Non-equilibrium critical dynamics and its application

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2013.8.19-23


West Lake Oct.


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Non-equilibrium critical dynamics

Two review article:

1. **B. Zheng, *Monte Carlo simulations of short-time critical dynamics*, Int. J. Mod. Phys., B12 (1998), 1419-1484. cited 193 times**

2. **E.V. Albano**, M.A. Bab, G. Baglietto, R.A. Borzi, T.S. Grigera, E.S. Loscar, D.E. Rodriguez, M.L.R. Puzzo, and G.P. Saracco, **Rep. Prog. Phys., 74 (2011) 026501**

http://zimp.zju.edu.cn/~cpsp

Non-equilibrium critical dynamics

23. H.J. Luo, L. Schülke and B. Zheng, Dynamic approach to the fully frustrated XY model, Phys. Rev. Lett., 81 (1998), 180-183. cited 104 times
26. A. Jaster, J. Mainville, L. Schülke and B. Zheng, Short-time critical dynamics of the three-dimensional Ising model, J. Phys., A32 (1999), 1395 - 1406. cited 63 times
29. B. Zheng, M. Schulz and S. Trimper, Dynamic simulations of the Kosterlitz-Thouless phase transition, Phys. Rev., E59 (1999), R1351-1354, Rapid Comm.. cited 40 times
32. B. Zheng, M. Schulz and S. Trimper, Deterministic equations of motion and dynamic critical phenomena, Phys. Rev. Lett., 82 (1999), 1891-1894. cited 57 times
35. L. Schülke and B. Zheng, Dynamic approach to weak first-order phase transitions, Phys. Rev., E62 (2000), 7482-7485. cited 37 times

49. **B. Zheng**, F. Ren and H. Ren, Corrections to scaling in 2D dynamic XY and fully frustrated XY models, **Phys. Rev**. **E68** (2003) 046120.

57. J.Q. Yin, **B. Zheng** and S. Trimper, Critical behavior of 2D random-bond Potts Model: a short-time dynamic approach, **Phys. Rev. E70** (2004) 056134.

60. J.Q. Yin, **B. Zheng** and S. Trimper, Dynamic Monte Carlo simulations of the three-dimensional random-bond Potts model, **Phys. Rev. E72** (2005) 036122.

61. S.Z. Lin, **B. Zheng** and S. Trimper, Computer simulations of 2D melting with dipole-dipole interactions, **Phys. Rev. E73** (2006) 066106.

71. X.W. Lei and **B. Zheng**, Short-time critical dynamics and ageing phenomena in the two-dimensional XY model, **Phys. Rev. E75** (2007) 040104, **Rapid. Comm..**

Relevant topics

- **Spin-glass phase transition and dynamics**
- **Interface and surface growth dynamics**
- **Phase ordering dynamics and spinodal decomposition dynamics**
- Damage spreading and dislocation dynamics

Contents

I Second-order phase transitions

II Weak First-order phase transitions

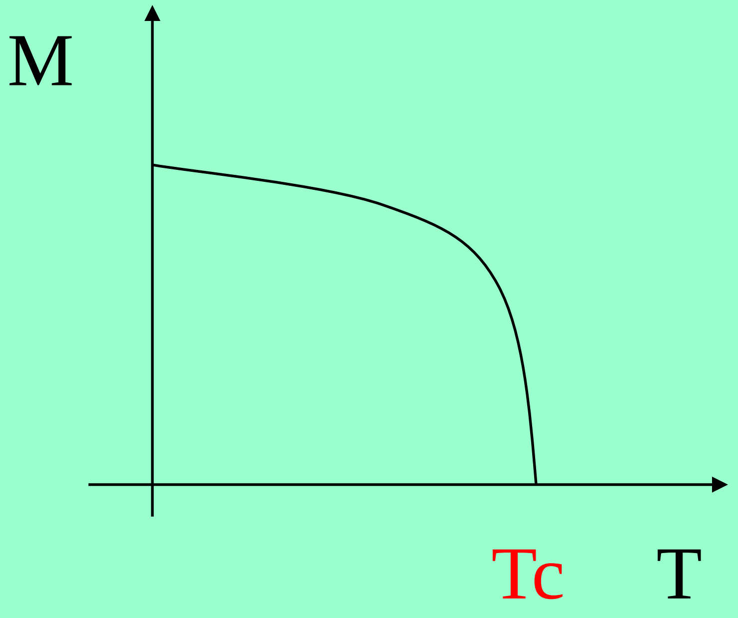
III Kosterlitz-Thouless phase transitions

Ising model and phase transitions

$$-H/kT = K\sum_{<i,j>} s_i s_j + h\sum_i s_i \qquad s_i = \pm 1$$

$$M \equiv \frac{1}{Z}\sum_{\{s_i\}} \frac{1}{L^d}\sum_i s_i \; e^{-H/kT}$$

$$Z = \sum_{\{s_i\}} e^{-H/kT}$$



$$h = 0$$

$$M = \begin{cases} 0 & T \geq T_C \\ (-\tau)^{\beta} & T < T_C \end{cases}$$

$$\tau = (T - Tc)/Tc$$

Features of second order transitions

* **Scaling form**

$$M(\tau) = b^{-\beta/\nu}\ M\left(b^{1/\nu}\ \tau\right) \Rightarrow \quad power\ \ law$$

It represents self-similarity

$\beta, \quad \nu$ **are critical exponents**

* **Universality**

Scaling functions and critical exponents depend only on symmetry and spatial dim.

Physical origin

divergent spatial correlation length and fluctuations

How to simulate phase transitions and determine *Tc* and critical exponents ?

