Quenches across phase transitions: the density of topological defects

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J. Stat. Mech. P02032 (2011).

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## 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.

# **Motivation**

#### From the statistical physics perspective

Classical systems with well-known equilibrium phases & transitions.

- Applications in, *e.g.* soft condensed-matter, phase separation.
- Hard problem to solve analytically : non-linear interacting field theory.
- Out of equilibrium dynamics in macroscopic systems with mechanisms for relaxation that are understood.
- Comparison to more complex systems for which the phases and phase transitions are not as well known, *e.g.* glassy systems.

Some open issues mentioned in orange Quantum counterparts mentioned at the end.

# Plan of the talk

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 order transit.

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

#### 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 the symmetric phase:
  - Dynamic scaling, the typical ordering length, and the density of topological defects.
     Corrections to the KZ scaling

# **Density of topological defects**

#### **Kibble-Zurek mechanism 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.

• results are universal.

and one scaling law

that we critically revisit within 'thermal' phase transitions



#### **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)



Defects exist and progressively annihilate even after an instantaneous quench into the symmetry-broken phase.

During the time spent in the critical region and/or in the ordered phase the system evolves and the number of topological defects be them domain walls, vortices or other - decreases.

How much it does depends on how long it remains close or below the critical point.



Show these claims using a simple and well-understood system

Find a new scaling law

# *d*-dimensional magnets

#### **Archetypical examples**

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{s_i} \cdot \vec{s_j}$$

J > 0  $\sum_{\langle ij \rangle} s_i = \pm 1$   $\vec{s}_i = (s_i^x, s_i^y)$   $\ell^d \vec{\phi}(\vec{r}) = \sum_{i \in V_{\vec{r}}} \vec{s}_i$  L $T_c > 0$  Ferromagnetic coupling constant.

Sum over nearest-neighbours on a d-dim. lattice. Ising spins.

xy two-component spins.

Coarse-grained field over the volume  $V = \ell^d$ 

Linear size of the system  $L \gg \ell$ 

for d > 1 and  $L \to \infty$ .

Non-conserved order parameter dynamics [*e.g.*,  $\uparrow\downarrow$  towards  $\uparrow\uparrow$ ] allowed. Other microscopic rules - local order parameter conserved, *etc.* 

# **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

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

Dissipation Deterministic Noise

with  $\vec{F}(\vec{\phi}) = -\delta f(\vec{\phi})/\delta \vec{\phi}$ 

(see next-to-next slide for f)

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

Stochastic Gross-Pitaevskii equation

# **Equilibrium configurations**

#### Up & down spins in a 2d Ising model



 $\langle s_i \rangle_{eq} = 0 \qquad \langle s_i \rangle_{eq} = 0 \qquad \langle s_i \rangle_{eq^+} > 0$   $\phi(\vec{r}) = 0 \qquad \phi(\vec{r}) = 0 \qquad \phi(\vec{r}) > 0$ 

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 eq. correlation length

#### From the spatial correlations of equilibrium fluctuations

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



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

In KT transitions,  $\xi_{eq}$  diverges exponentially on the disordered and it is  $\infty$  in the quasi long-range ordered side of  $g_c$ , that is a critical phase, *e..g.* 2d xy model.

# **Topological defects**

#### **Definition via one example**

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

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

u < 0 with finite localized energy.

 $d = 1 \text{ domain wall} \qquad \phi$   $\phi(x,t) \propto \sqrt{\frac{-u}{\lambda}} \tanh\left(\sqrt{\frac{-u}{\lambda}} x\right)$ 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

 $\mathcal{X}$ 

# 2d lsing model

#### Snapshots after an instantaneous quench at t=0



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



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



In both cases one sees the growth of 'red and white' patches and interfaces surrounding such geometric domains.

More precisely, spatial regions of local equilibrium (with vanishing or non-vanishing order parameter) grow in time and

a growing length R(t,g) can be computed with the help of dynamic scaling.

