Coarsening dynamics in NLC

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PLAN

1) Domains and I-N phase transition:

   some known facts & open problems

2) Semi-microscopic model

3) Coarsening dynamics

4) Equilibrium domain structure of weakly perturbed systems

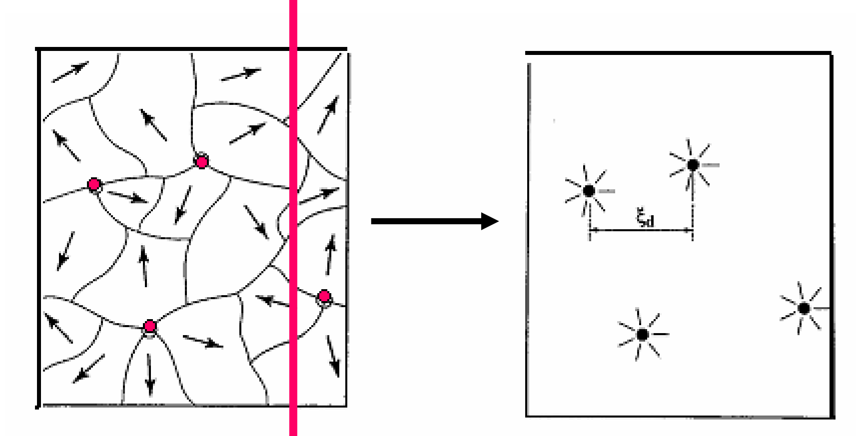
5) Summary

I-N quench

Domains & phase transition:

i) continuous symmetry breaking

ii) causality



Signature : **Goldstone mode**

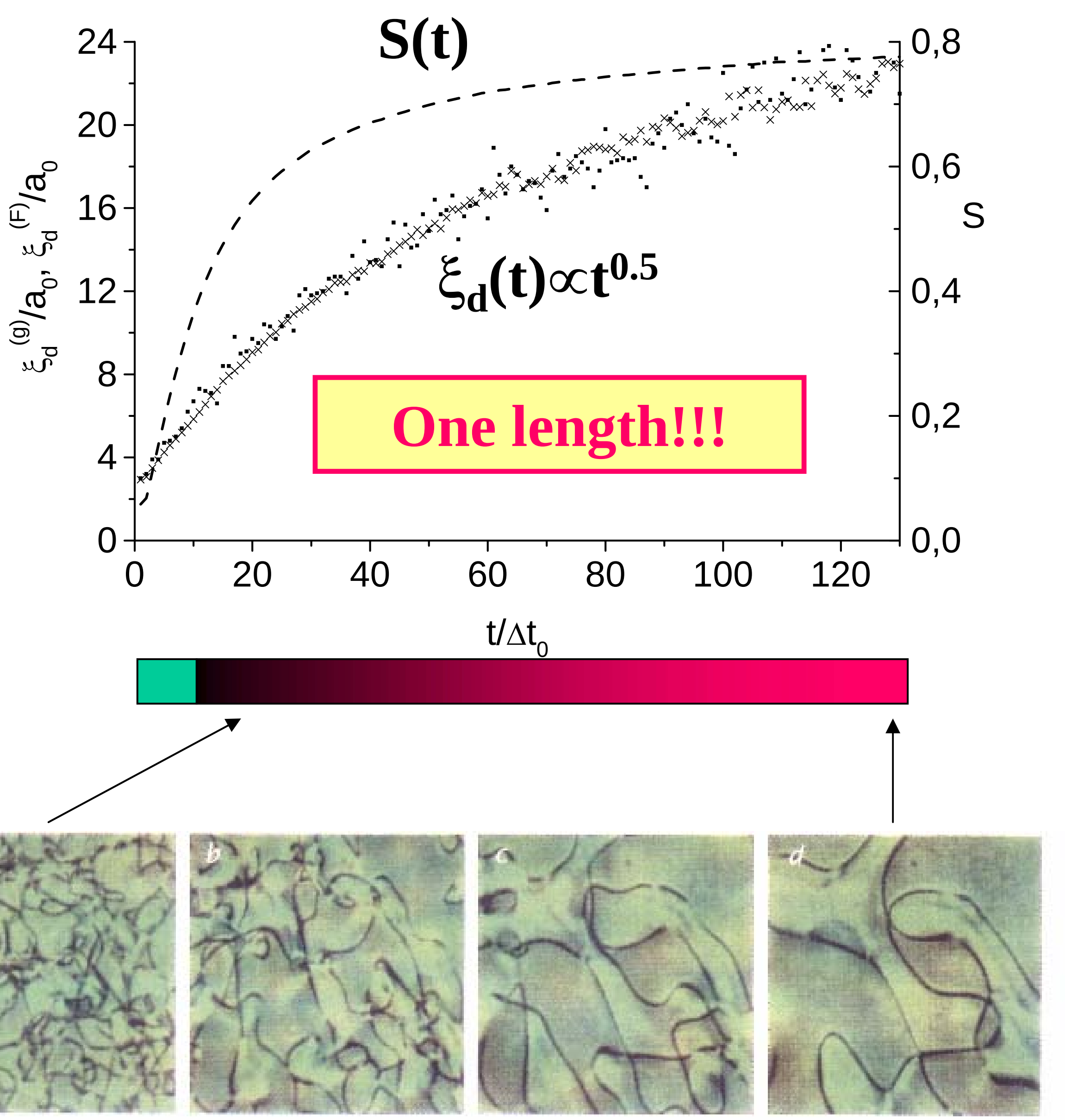
I-N phase transition :

i) continuous symmetry breaking of orientational ordering,

ii) growth of non-conserved order parameter

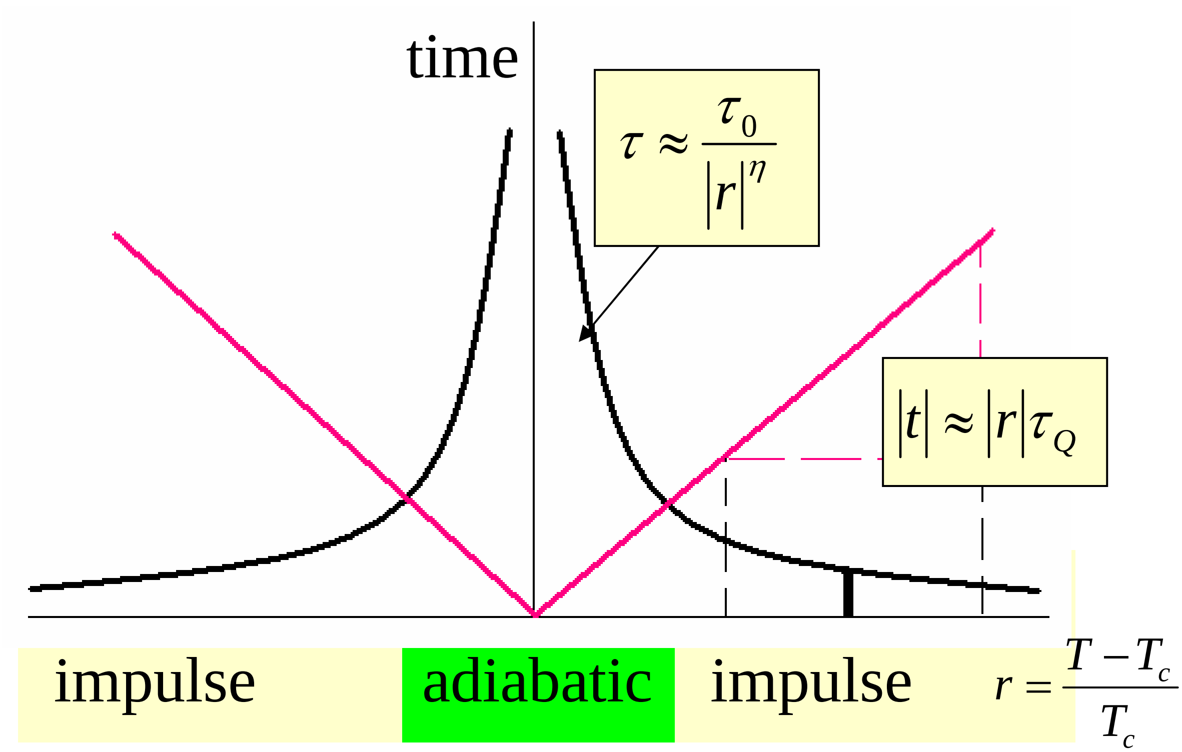
I-N quench: qualitatively different regimes

- early regime -> exponential S(t) growth
- domain regime –> domains are visible
- late-stage regime -> defects are visible



Kibble – Zurek mechanism ?