* **Direct measurement of magnetization?**

* **Finite size scaling form**

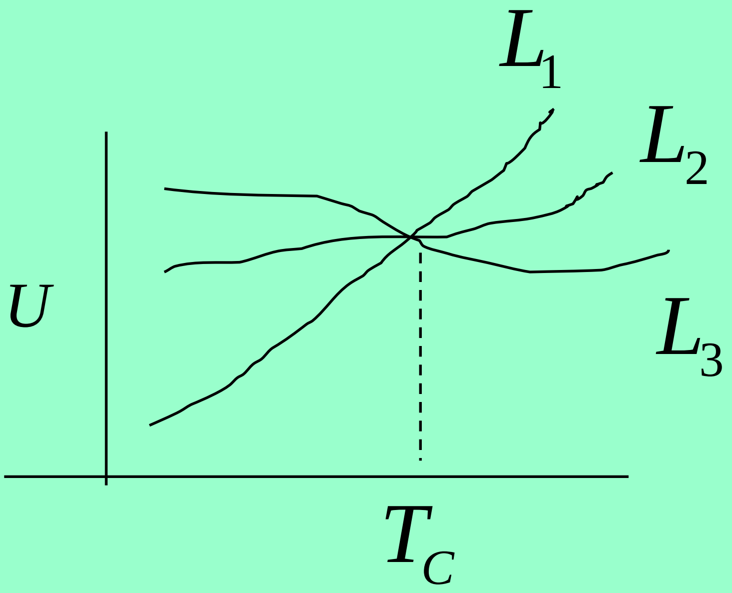
$$M^{(k)}(\tau, L) = b^{-k\beta/\nu} M^{(k)}\left(b^{1/\nu}\tau, b^{-1}L\right)$$

Binder cumulant

$$U = 1 - \frac{M^{(4)}}{3\left(M^{(2)}\right)^2}$$

Scaling behavior of *U*

$$U(\tau, L) = U\left(b^{1/\nu}\tau, b^{-1}L\right)$$
$$= U\left(L^{1/\nu}\tau, 1\right)$$



$$\frac{\partial U(\tau, L)}{\partial \tau}\Big|_{\tau=0} = L^{1/\nu}\frac{\partial U(\tau', 1)}{\partial \tau'}\Big|_{\tau'=0}$$

From $M^{(2)}(0,L) = L^{-2\beta/\nu}M^{(2)}(0,1)$**, one obtains** β/ν

Dynamic fluctuations in equilibrium

For sufficient large lattice, large time *t*, the auto-correlation function

$$A(t) \equiv \frac{1}{L^d} \sum_{t'} \langle S_i(t') S_i(t'+t) \rangle \quad \sim \quad t^{-\lambda}$$

For a finite lattice, large time *t*

$$A(t) \sim \exp(-t/\tau) \qquad \tau \sim L^Z$$

***z* is the dynamic exponent, i.e., the correlating time is divergent, and this is the so-called critical slowing down**

How to overcome critical slowing down?

Cluster algorithms

- **Swendsen-Wang algorithm**
- **Wolff algorithm**

z **is small, but accurate values are unknown**

-- the algorithms are not ‘universal’

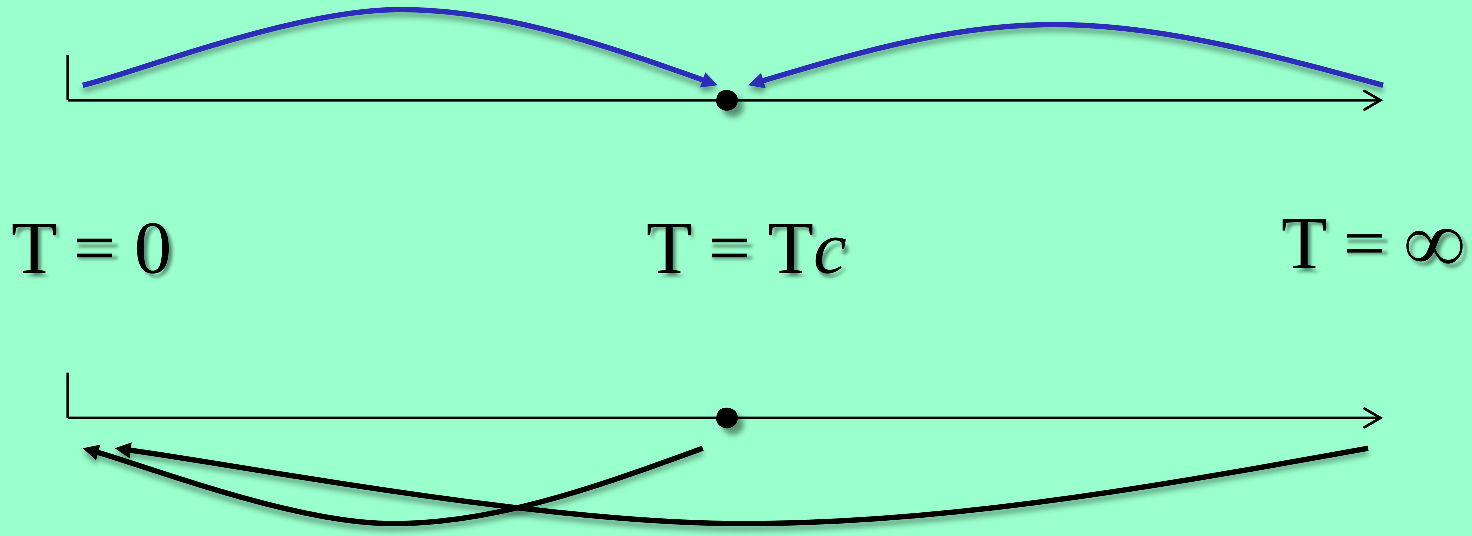
-- do not apply to study the local dynaics

