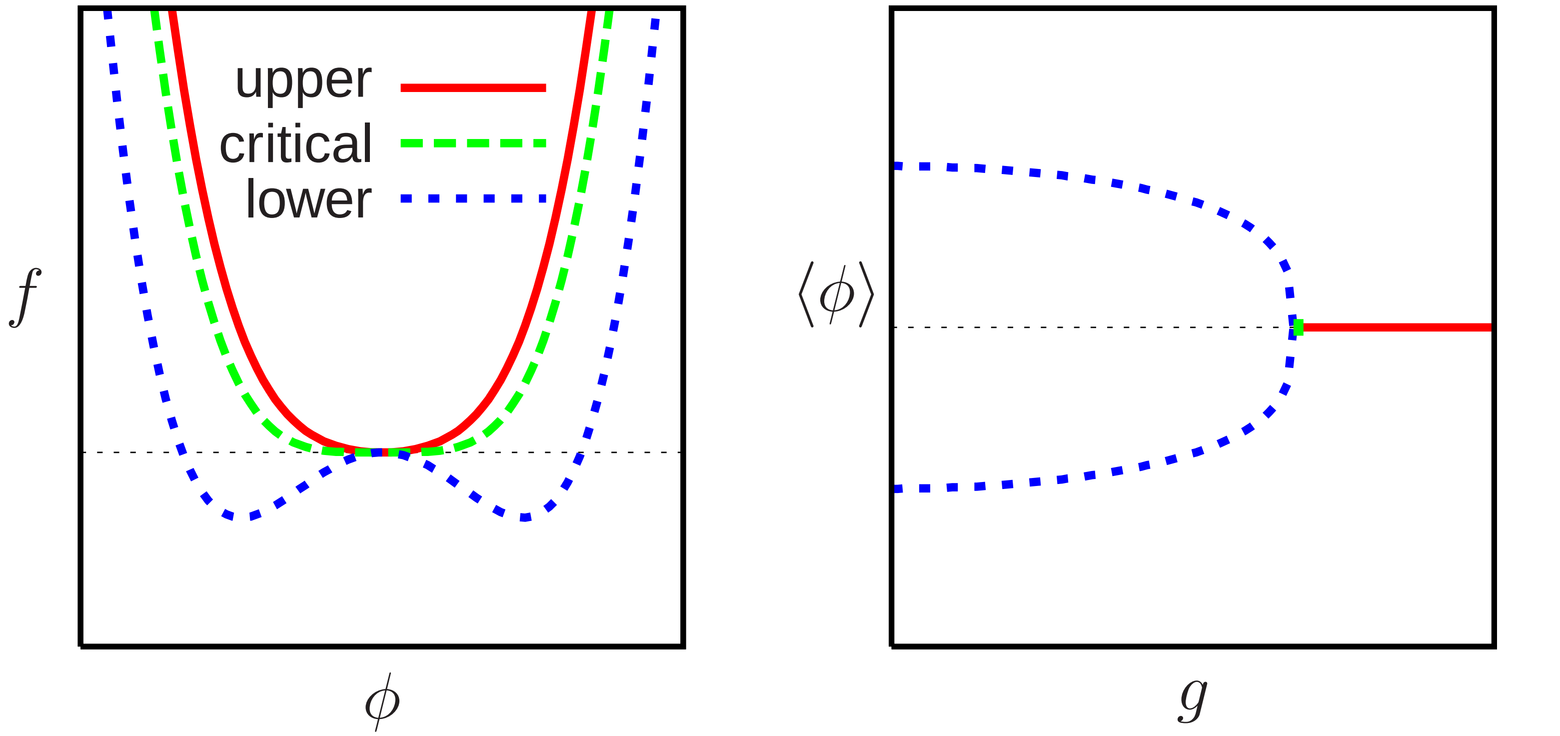
⋆ Dynamic scaling analysis :