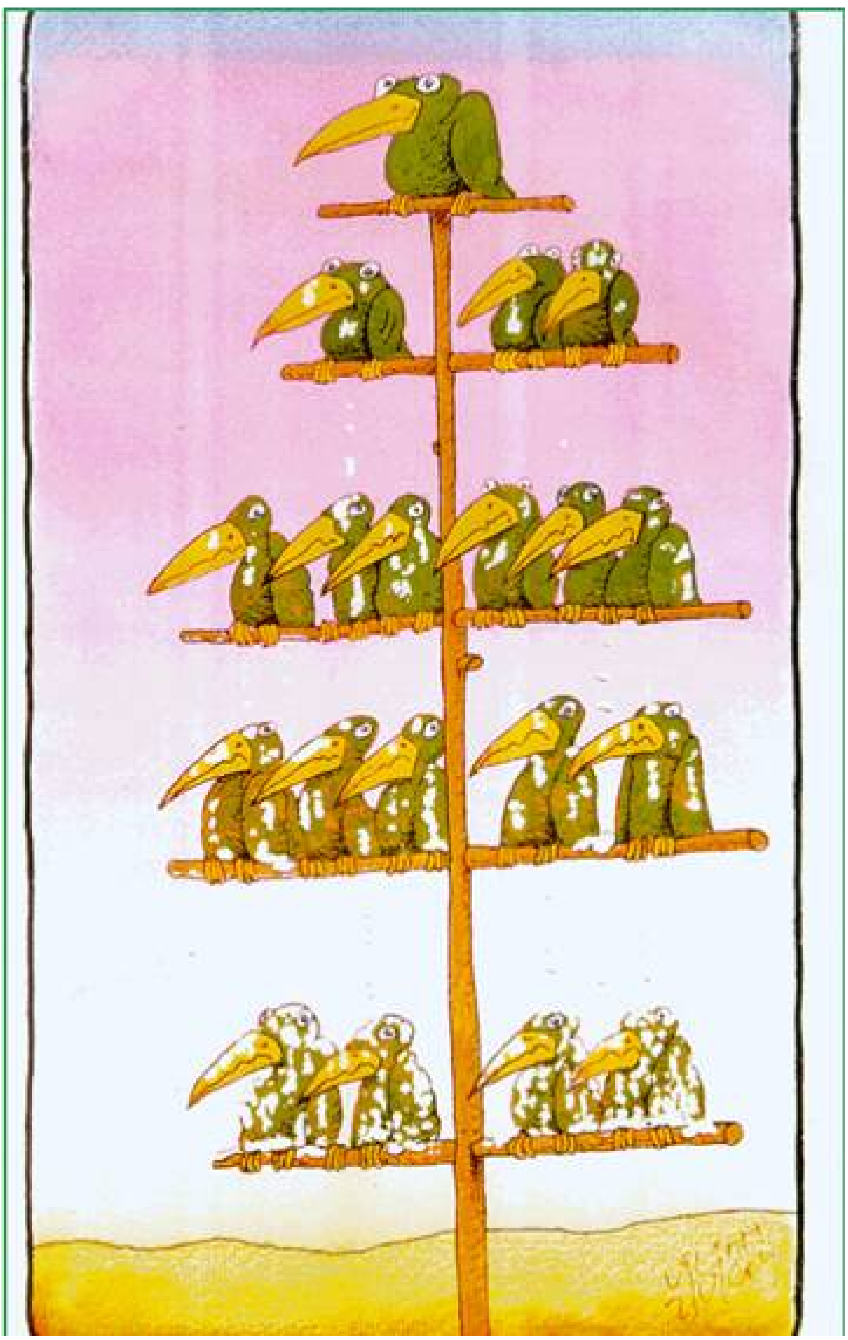
$$r = \frac{T - T_{IN}}{T_{IN}} = -\frac{t}{\tau_Q}\;; \quad \tau \approx \frac{\tau_0}{|r|^\eta} \quad , \quad \xi \approx \frac{\xi_0}{|r|^\nu}$$



$$\xi_f \equiv \xi_d(t_z) \approx \xi_0 \left(\frac{\tau_Q}{\tau_0}\right)^{\frac{\nu}{1+\eta}}$$

$$LCs: \quad \nu = \frac{1}{2}, \quad \eta = 1 \longrightarrow \boxed{\xi_f = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{1}{4}}}$$

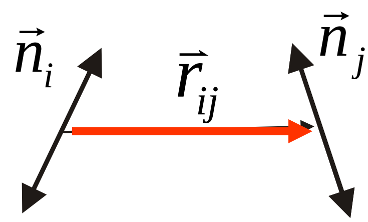
? **How "universal" is this behavior?**



MODEL

Molecules in the lattice interact via the modified induced dipole-induced dipole coupling.

$$f_{ij} = -J\left(\frac{a}{r_{ij}}\right)^6 \left(\vec{n}_i.\vec{n}_j - 3\varepsilon \frac{(\vec{n}_i.\vec{r}_{ij})(\vec{n}_i.\vec{r}_{ij})}{r_{ij}^2}\right)^2$$



$$\vec{n} = \vec{e}_x \sin\theta\cos\phi + \vec{e}_y \sin\theta\sin\phi + \vec{e}_z \cos\theta$$

Molecular Brownian Dynamics.

$$\theta_i(t+\Delta t) = \theta_i(t) + \theta_{i,torque} + \theta_{i,random}$$

$$\phi_i(t+\Delta t) = \phi_i(t) + \phi_{i,torque} + \phi_{i,random}$$

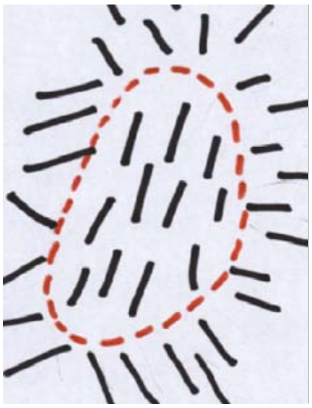
In the molecelar eigen frame (x',y',z')

$$\vartheta_i^{(x',y')} = -\frac{D\delta t}{kT}\sum_{j\neq i}\frac{\partial f_{ij}}{\partial \vartheta_i^{(x',y')}} + \vartheta_{i,random}^{(x',y')}$$