Our motivation

- Critical dynamics far from equilibrium

- Overcome critical slowing down

Critical dynamic relaxation



Phase ordering dynamics

Dynamic process far from equilibrium

e.g. t = 0 , T = ∞ ; a small m_0

t > 0 , T = Tc

Monte Carlo dynamics

Dynamic scaling form in the short-time regime

$$M(t,\ \tau,\ m_0) = b^{-\beta/\nu} M(b^{-z}t,\ b^{1/\nu}\tau,\ b^{x_0} m_0)$$

x_0 : a “new” critical exponent

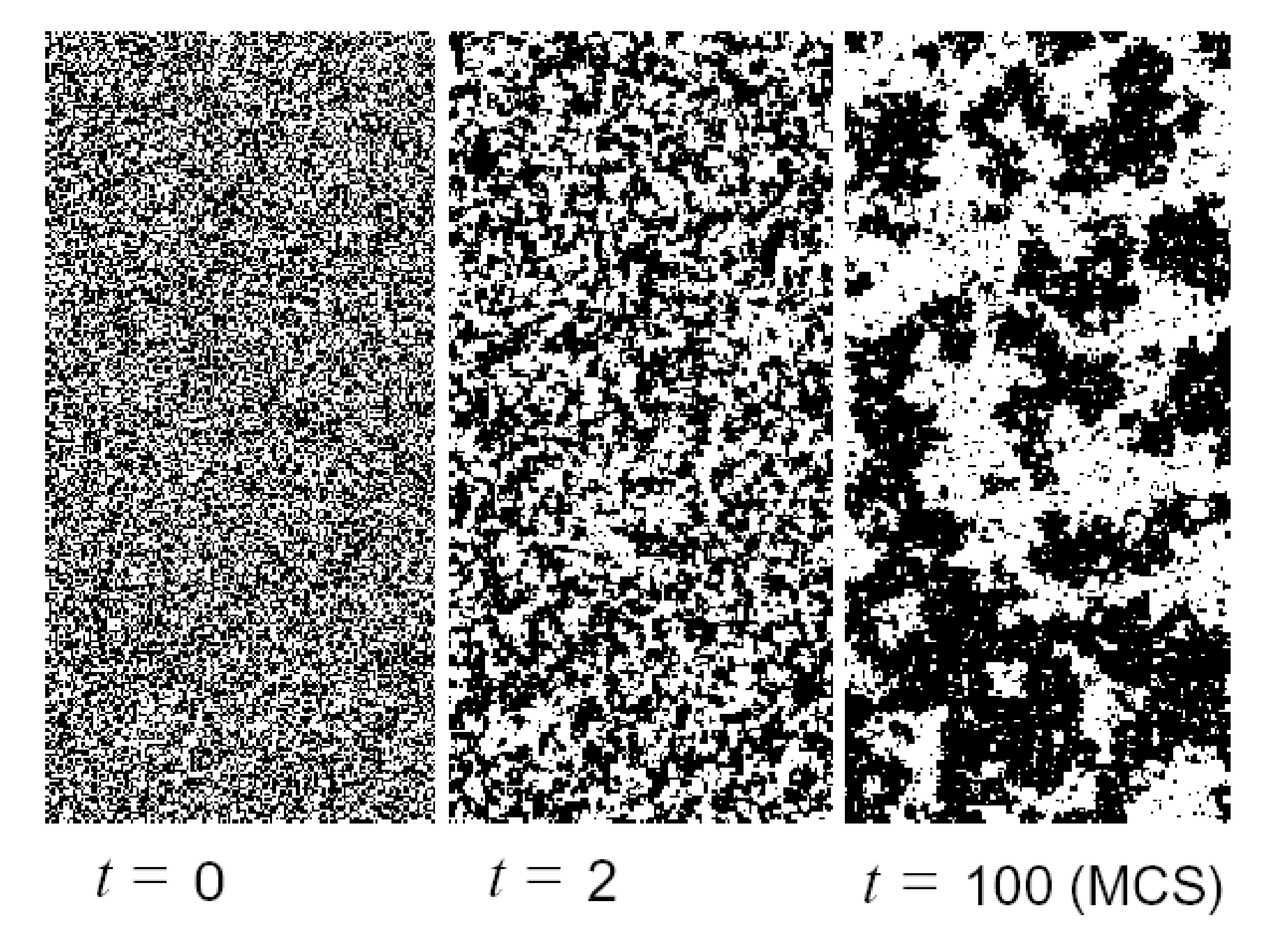
Origin: divergent correlating time

Important

* Distinguish microscopic and macroscopic time scales and spatial scales

* Comparison: surface critical phenomena

Self-similarity in time direction, Ising model



Auto-correlation

$$\tau = 0, \qquad m_0 = 0$$

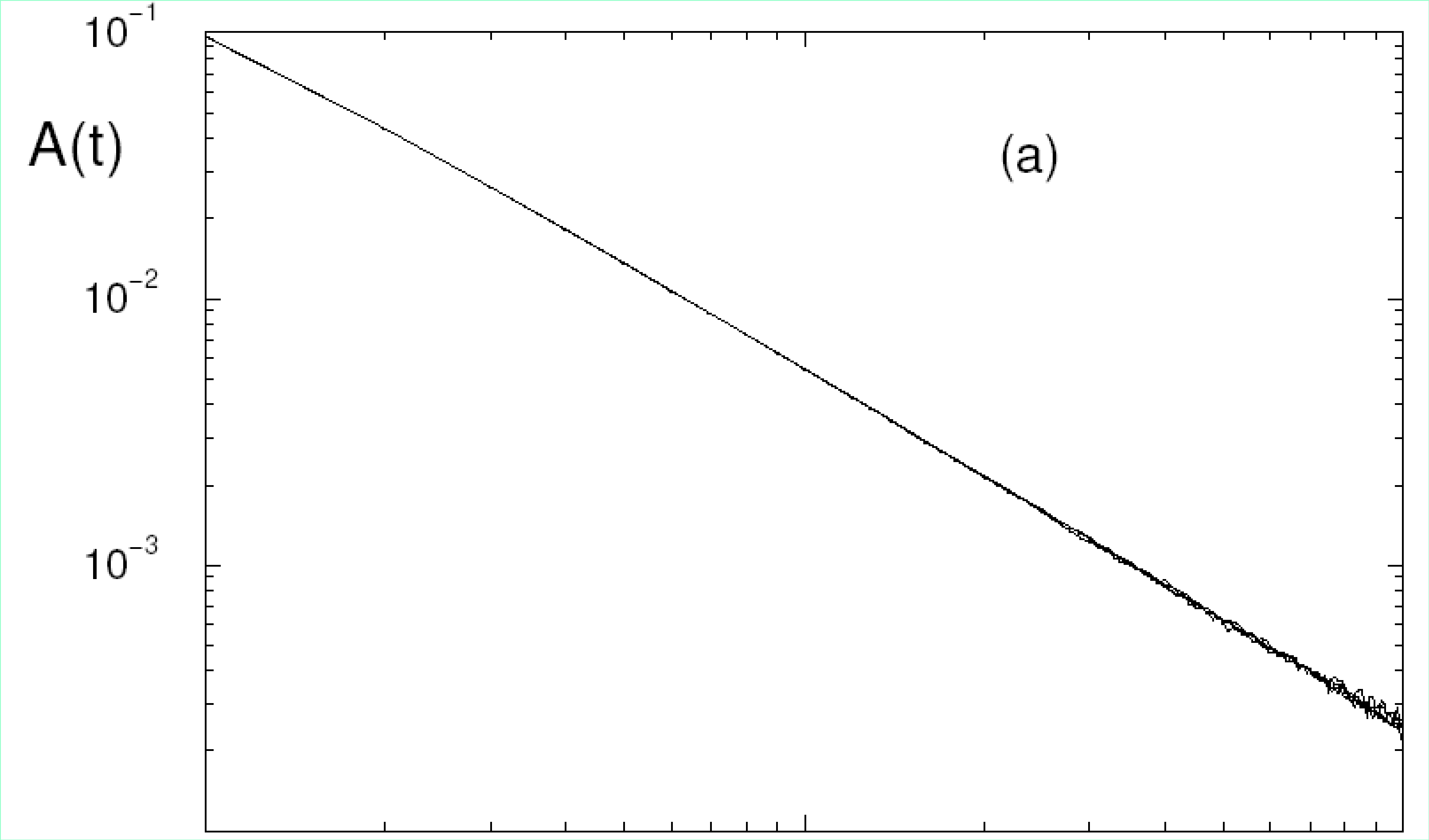
$$A(t) \equiv \frac{1}{L^d} \sum \langle S_i(0)\, S_i(t) \rangle \quad \sim \quad t^{-d/z+\theta}$$