### Instantaneous quench

#### **Dynamic scaling**

very early MC simulations Lebowitz et al 70s & experiments

One identifies a growing linear size of equilibrated patches

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

R(t,g)

At $g_f = g_c$	$C(r,t) \simeq C_{eq}(r) f_c(\frac{r}{\mathcal{R}_c(t)})$	proven w/dyn-RG
At $g_f < g_c$	$C(r,t) \simeq C_{eq}(r) + f(\frac{r}{\mathcal{R}(t,g)})$	argued & MF

and the number density of interfaces should scale as

$$n(t,g) = N(t,g)/L^d \simeq [R(t,g)]^{-d}$$

Reviews Hohenberg & Halperin 77 (critical) Bray 94 (sub-critical)

### Instantaneous quench

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

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### Instantaneous quench

#### **Control of cross-overs**



### **Instantaneous quench to** $g_c + \epsilon$

#### **Growth and saturation**

The length grows and saturates

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

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  $R(\tau_{eq}(g),g) \simeq \xi_{eq}(g)$ 

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

Dynamic RG calculations Bausch, Schmittmann & Jenssen 80s.

### Instantaneous quench to $g_c$

#### **Non-stop growth**

The length grows

$$R(t,g) = \mathcal{R}_c(t) \simeq t^{1/z_c} \qquad t \ll \tau_{eq}(g) \to \infty$$

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

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

Dynamic RG calculations Bausch, Schmittmann & Jenssen 80s.

### Instantaneous quench to $g < g_c$

#### **Deep quenches**

The length grows as

$$R(t,g) = \mathcal{R}(t,g) \approx \zeta(g) t^{1/z_d} \qquad t \gg \tau_{eq}$$

with  $\tau_{eq}$  the equilibrium relaxation time.

Non-conserved scalar order parameter

 $z_d = 2$ 

Proven for time-dependent Ginzburg-Landau equation Allen & Cahn 79 & arguments for lattice models Kandel & Domany 90, Chayes et al. 95

Not really a 'formal' proof & even harder for vector order parameter and/or conservation laws

## Instantaneous quench to $g < g_c$

#### **Deep quenches**

The length grows as

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Non-conserved scalar order parameter

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Weak quench disorder effect on  $\mathcal{R}$ ? Is there an  $\mathcal{R}$  with strong disorder?

### Instantaneous quench to $g_c - \epsilon$

#### **Control of cross-overs**

The length grows with different laws

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

with  $\xi_{eq}$  and  $\tau_{eq}$  the equilibrium correlation length and relaxation time.

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

Arenzon, Bray, LFC & Sicilia 08

Note that  $z_c \ge z_d$ 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**

#### configurations after a sub-critical instantaneous quench



$$n(t,g) = N(t,g)/L^d \simeq [R(t,g)]^{-d}$$

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

# Finite rate quenching protocol

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



 $\Delta g \equiv g(t) - g_c = -t/\tau_O$ with

Standard time parametrization

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

Simplicity argument: linear cooling could be thought of as an approximation of any cooling procedure g(t) 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,  $\tau_{eq}$ , is of the order of the typical time-scale over which the control parameter, g, changes :

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

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

Zurek 85

and the claim is that it gets blocked at this value ever after

### Sketch of Zurek's proposal for $R_{\tau_Q}$



#### **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,  $R^* \simeq \xi_{eq}(g^*)$ .

For a linear cooling a simple calculation yields

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

(if the scaling for an infinitely rapid critical quench,  $\Delta R(\Delta t) \simeq \Delta t^{1/z_c}$ , with  $\Delta t = t^* - \hat{t}$  the time spent since entering the critical region holds) No change in leading scaling with  $\tau_Q$ .

However, for a non-linear cooling, e.g.  $\Delta g = (t/\tau_Q)^x$  with x > 1,

 $R^*\simeq au_Q^a$  with  $a>
u/(1+
u z_c)$  for x>1

### Contribution from critical relaxation, $R^*_{\tau_O}$



#### Far from the critical region, in the coarsening regime

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

#### Working assumption for the slow quench



with  $\Delta t$  the time spent since entering the sub-critical region at  $R^*$ .

 $\infty$ -rapid quench with  $\rightarrow$  finite-rate quench with  $g = g_f$  held constant g slowly varying.

#### The two cross-overs

One needs to match the three regimes :

equilibrium, critical and sub-critical growth.

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

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

Scaling on both sides of the critical (uninteresting for a linear cooling) region

Crossover at  $t\simeq t^*\simeq \tau_Q^\alpha$  with  $\alpha<1$  ensured

# Finite rate quenching protocol

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

$$\left| R \simeq \left( t/\tau_Q \right)^{-\nu + \frac{\nu z_c}{z_d}} t^{\frac{1}{z_d}} \simeq \left| \Delta g \right|^{-\nu + \frac{1+\nu z_c}{z_d}} \tau_Q^{\frac{1}{z_d}} \right|$$



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

R depends on ]t and  $\tau_Q]$  or on  $[\Delta g \text{ and } \tau_Q]$  independently R increases with  $[\Delta g \text{ and } \tau_Q]$ 

### Sketch of the effect of $au_Q$ on 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.

## **Number of domain walls**

Test of universal scaling in the 2dIM with NCOP dynamics

Dynamic scaling implies

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

with d the dimension of space

Therefore

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

depends on *both* times t and  $\tau_Q$ .