  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**



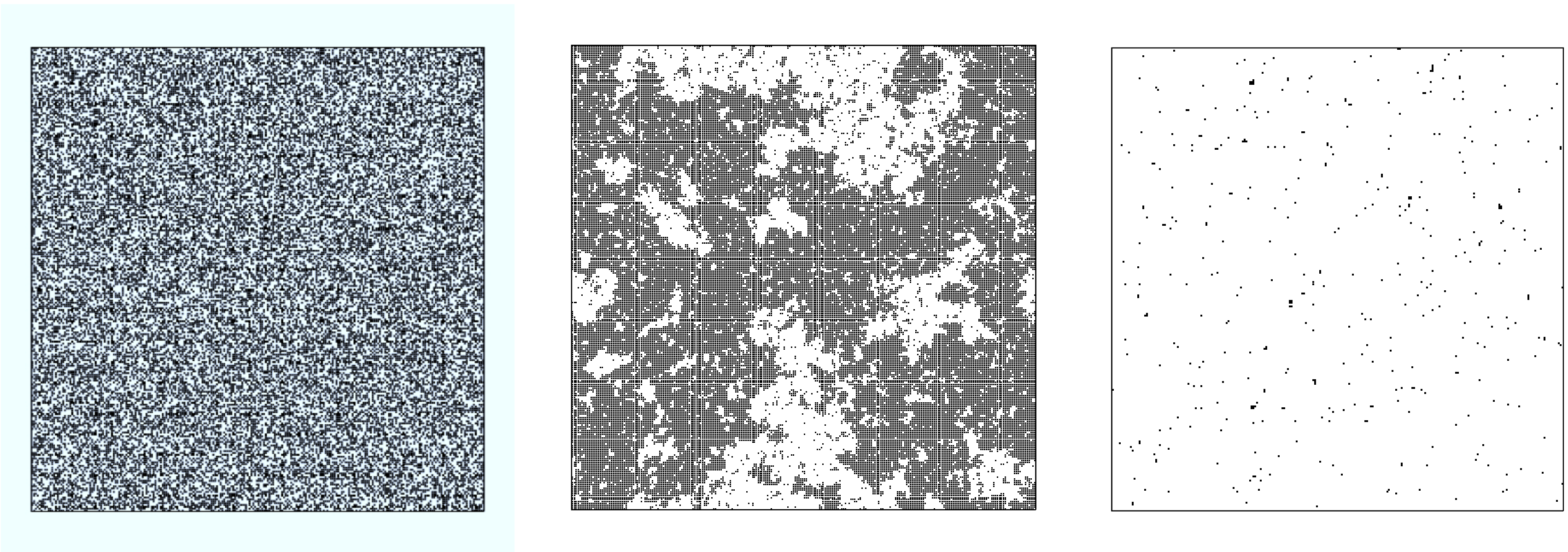
Ginzburg-Landau free-energy

Scalar order parameter

Equilibrium configurations

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

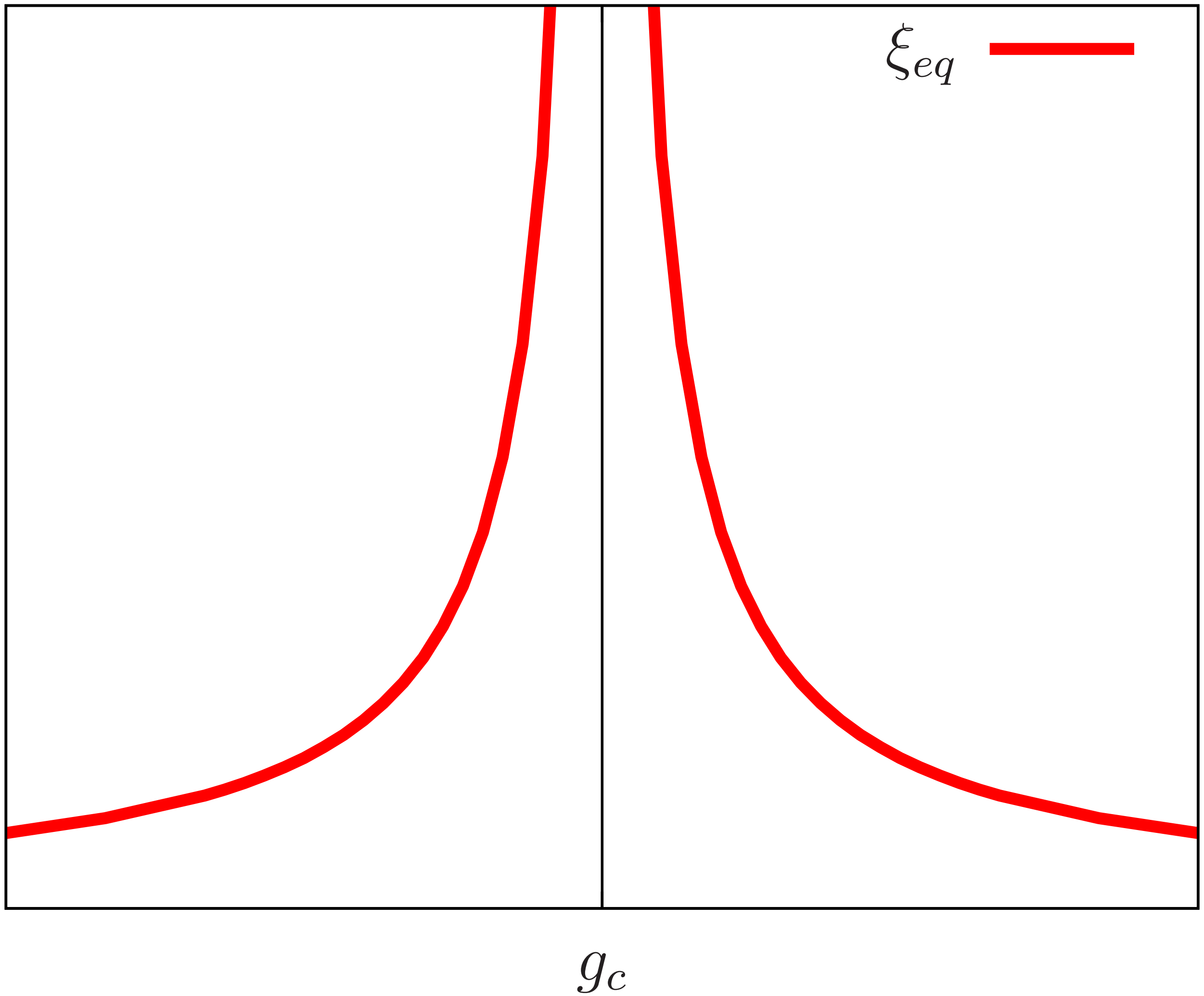
$\langle \phi \rangle = 0$ $\quad\quad$ $\langle \phi \rangle = 0$ $\quad\quad$ $\langle \phi \rangle \neq 0$



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

In a canonical setting the control parameter is $g = T/J$.

The eq. correlation length



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

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, Glauber**).

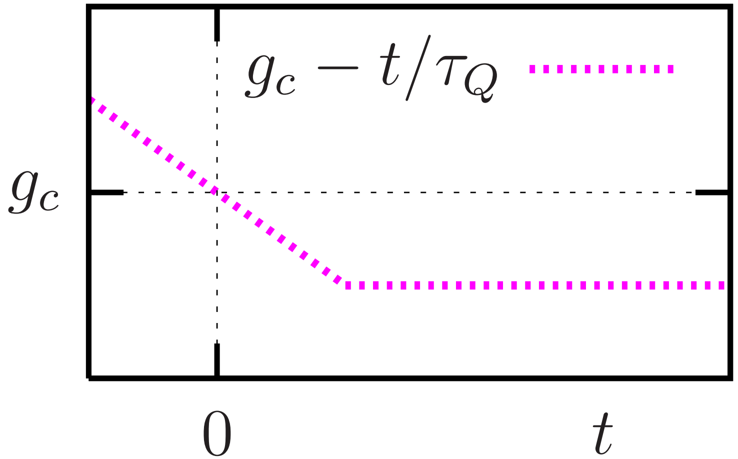
- **Coarse-grained** : average the microscopic variables over a coarse-