Even if $m_0 = 0, \quad \theta$ **enters dynamic behavior**

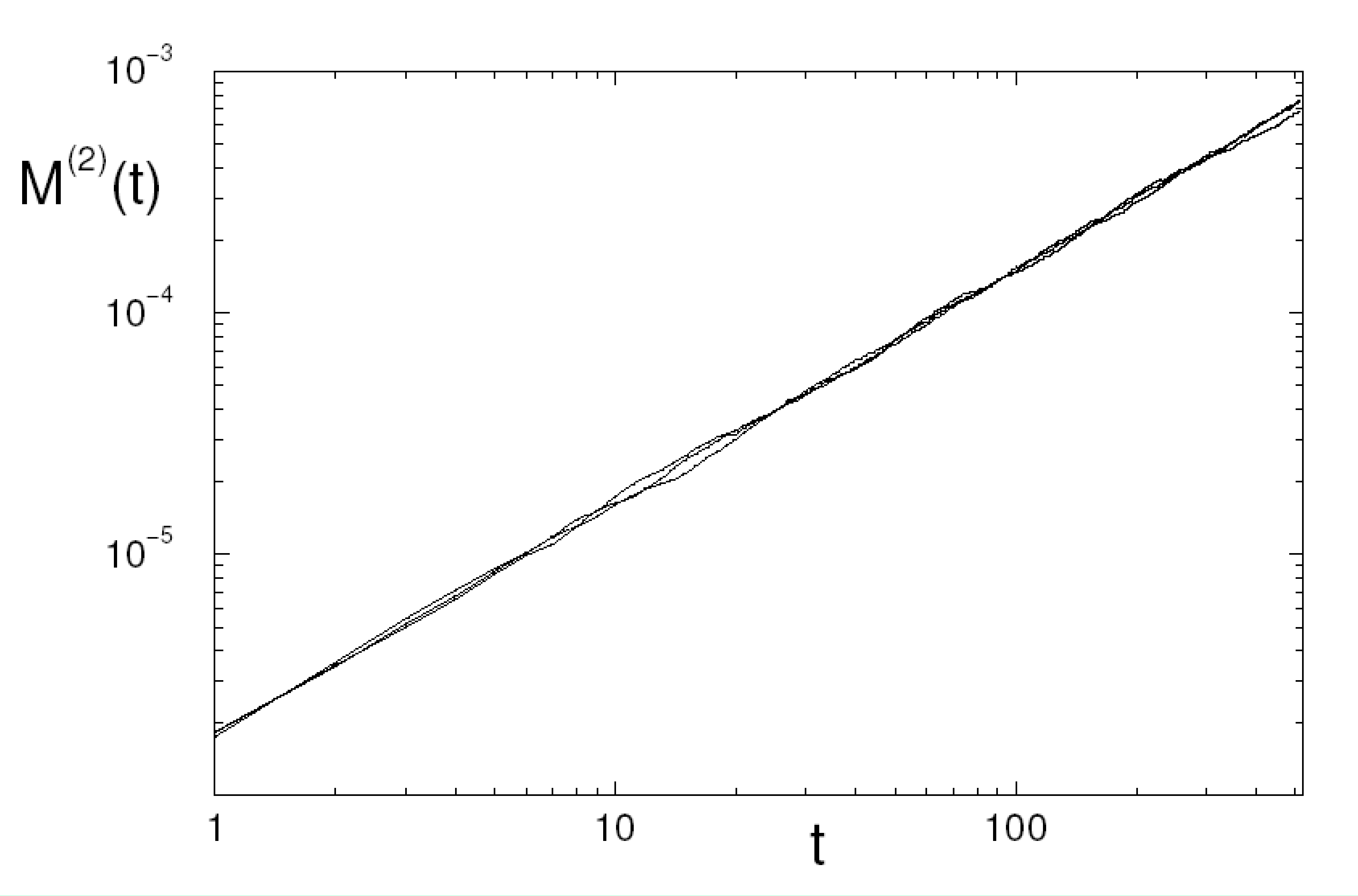
Second moment

$$M^{(2)}(t) \equiv \frac{1}{L^{2d}} \left\langle \left(\sum_i S_i(t) \right)^2 \right\rangle \sim t^c \qquad c = \left(d - 2\beta/\nu\right)/z$$

3D Ising Model J. Phys. A (1999)



3D Ising Model J. Phys. A (1999)



Summary

* **Short-time dynamic scaling**

a new exponent

* **Scaling form ==>** θ, z

==> static exponents

Zheng, IJMPB (98), review

Zheng, PRL(98,99)

Conceptually interesting and important

Dynamic approach does not suffer from

critical slowing down

Compared with cluster algorithms,

it applies to local dynamics

2D FFXY model

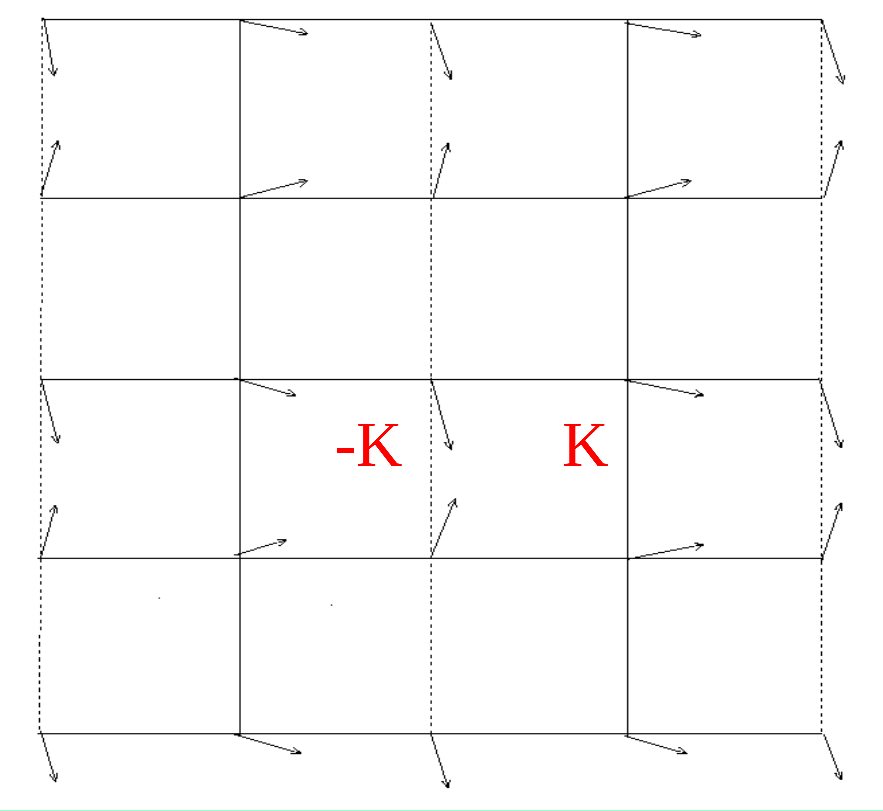
$$-H/kT = \sum_{<i,j>} K_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