NB t can be much longer than  $t^*$  (time for starting sub-critical coarsening); in particular t can be of order  $\tau_Q$  while  $t^*$  scales as  $\tau_Q^{\alpha}$  with  $\alpha < 1$ . Since  $z_c$  is larger than  $z_d$  this quantity grows with  $\tau_Q$  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 scaling yields  $N_{\rm KZ}\simeq au_Q^{u/(1+
u z_c)}\simeq au_Q^{-0.31}.$ 

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

# **Topological defects**

#### **Definition via another example**

A vector field

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

in d=2 for  $\vec{\phi}=(\phi^x,\phi^y)$  leads to a two dimensional vortex



Picture from the Cambridge Cosmology Group webpage

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

# 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

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

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  $T_{\rm KT}$ 

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

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

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

Logarithmic corrections to the sub-critical growing length

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

with  $z_d = 2$  for NCOP

# Dynamics in the 2d XY model

**KT phase transition & coarsening** 

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



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

# Work in progress

Quench rate dependencies in the dynamics of the

3d O(2) relativistic field theory  $c^{-2}\partial_t^2\psi(\vec{r},t) + \gamma_0\partial_t\psi(\vec{r},t) = [\nabla^2 - g(|\psi|^2 - \rho)] \psi(\vec{r},t) + \xi(\vec{r},t)$ 

and the stochastic Gross-Pitaevskii equation

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

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

Study of vortex lines.

Kobayashi & LFC

# **Beyond density of defects**



2d Ising & voter models Finite size effects & short-time dynamics. **Distributions & geometry** Percolation & fractality Arenzon, Blanchard, Bray Corberi, LFC, Picco, Sicilia & Tartaglia Krapivsky & Redner

# 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.



#### Annealing in quantum dissipative systems

Same arguments apply though harder problem since

Quantum environment usually implies non-Ohmic 'noise' & non-Markov 'dissipation'.

- Critical quenches  $\mathcal{R}_c(t) \simeq t^{1/z_c}$ 

**Bonart, LFC & Gambassi 11** (classical non-Ohmic) **Gagel, Orth & Schmalian 14** (quantum non-Ohmic)

- Quantum coarsening  $\mathcal{R}(t) \simeq t^{1/z_d}$ 

Rokni & Chandra 04

Aron, Biroli & LFC 08

Slow quenches in a XY quantum spin chain coupled to a bath

Patané, Amico, Silva, Fazio, Santoro 09

## Finite rate quenching protocol

#### **Some details**



2dIM :  $\hat{t} \simeq \tau_Q^a$  with  $a \simeq 0.68$ ,  $\Delta \hat{g} \simeq \tau_Q^{-b}$  with  $b \simeq 0.31$ ,  $\hat{R} \simeq \tau_Q^c$  with  $c \simeq 0.31$ .

### Finite rate quenching protocol

#### **Some details**

Say 
$$g(t) = g_c - (t/\tau_Q)^x$$
 after  $-\hat{t}$   $(t_{max} = \tau_Q^x g_c)$ 

Non-trivial growth within the critical region

$$R^* \simeq |\Delta g^*|^{-\nu} \simeq (t^*/\tau_Q)^{-x\nu} \simeq \hat{R} + c \, |t^* - \hat{t}|^{1/z_c}$$

yields  $t^*$  and

$$R^* \simeq \begin{cases} \hat{R} & x < 1\\ \hat{R} \tau_Q^{(x-1)/[xz_c(1+\nu z_c)]} & x \ge 1 \end{cases}$$

 $\begin{array}{ll} 2d \text{IM and, } \textit{e.g., } x = 2: & \hat{R} \simeq \tau_Q^{0.31} \text{ and } R^* \simeq \tau_Q^{0.39} \\ 2d \text{IM and, } \textit{e.g., } x \rightarrow \infty: & \hat{R} \simeq \tau_Q^{0.31} \text{ and } R^* \simeq \hat{R}^{\frac{1+\nu z_c}{\nu z_c}} \simeq \tau_Q^{1/z_c} \simeq \tau_Q^{0.46} \end{array}$