Developed by Zlatko Bradac for his PhD

Determination of ξ_d

i) Geometrical approach



$$V \approx \frac{4\pi {\xi_d^{(g)}}^3}{3}$$

ii) Energy appoach

$$\Delta F_{excess} = F - F_{bulk}$$

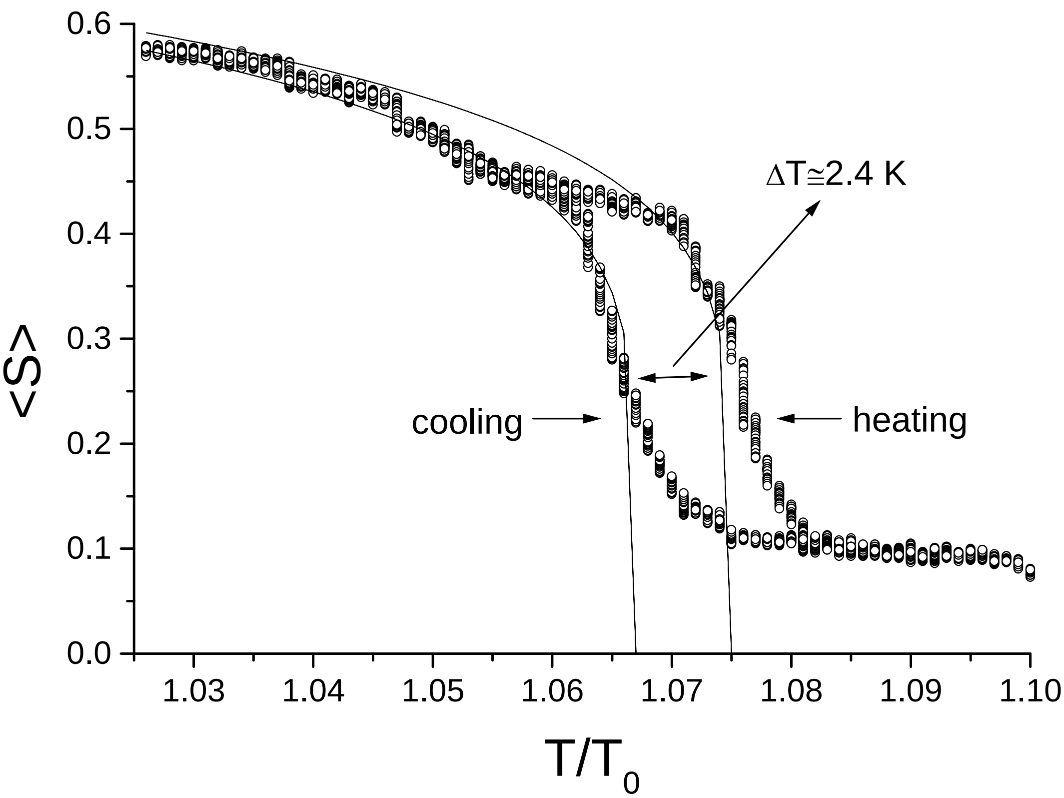
$$\frac{\Delta F_{excess}}{V} \approx \frac{f_{wall} V_{domain-wall}}{V_{domain}} \approx \frac{f_{wall}\xi_d^2 d_w}{\xi_d^3}$$

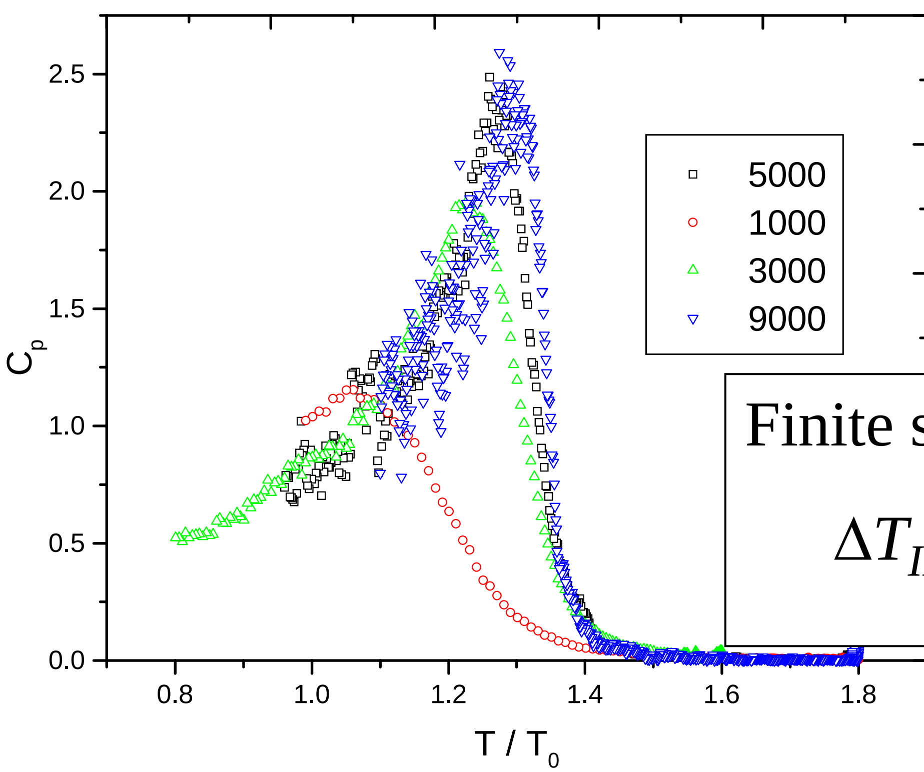
$$\xi_d^{(f)} \propto \frac{1}{\Delta F_{excess}}$$

$$S \approx \frac{S_{bulk}(V - V_{wall}) + S_{wall} V_{wall}}{V}$$

$$S \approx S_{bulk}(1 - \frac{V_{wall}}{V}) \approx S_{bulk}(1 - \frac{d_w}{\xi_d})$$