Chiral degree of freedom

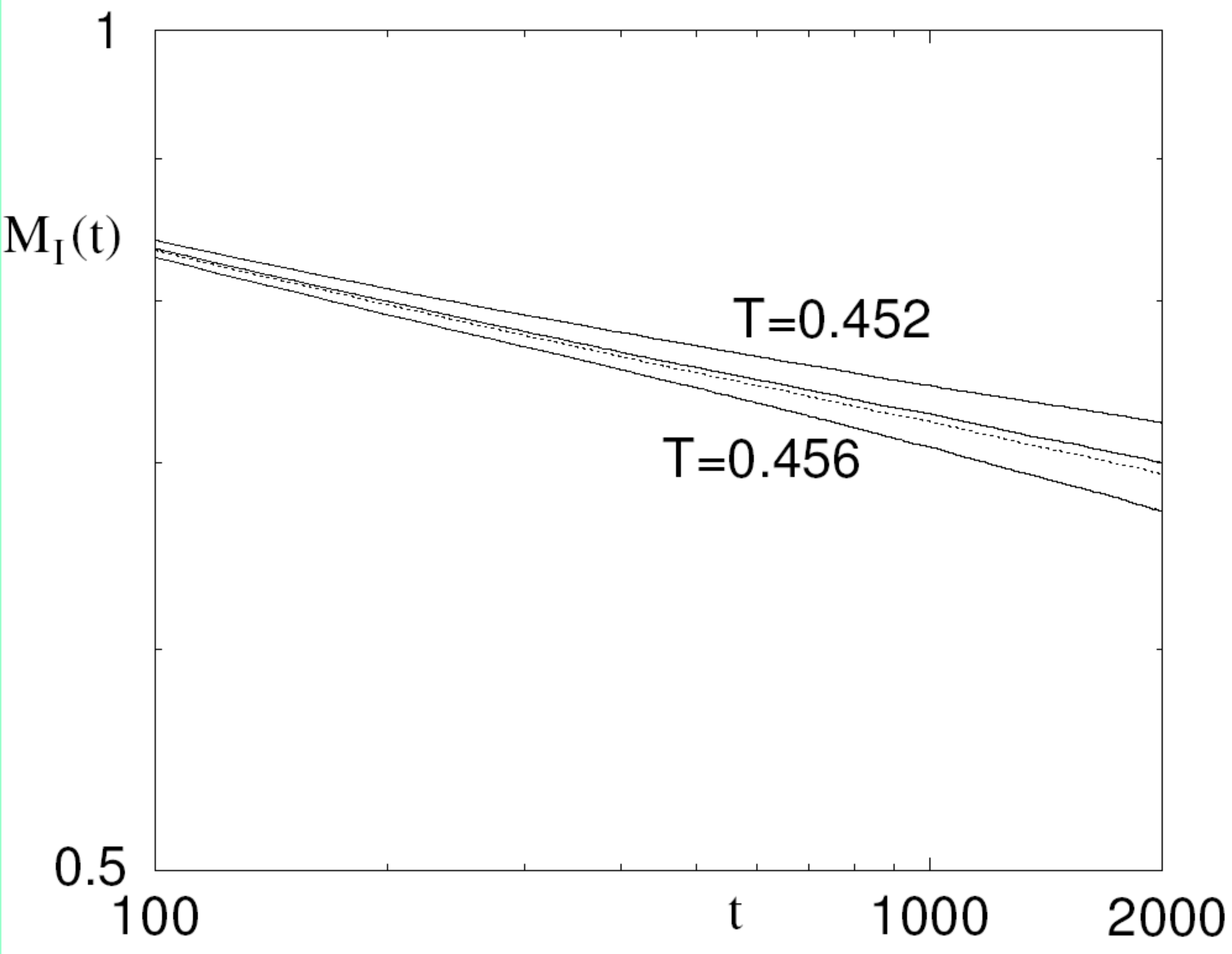
Order parameter:

Project of the spin-configuration

onto the ground state



2D FFXY model,   Chiral degree of freedom



2D FFXY model, Chiral degree of freedom

Luo,Schuelke,Zheng, PRL (98)

	Tc	θ	Z	2β/ν	ν
93	.454(3)			.38(2)	.80(5)
94	.454(2)			.22(2)	.813(5)
95	.452(1)				1
96	.451(1)				.898(3)
OURS (98)	.4545(2)	.202(3)	2.17(4)	.261(5)	.81(2)
Ising		.191(3)	2.165(10)	.25	1

Ozeki, Ito PRE, PRB (2003)

Deterministic dynamics

Now it is NOT traditional 'statistical physics', rather molecular dynamics based on fundamental equations of motion

Φ^4 theory, isolated

$$H=\sum_i\left(\frac{1}{2}\pi_i^2+\frac{1}{2}\sum_\mu\left(\Phi_{i+\mu}-\Phi_i\right)^2-\frac{1}{2}m^2\Phi_i^2+\frac{1}{4!}\lambda\Phi_i^4\right)$$

$$\Rightarrow\quad \ddot{\Phi}_i=\sum_\mu\left(\Phi_{i+\mu}+\Phi_{i-\mu}-2\Phi_i\right)+m^2\Phi_i-\frac{1}{3!}\lambda\Phi_i^3$$

Zheng, Trimper, Schulz, PRL (99)

	θ	Z	$2\beta/\nu$	ν
Φ^4	.176(7)	2.148(20)	.24(3)	.95(5)
Ising	.191(1)	2.165(10)	.25	1

Φ^4 **theory does describe both statics and dynamics around phase transition**

Macroscopic initial condition violate Lorentz invariance

Other progress

* Disordered systems
* Aging phenomena
* Dynamic and irreversible phase transitions
* Melting transitions
* Self-organized criticality

Contents

How to distinguish

weak first order phase transitions from second order or KT phase transitions?

e.g. 2-dimensional melting transitions

traditionally: weak first order

recently: possibly TWO KT transitions

Experiments: Phys.Rev.Lett. 82 (1999) 2721

85 (2000) 3656

Methods: dynamic approach

(in equilibrium)

First effort:

distinguish weak first order transitions from second order transitions

Methods:

Non-equilibrium dynamic approach:

for a 2nd order transition: at Kc (~ 1/Tc)