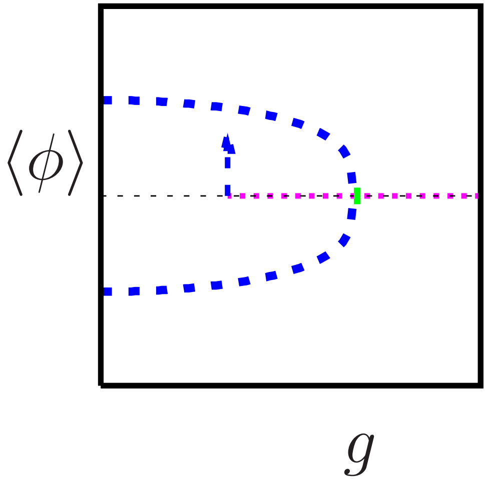
  graining length to construct a field $\phi(x,t)$;

  propose a differential equation for its dynamics (**e.g. time-dependent**

  $\lambda\phi^4$ **Ginzburg-Landau with noise & friction**).

Quenching protocol



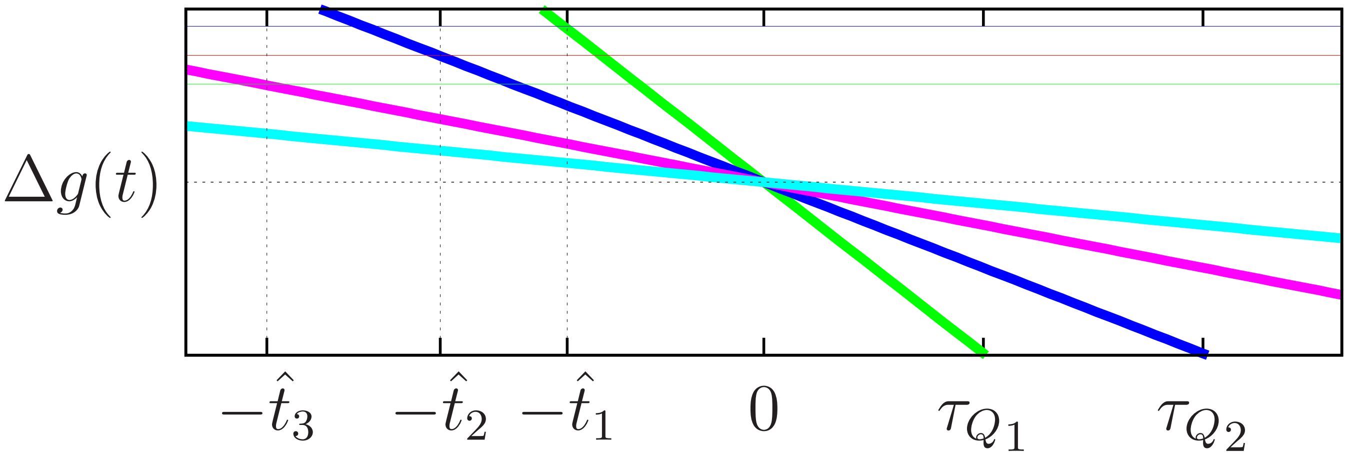


$\boxed{\langle\phi\rangle(t,g) \neq \textbf{ct}}$: **Non-conserved order parameter**

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

Due to dissipation the energy is not conserved either : $\boxed{E(t,g) \neq \textbf{ct}}$.