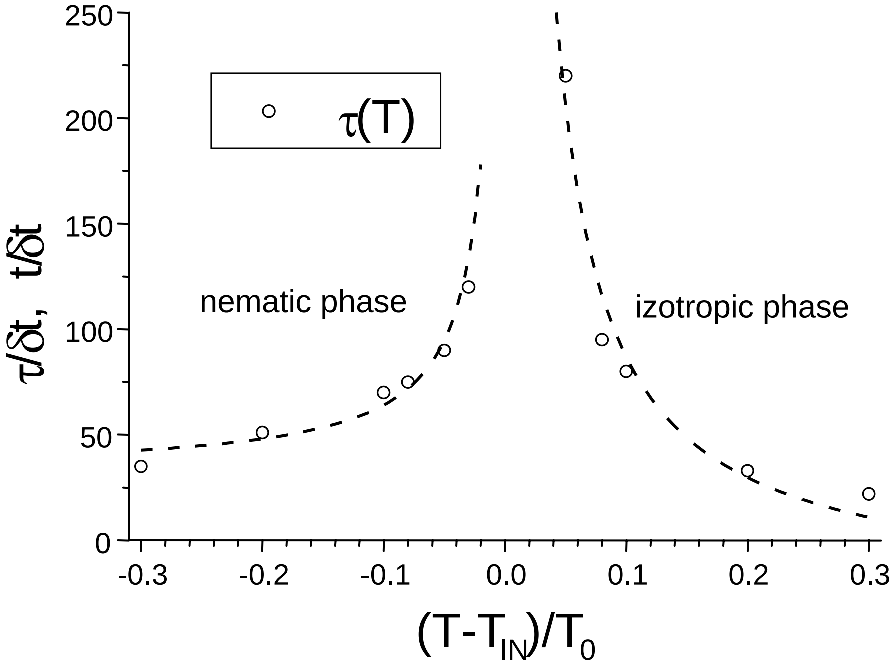
Equlibrium behavior



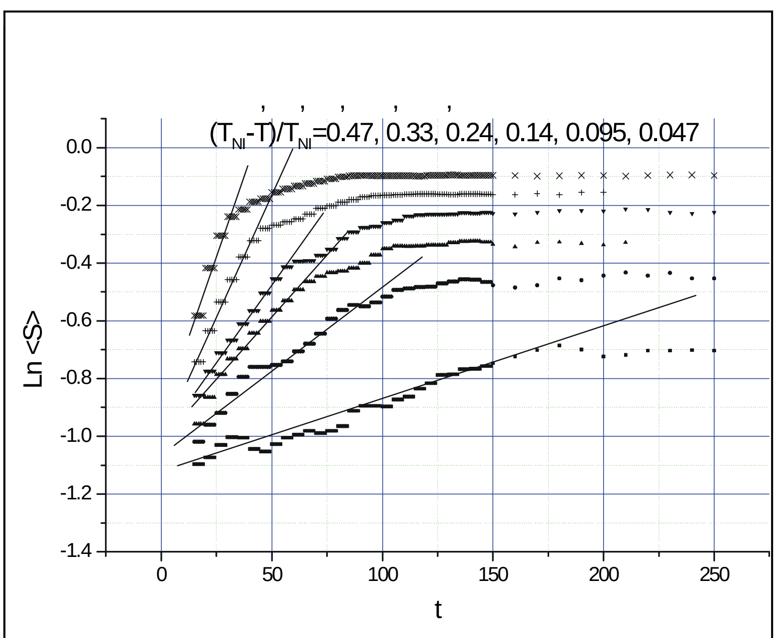


Finite size scaling

$$\Delta T_{IN} \propto \frac{1}{R^3}$$

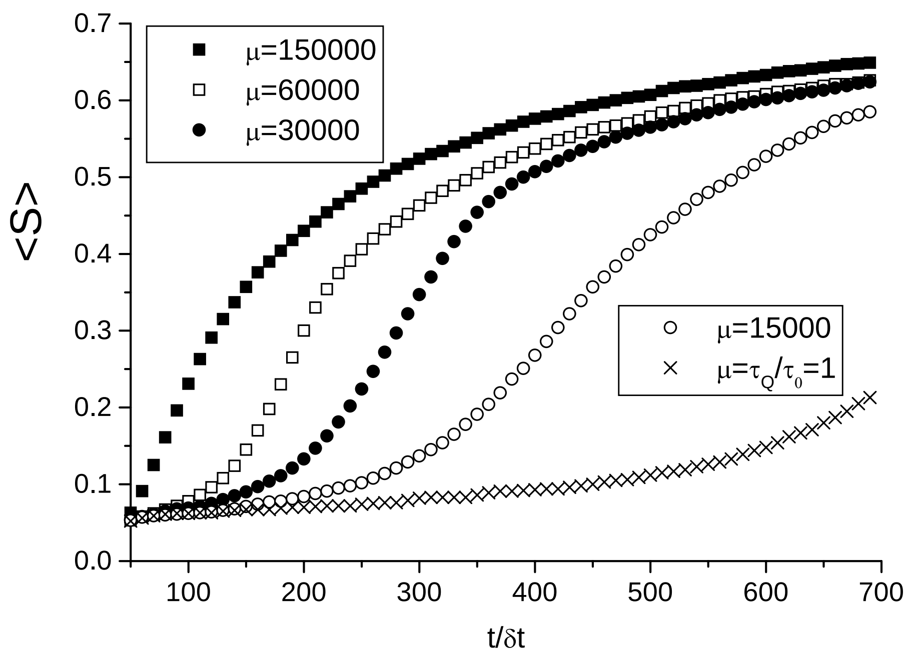


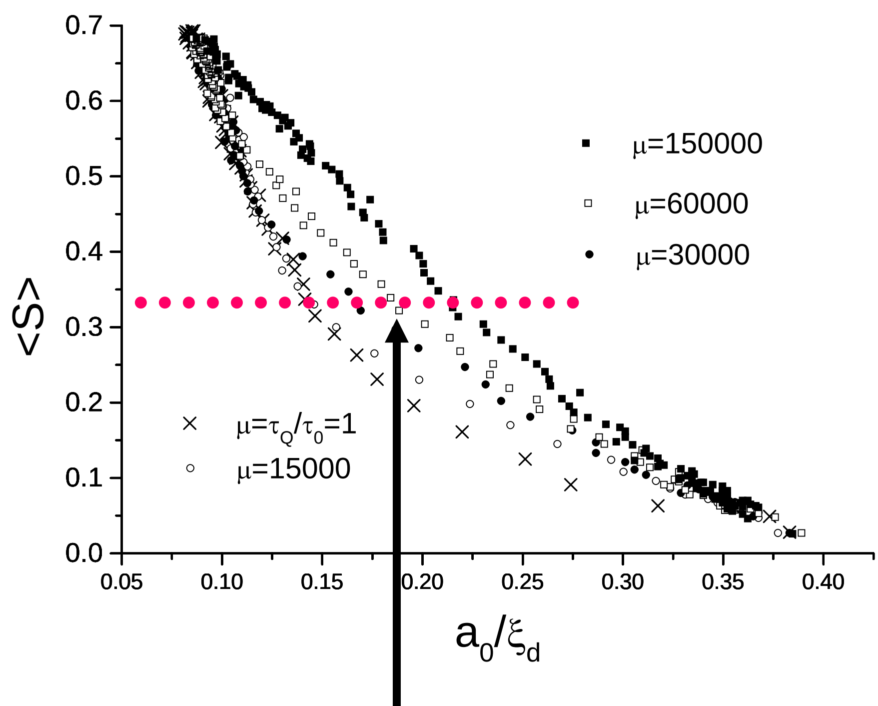
τ(T)
nematic phase
izotropic phase
τ/δt, t/δt
(T-T_IN)/T_0



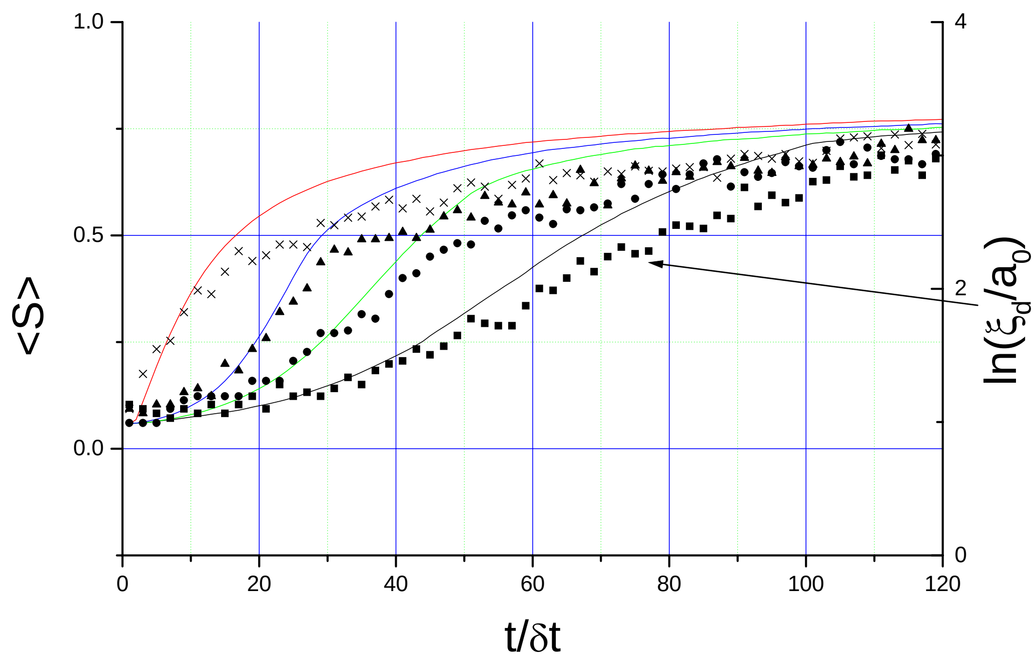
(T_NI-T)/T_NI=0.47, 0.33, 0.24, 0.14, 0.095, 0.047
Ln <S>
t