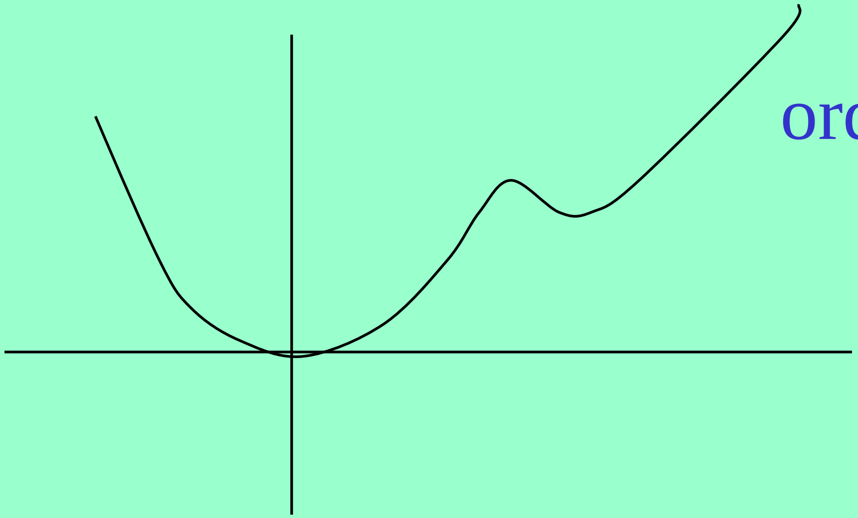
there is power law behavior

for a weak 1^{st} order transition: at Kc

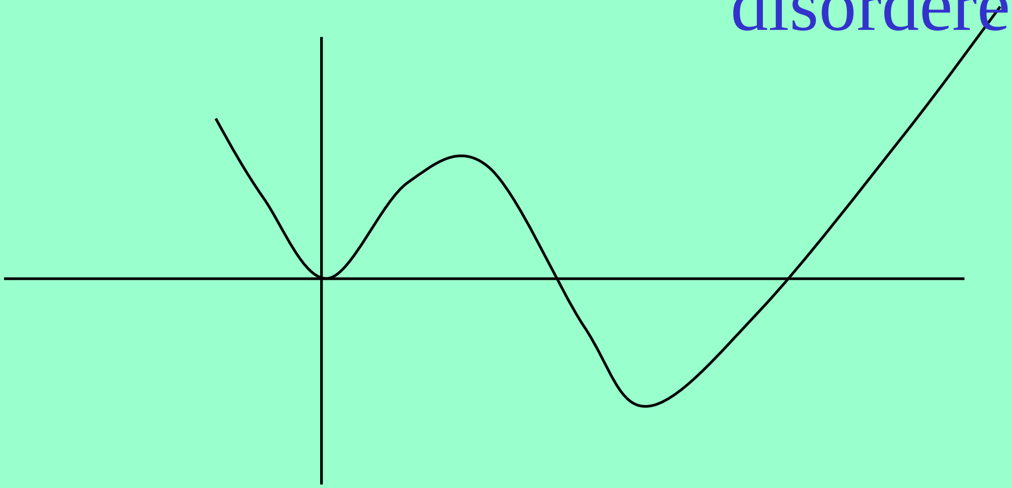
there is NO power law behavior

However, there exist pseudo critical points!