Annealing or finite τ_Q quenches

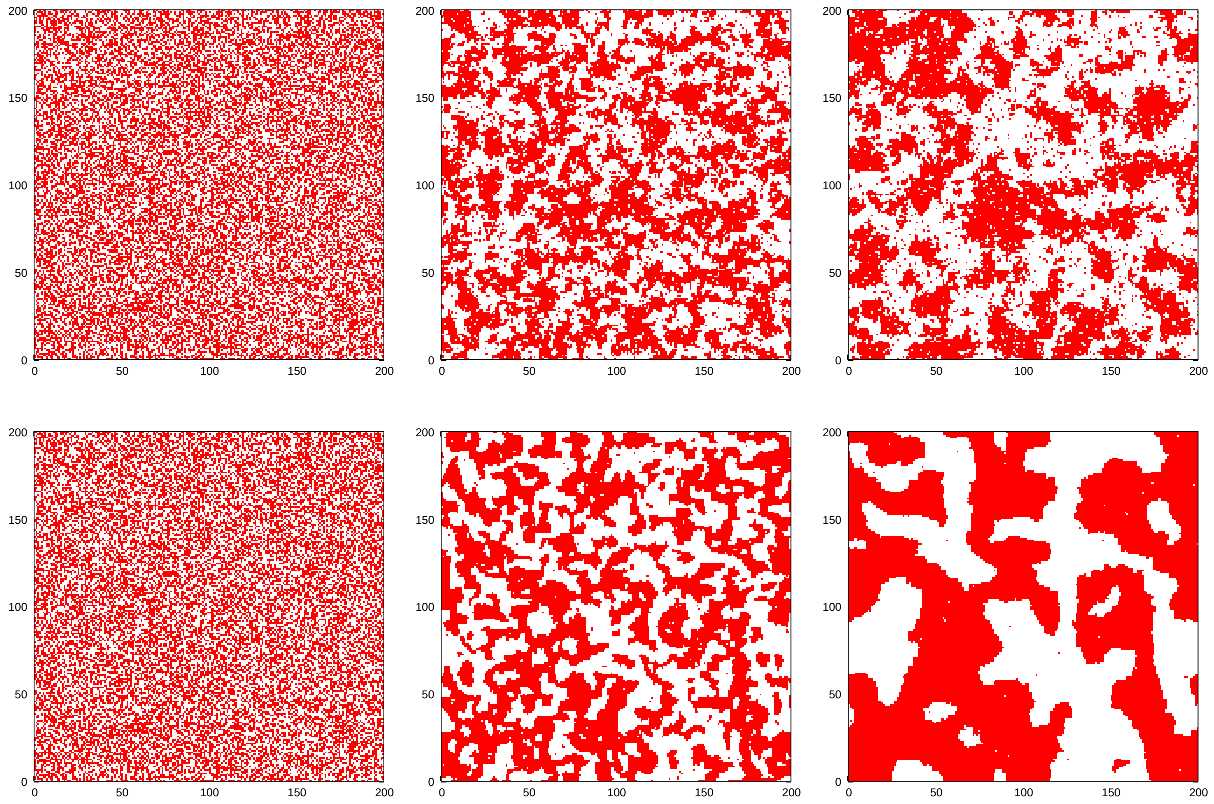


$\Delta g \equiv g(t) - g_c$

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.

$2d$ **Ising model**



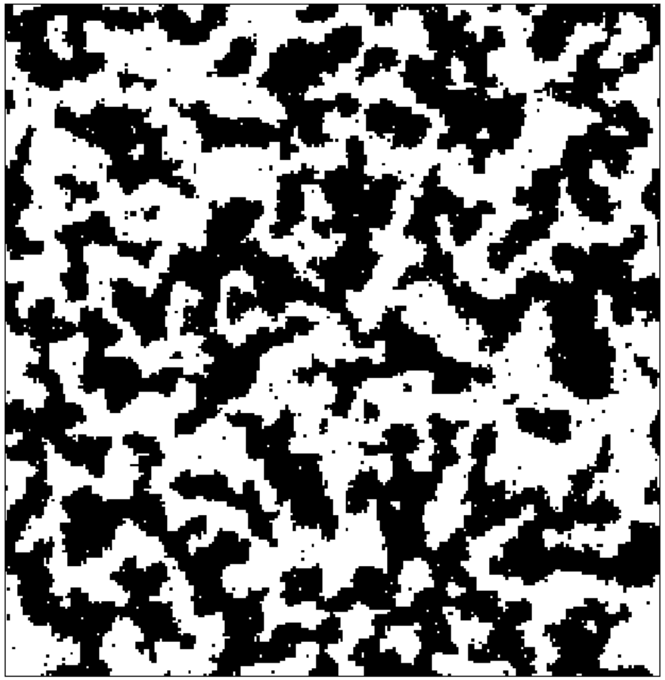
$$g_f = g_c$$

$$g_f < g_c$$

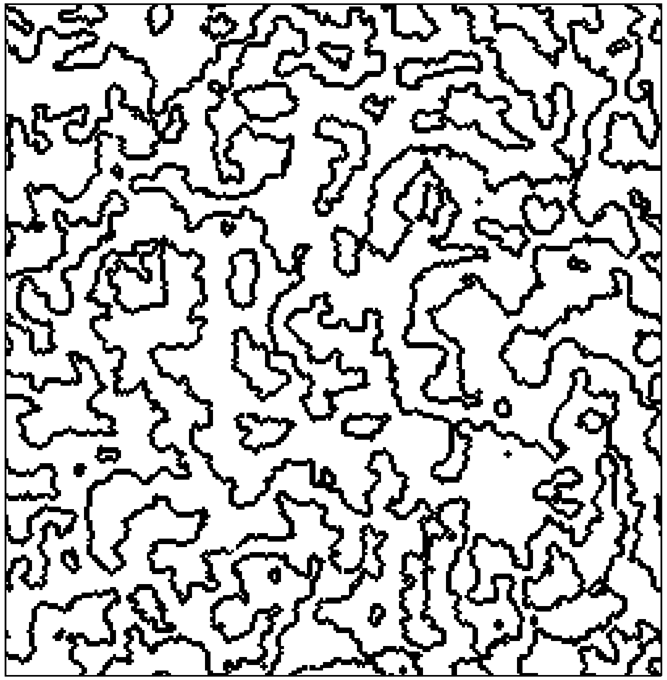
Question : starting from equilibrium at g_i and changing g to g_f with some protocol, how is equilibrium at g_f approached ?

Topological defects : walls

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



Domains



Walls

Look at the initial ($T \to \infty$) distribution, walls are already there !

Annealing : the Z argument

In equilibrium well above g_c

The system follows the pace imposed by the changing conditions, $g(t) = g_c - t/\tau_Q$, 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, 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 $$\boxed{\hat{n} \simeq \xi_{eq}^{-d}(\hat{g}) \simeq (\Delta \hat{g})^{\nu d} \simeq \tau_Q^{-\nu d/(1+\nu z_c)}}$$

and gets blocked at this value ever after.

Zurek 85

Recall : ∞-rapid quench

- At $g_f = g_c$ the system grows ordered 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 a **growing linear size of equilibrated patches**

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

(equilibrium thermal fluctuations are within).