Quench dynamics

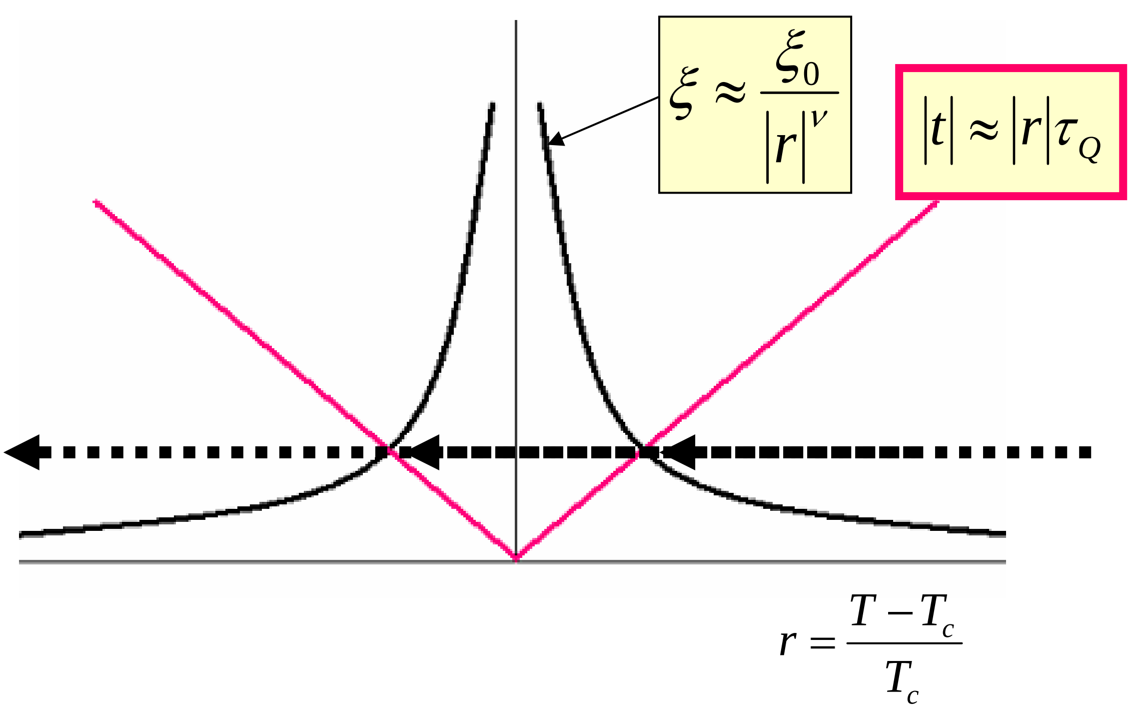




$\xi_f = \xi_f(\tau_Q)$



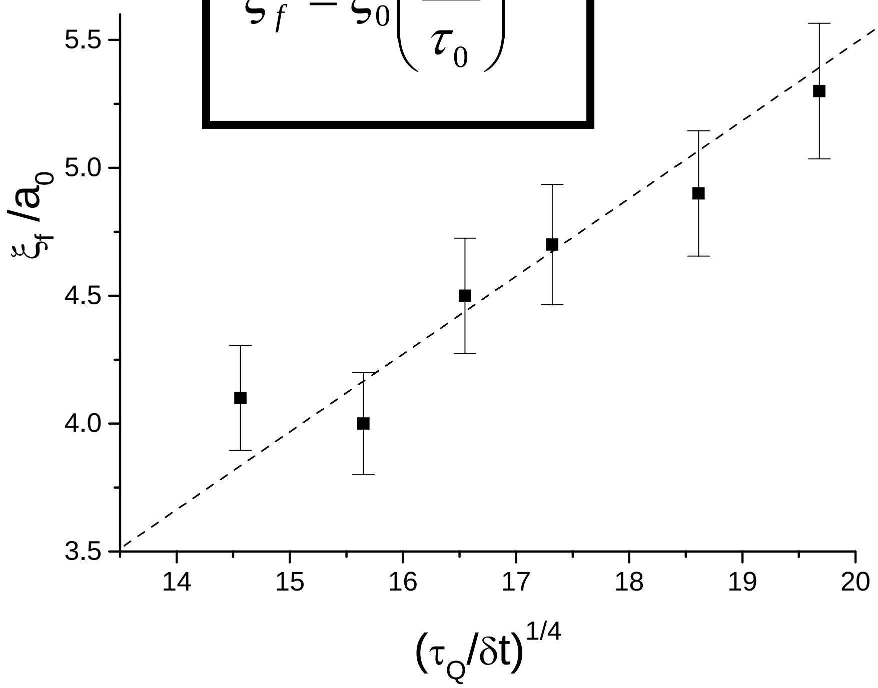
1.0
0.5
0.0
<S>
0
20
40
60
80
100
120
t/δt
4
2
0
$\ln(\xi_d/a_0)$



$\xi \approx \frac{\xi_0}{|r|^\nu}$
$|t| \approx |r|\tau_Q$
$r = \frac{T - T_c}{T_c}$

Main result

$$\xi_f = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{1}{4}}$$

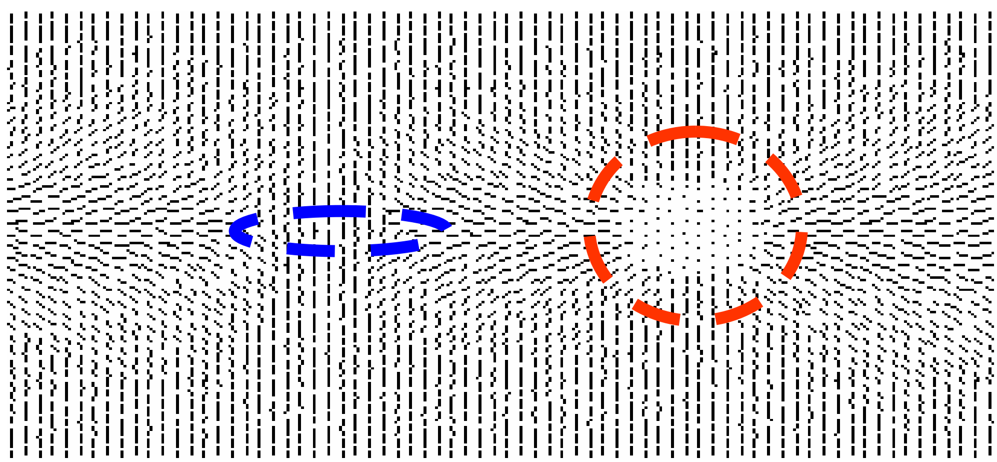


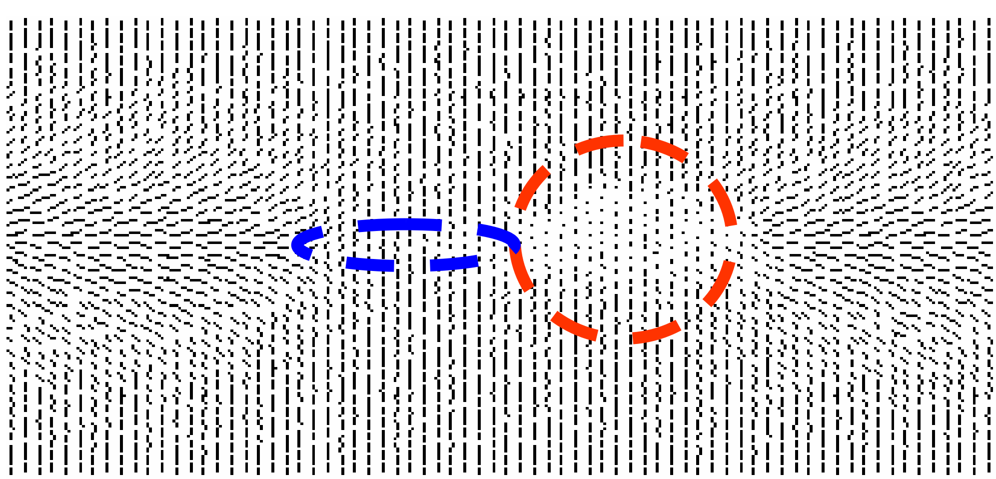
Bradac&Kralj&Zumer, submitted

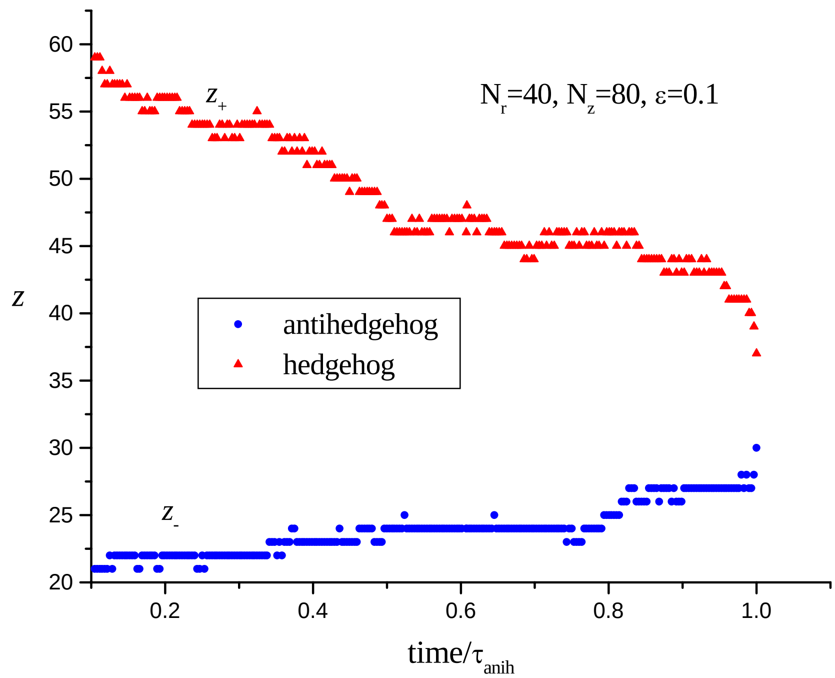
Application ?

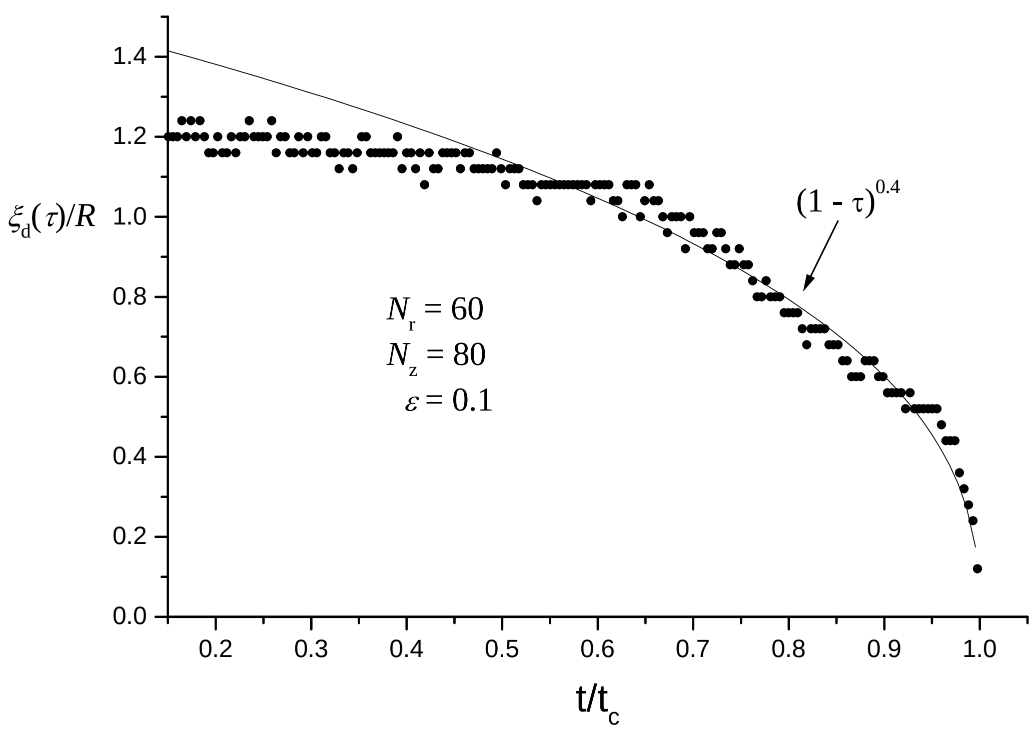
Late regime : annihilation of defects

Introduction: Andre Sonnet's lecture on Monday









Svetec&Kralj&Bradac&Zumer, submitted in a week or three

Equilibrium domain (?) structure of weakly perturbed nematic phase

Known analogies and open problems:

Imry-Ma argument (PRL 1975) -> domains exist (?)

- Coarsening dynamics and pinning?
- Single ξ_d?
- Thermal&static fluctuations?
- Phase (i.e., LC – "impurities") separation?

Imry-Ma argument and domains

System:

• magnetic spins, tend to order homogeneously

• pure phase exhibits Goldstone mode (**continuous sym. breaking**)

• an **uncorrelated quenched** disorder of strength W is acting on them (field conjugated to the order parameter)

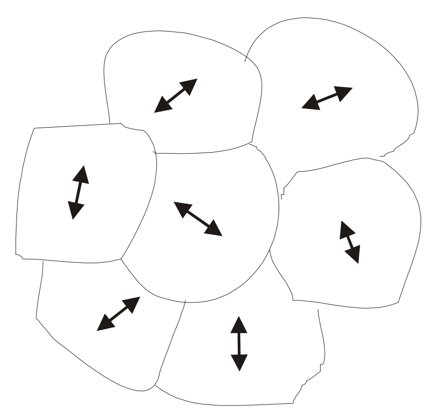
Phase structure (Imry&Ma 1975):

• predicts the size ξ_d of ordered domains in 3d

• Short Range Order

$$\xi_d \propto W^{-\frac{2}{4-d}},$$

$$\text{e.g., } d = 3: \quad \xi_d \propto W^{-2}$$



Simple MFA for nematics

Disorder and ξ_d

Random Anisotropy Nematic model **(Sluckin, 93),**

surface field enforces random orientations:

$$f_i^{(n)} = -W_n \vec{\nu}.\underline{Q}.\vec{\nu} = -\frac{W_n S}{2}\left(3(\vec{n}.\vec{\nu})^2 - 1\right),$$