Dynamic scaling

Consequence

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

very early MC simulations **Lebowitz et al 70s** ; review **Bray 90s**

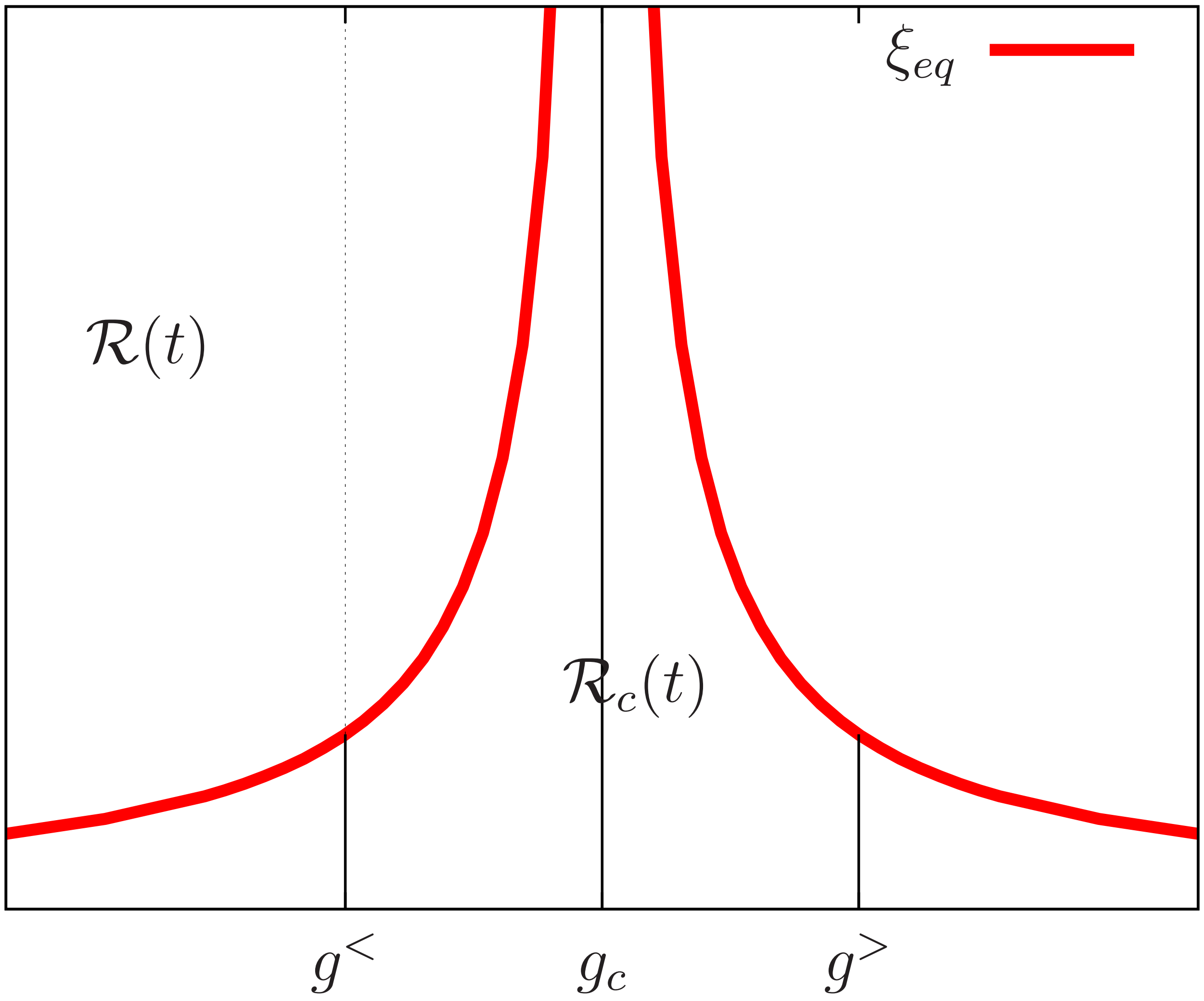
Then one has

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

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

∞-rapid quenches

Control of cross-over



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

Control of cross-over

The **‘typical length’** scales as

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

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

Crossover 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 2dIM with NCOP** .

RG calculation **Bausch, Schmittmann and Jenssen 80s**.

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

Control of cross-over

The **'typical length'** scales as

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

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

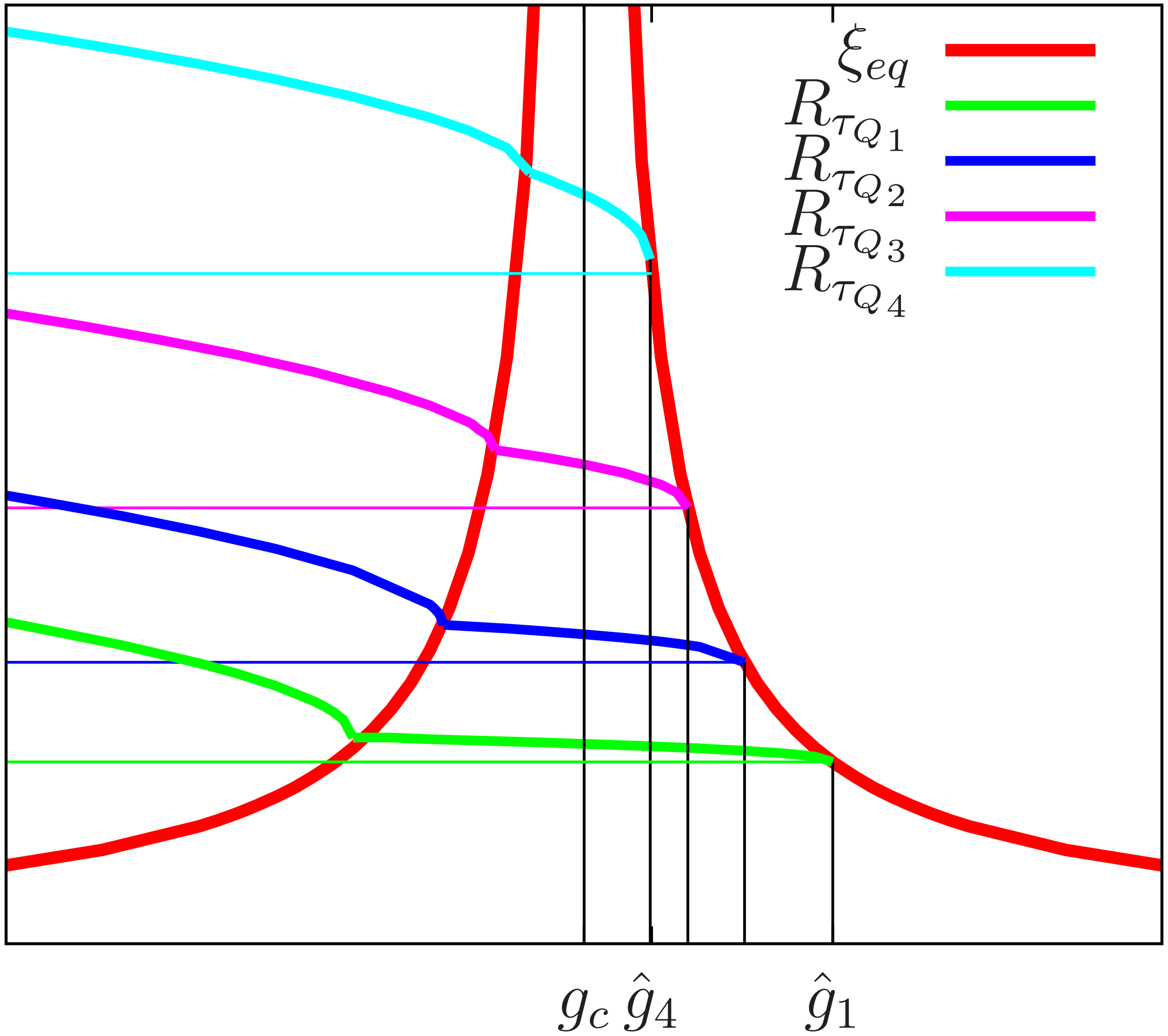
Crossover at $t \simeq \tau_{eq}(g)$ when $\boxed{\mathcal{R}(\tau_{eq}(g), g) \simeq \xi_{eq}(g)}$.