$\vec{\nu}$: random site variation

Within an average domain:

$$\left\langle F_i^{(n)} \right\rangle_{domain} \approx \left\langle f_i^{(n)} \right\rangle c V_d = -\frac{|W_n| S}{2} \frac{1}{\sqrt{N}} c V_d$$

$$\frac{1}{\sqrt{N}} \approx \left\langle \frac{3(\vec{n}.\vec{\nu})^2 - 1}{2} \right\rangle, \quad N \approx \left(\frac{\xi_d}{\xi_{random}} \right)^3$$

N : number of random sites in 3d

V_d : domain volume

c : surface/volume ratio

Typical competition:

$$\langle f \rangle V^d \approx +\frac{LS^2}{\xi_d^2} V^d - \frac{S|W_\mu|}{2}\left(\frac{\xi_{random}}{\xi_d}\right)^{3/2} c V^d$$

$\xi_d \to \infty$

$\xi_d \to 0$

In d-dimensions:

$$\xi_d \approx \left(\frac{LS}{cW\xi_{random}^{d/2}}\right)^{\frac{2}{4-d}}$$

Imry-Ma result :

$$\xi_d \approx W^{-\frac{2}{4-d}}$$

$$f_e = Ls^2 \left| \nabla \vec{n} \right|^2$$

$$f = f_b + \frac{Ls^2}{\xi_d^2} - \frac{Ws}{\xi_d^{3/2}}$$

Discontinuous bulk behavior :

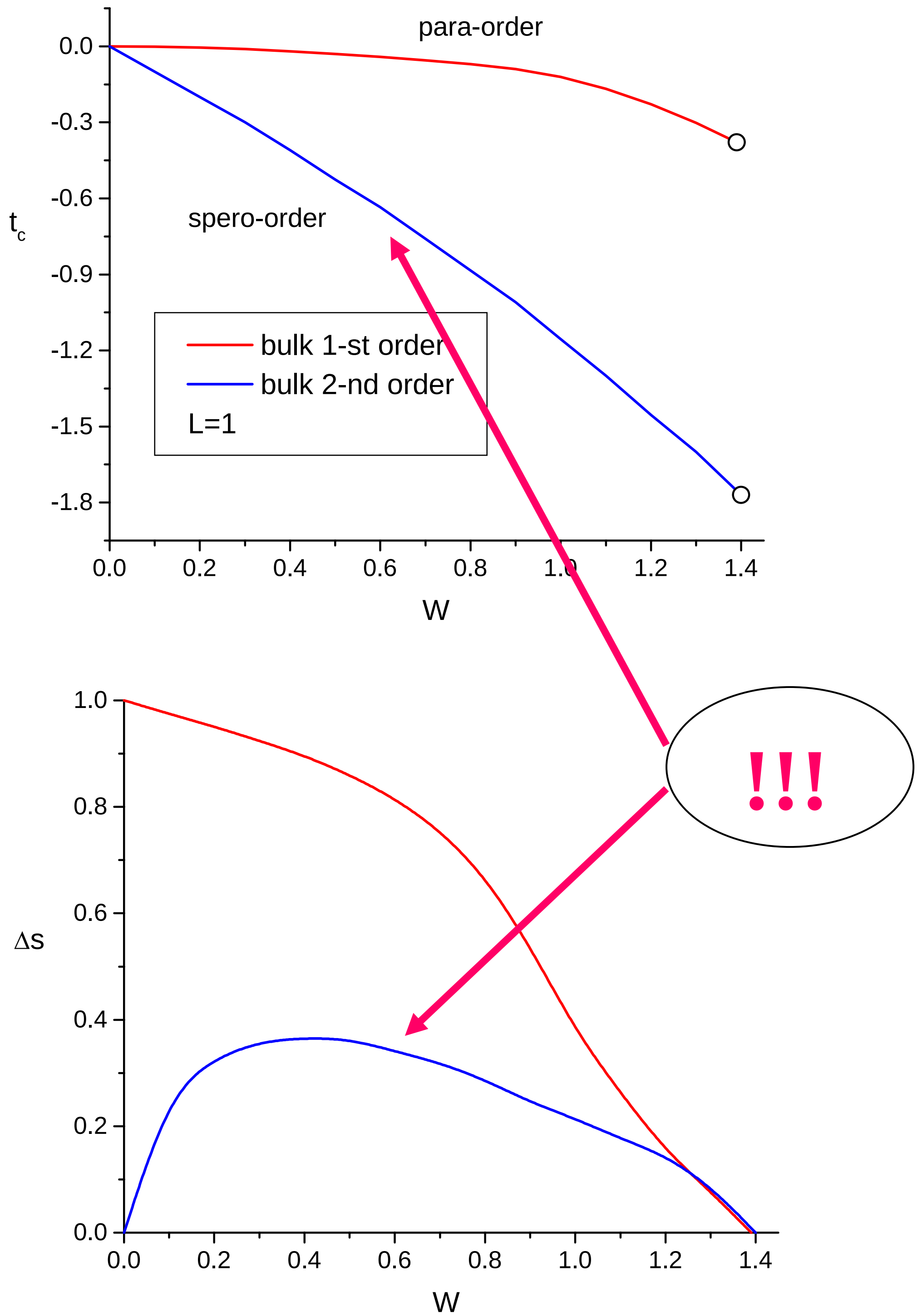
$$s(t^c) = 1, \quad t^c = 1, \quad t^* = -1, \quad t^{**} = \frac{1}{8}$$

$$s(t < t^c) = \frac{3}{4}\left(1 + \sqrt{1 - \frac{8}{9}(1+t)}\right)$$

$$f_b = ts^2 + s^2(1-s)^2$$

Continuous bulk behavior :

$$f_b = \frac{1}{2} ts^2 + \frac{1}{4} s^4$$



Popa-Nita&Kralj,PRE 2005

Disorder induced 1st order phase transition!

Similar: fluctuation induced 1st order PT in SmA,

Halperin-Lubensky-Ma effect

$$f \approx \frac{A}{2}|\psi|^2 + \frac{C}{4}|\psi|^4 + C_\perp q^2 |\psi|^2 \theta^2 + \frac{K}{2}|\nabla \theta|^2$$

Fourier expansion of θ, equipartitition theorem:

$$\left\langle |\theta_{\mathrm{k}}|^2 \right\rangle \propto \frac{k_B T}{K\left(k^2 + 1/\lambda^2\right)}, \quad \lambda = \sqrt{\frac{K}{2C_\perp q^2 \eta^2}}$$

$$\left\langle \theta(\vec{r})^2 \right\rangle \propto \int_0^{q_{\max}} \left\langle |\theta_{\mathrm{k}}|^2 \right\rangle k^2 dk \propto a - b|\psi|$$

Effective influence: $f \approx \frac{\tilde{A}}{2}|\psi|^2 - \frac{B}{3}|\psi|^3 + \frac{C}{4}|\psi|^4$