Arenzon, Bray, LFC, Sicilia 08

Note that $z_c \geq z_d$; e.g. $z_d = 2$ **for 2dIM with NCOP**.

Annealing

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



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, $\mathcal{R}(\Delta t) \simeq \Delta t^{1/z_c}$, with ΔT the time spent since the quench, 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**.)

Annealing

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

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

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		$g(\Delta t)$ slowly varying.

Annealing

Crossover

One needs to match the three regimes :

equilibrium, critical and sub-critical growth.

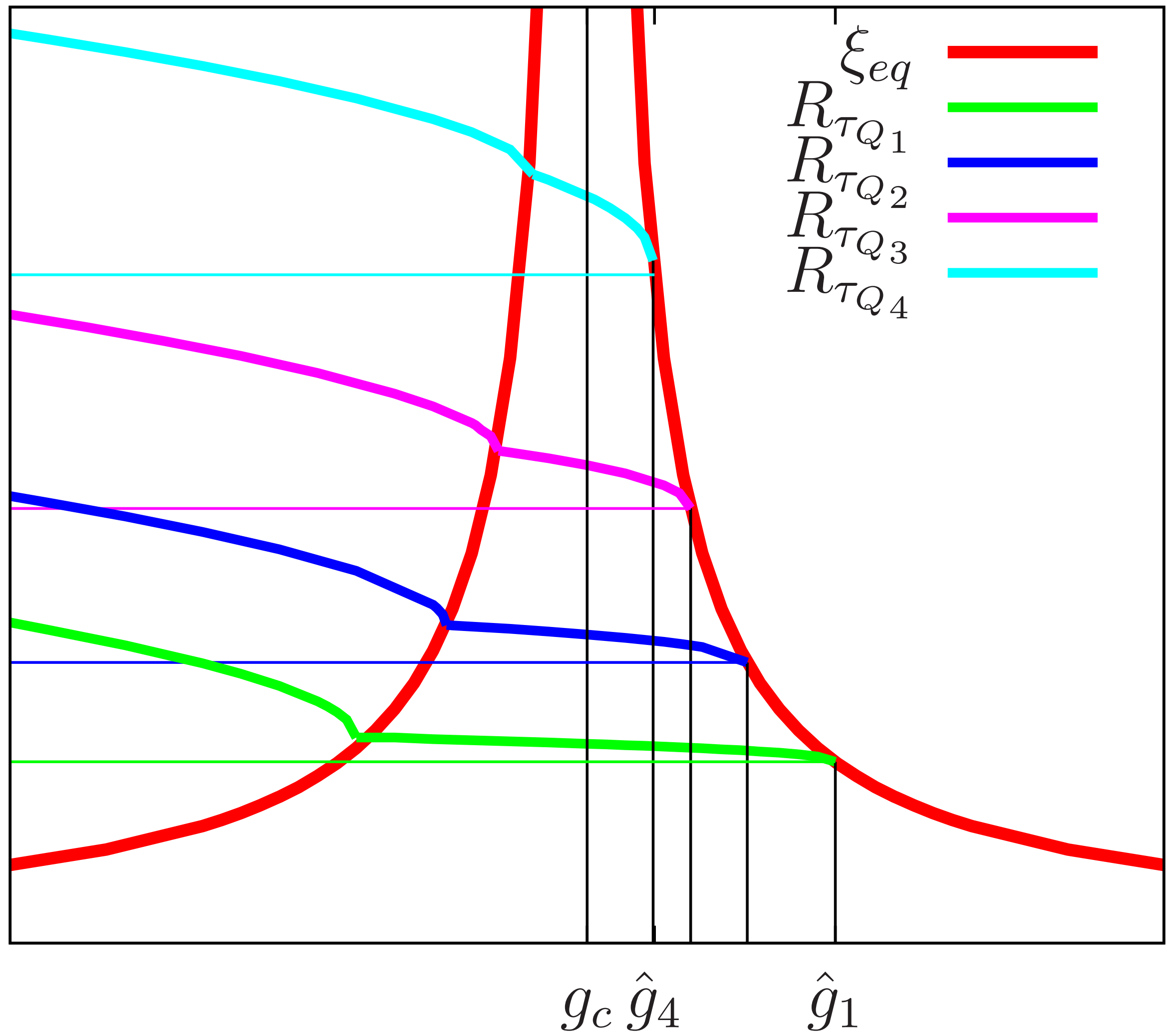
New **scaling assumption** for a linear cooling $|\Delta g(t)| = t/\tau_Q$:

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

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

Annealing

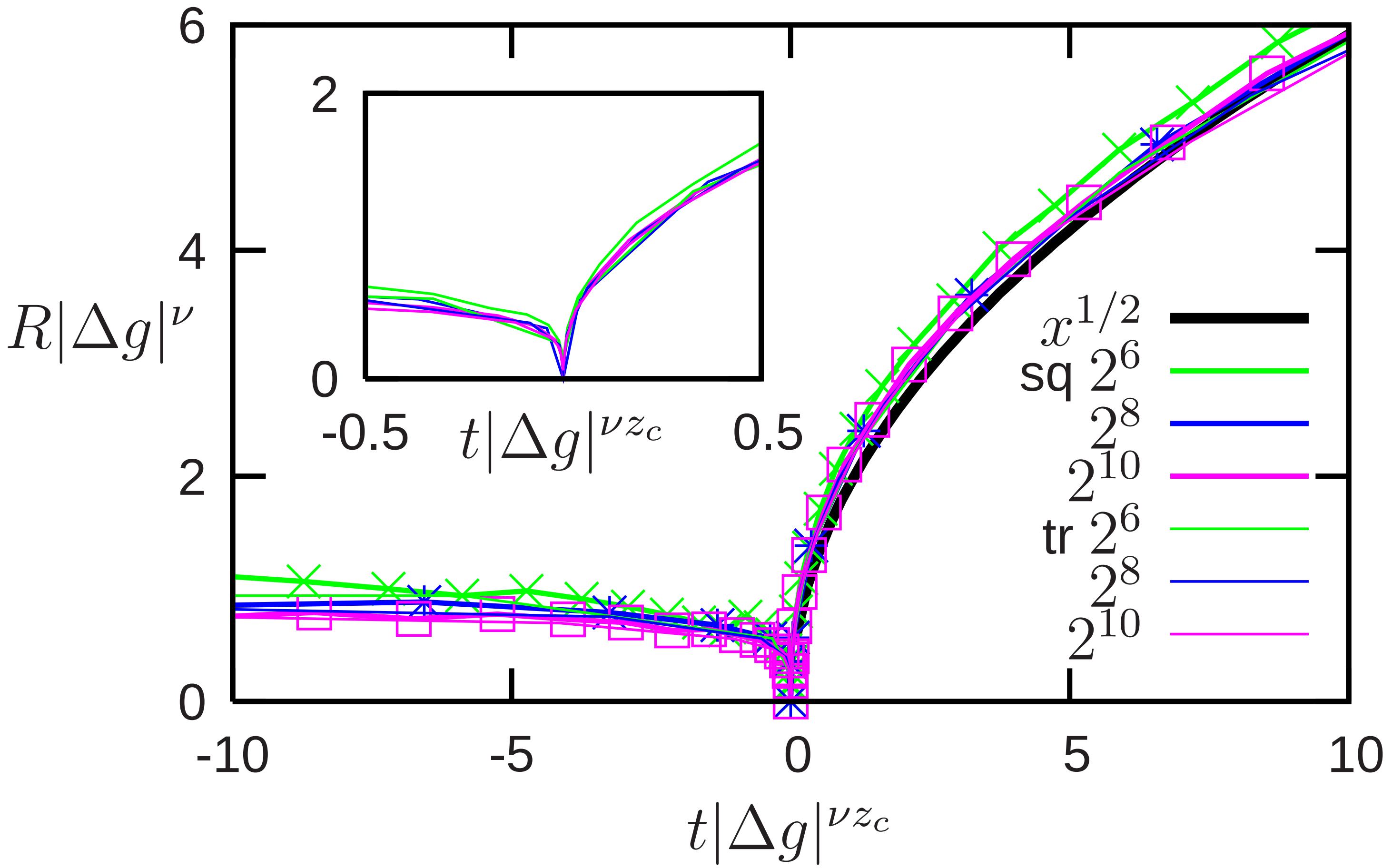
What is the effect of a finite cooling rate on $\mathcal{R}(t,g)$?



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

Simulations

Test of universal scaling in the 2dIM with NCOP dynamics



$z_c \simeq 2.17$ 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

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.

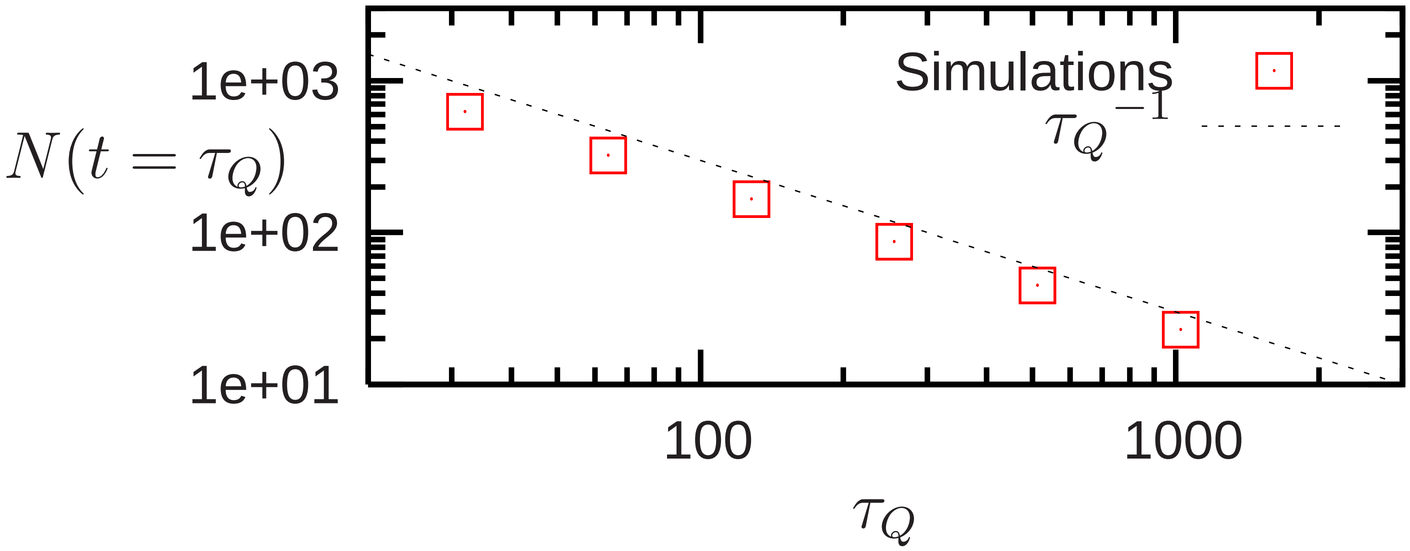
NB t can be much longer than t^* (time for starting sub-critical coarse-ning) ; in particular t can be of order τ_Q while t^* scales as τ_Q^α with $\alpha < 1$.