Phase separation and disorder

$$f = \Gamma\left(c\ln c + (1-c)\ln(1-c) + \chi c(1-c)\right) + (1-c)f_{LC}$$

$$f_{LC} = s^2(t+\lambda c) - 2s^3 + s^4$$

$$g = f - \mu c$$

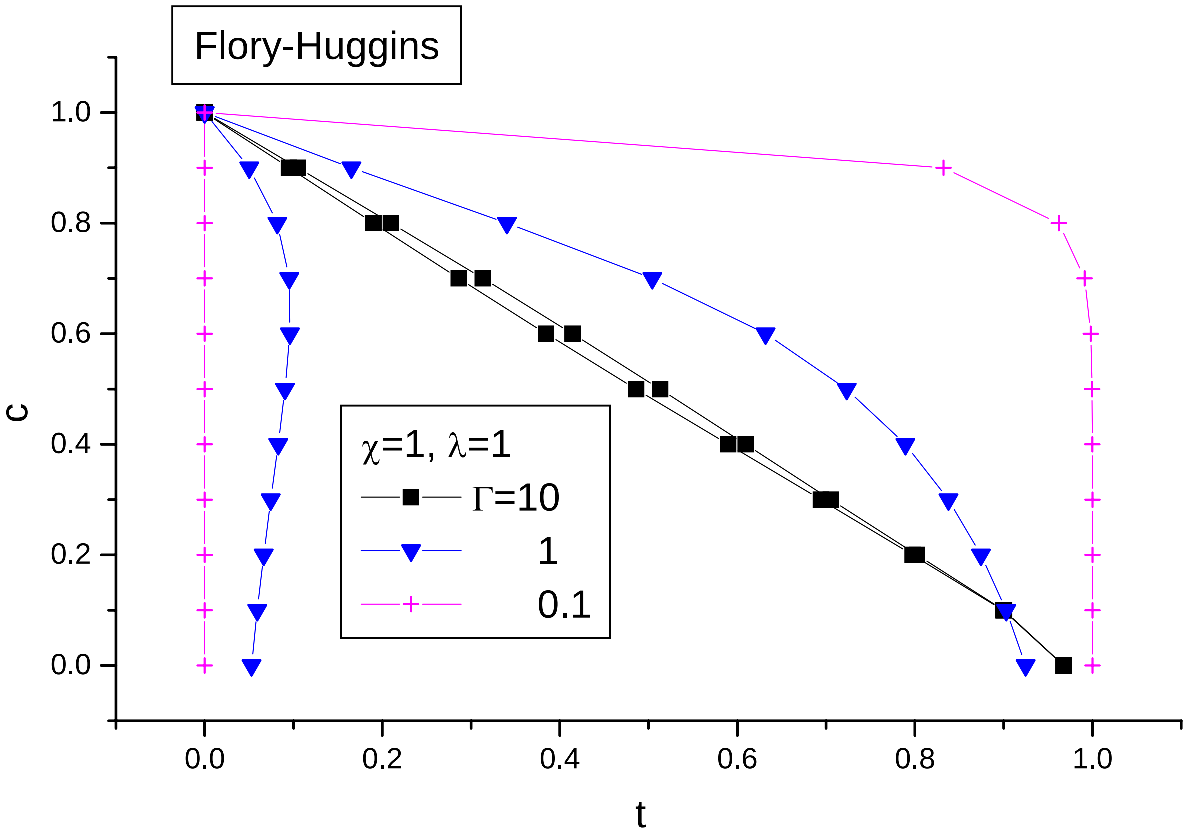
Most important term in the nematic phase:

$$\Delta f = c(1-c)\lambda s^2$$

Humphries&James&Luchurst, J.Chem.Soc, 1972

Popa-Nita&Sluckin&Kralj, PRE, 2005

$$f = \Gamma\left(c\ln c + (1-c)\ln(1-c) + \chi c(1-c)\right) + (1-c) f_{LC}$$



Random field contribution:

$$f_{LC} = s^2(t + \lambda c) - 2s^3 + s^4 + \frac{Ls^2}{\xi^2} - \frac{cWs}{\xi^{3/2}}$$

Renormalization of χ :

$$\chi_{eff} = \chi + \tfrac{1}{\Gamma}\left(s^2\lambda - \frac{Ws}{\xi^{3/2}}\right)$$

Random field weakens phase separation

Conclusions

Domain patterns in nematic phase

Quench dynamics:

Semi-microscopic description & Brownian molecular dynamics

- Early<->domain regime: Kibble-Zurek mechanism seems to work

- potential application: quench rate driven surface biaxiality for degenerate planar anchoring

- Late regime: annihilation of defects, reasonable modelling

Conclusions

Domain patterns in nematic phase

Static patterns stabilized by "impurities":

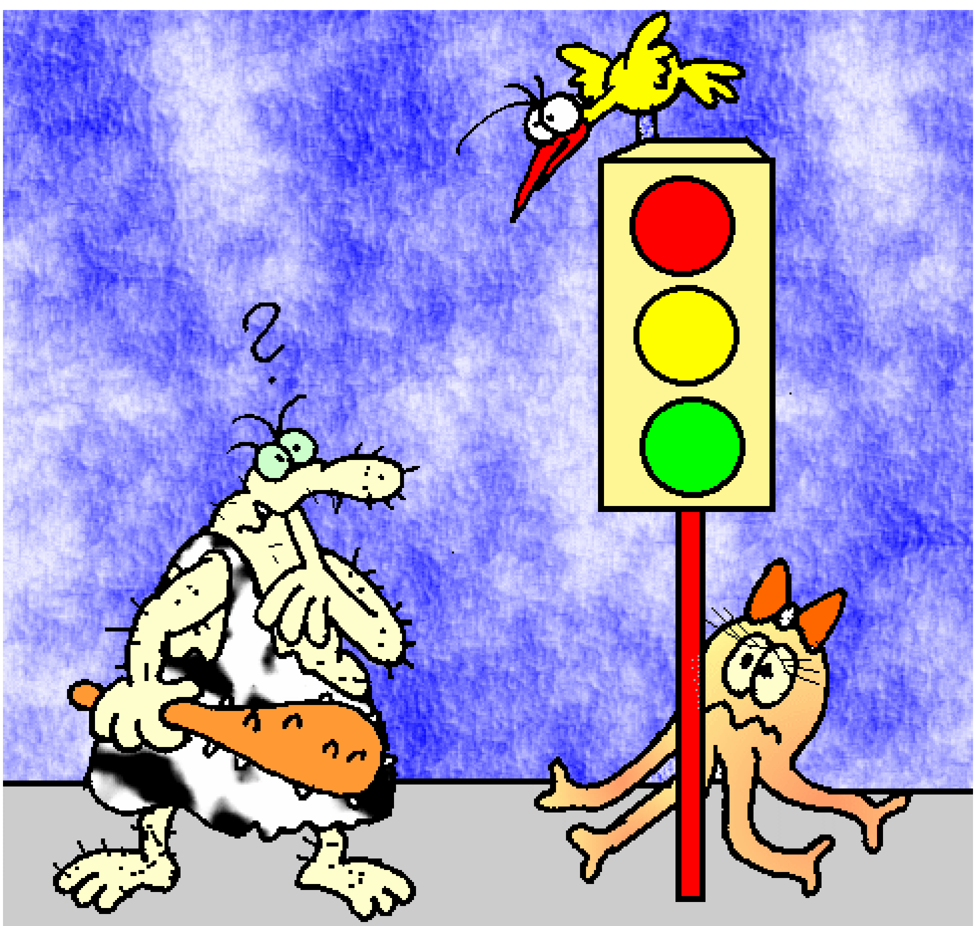
Simple mean-field modelling

- important "by-product": relatively weak uncorrelated quenched disorder converts continuous PT into discontinuous one
- random field seems to suppress LC-impurity phase separation

Main question

If $\xi_f < \Delta x$=average separation between impurities:

Static domain pattern ~ bulk domain pattern stabilized at SINGLE $\xi_d \sim \Delta x$?



In collaboration with:

Dynamics:

Svetec, Bradac, Repnik : University of Maribor

Zumer : University of Ljubljana

Virga: University of Pavia

Statics:

Sluckin : University of Southampton

Popa-Nita : University of Bucharest

Rosso : University of Pavia