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

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



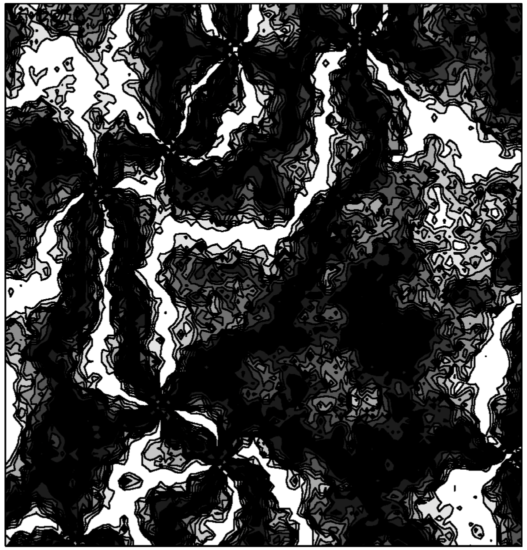
while the KZ mechanism yields $N_{KZ} \simeq \tau_Q^{-\nu/(1+\nu z_c)} \simeq \tau_Q^{-0.31}$.

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

Dynamics in the $2d$ XY model

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

Defects are vortices (planar spins turn around these points)



After a quench vortices annihilate and tend to bind in pairs

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

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

Density of vortices

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 $\Rightarrow$

$$\boxed{\hat{t} \simeq \tau_Q / \ln^2(\tau_Q/t_0)}$$

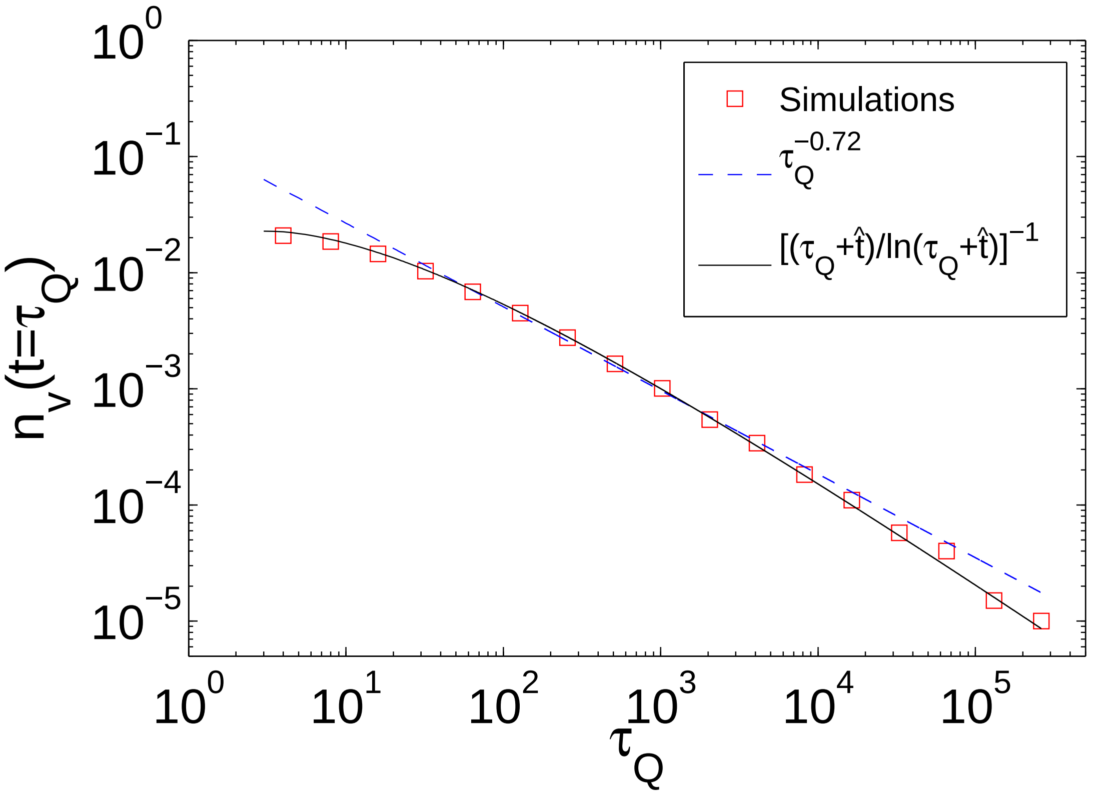
- Logarithmic corrections to the non-equilibrium growing length

$$\boxed{\mathcal{R}(t,T) \simeq [t/\ln(t/t_0)]^{1/z_d}} \qquad \text{with } z_d = 2 \text{ for NCOP.}$$

Density of vortices

Kosterlitz-Thouless phase transition

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



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

Conclusions

- The criterium to find the time when the system falls out of equilibrium above the phase transition ($-\hat{t}$) is correct ; see 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**, e.g. $3d$ xy model.
- **Annealing in quantum dissipative systems.**