ordered metastable state



disordered metastable state



disordered metastable state ➔ K* > Kc

M(0)=0 $M^{(2)}(t) \sim t^{(d-2\beta/\nu)/z}$

ordered metastable state ➔ K** < Kc

M(0)=1 $M(t) \sim t^{-\beta/\nu z}$

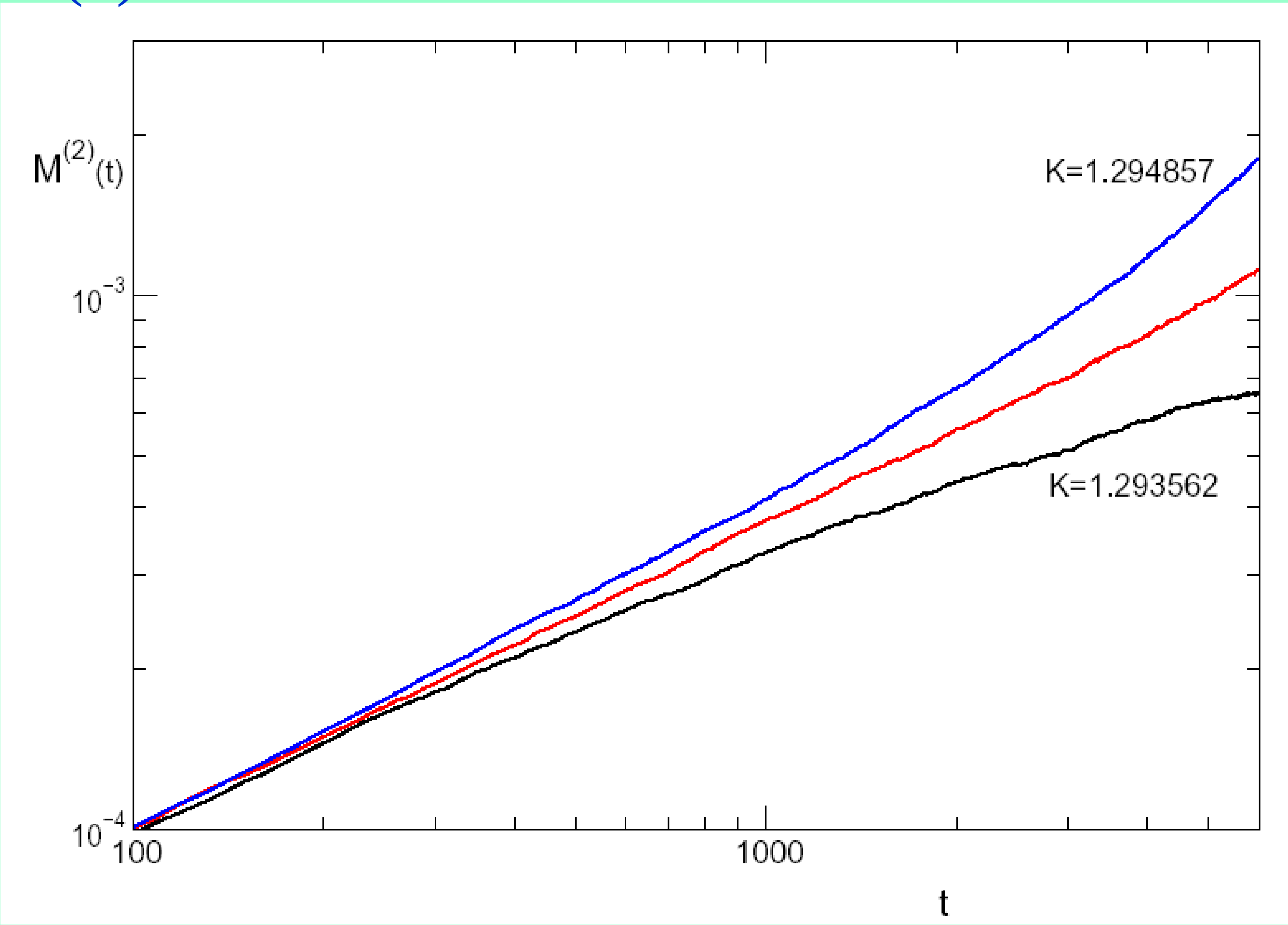
For a 2nd order transition, K* = K**

2D q-state Potts model

$$H = -K \sum_{<ij>} \delta_{\sigma i, \sigma j}$$

2D 7-state Potts model, heat-bath algorithm

M(0)=0

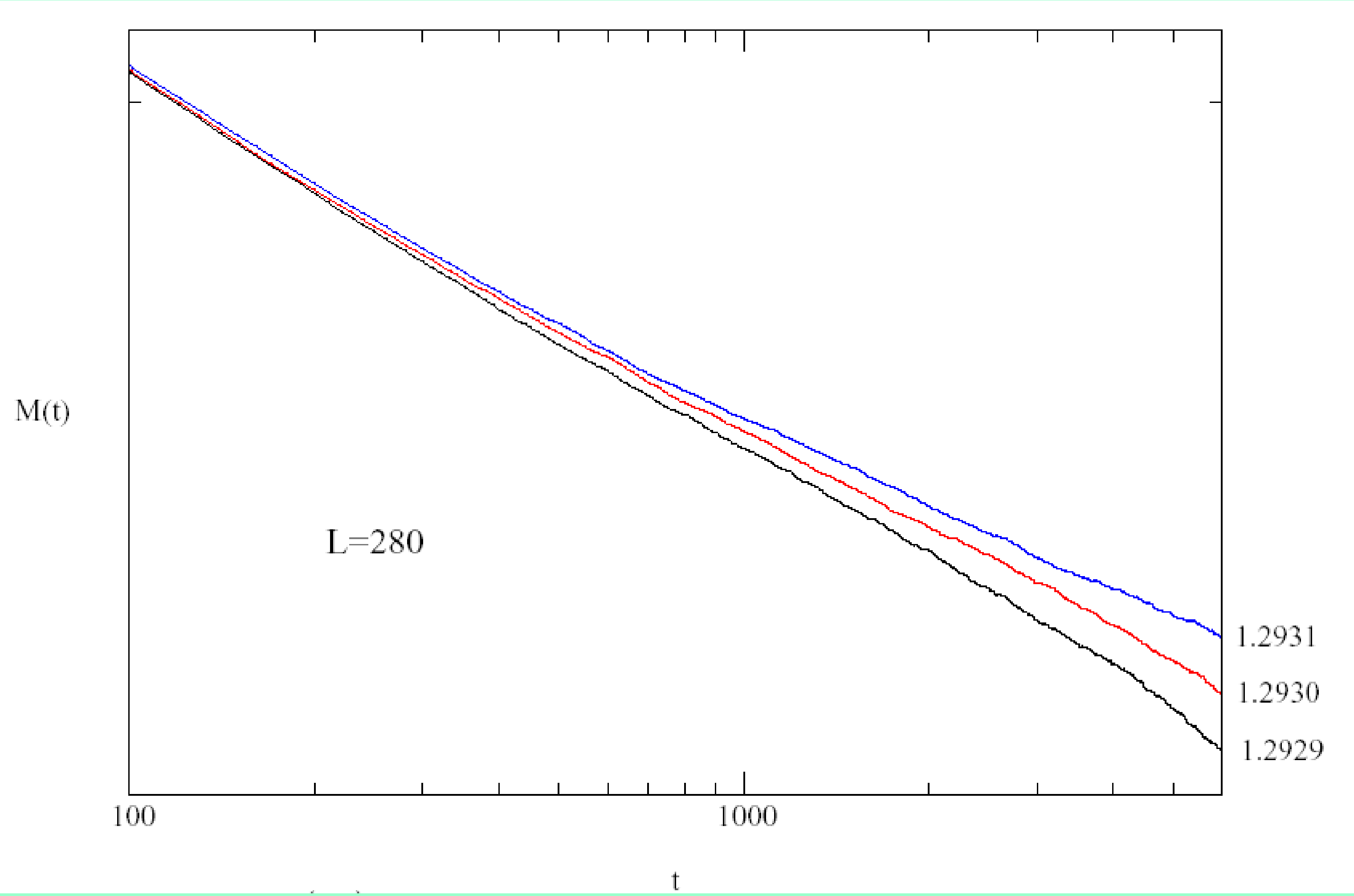


K*

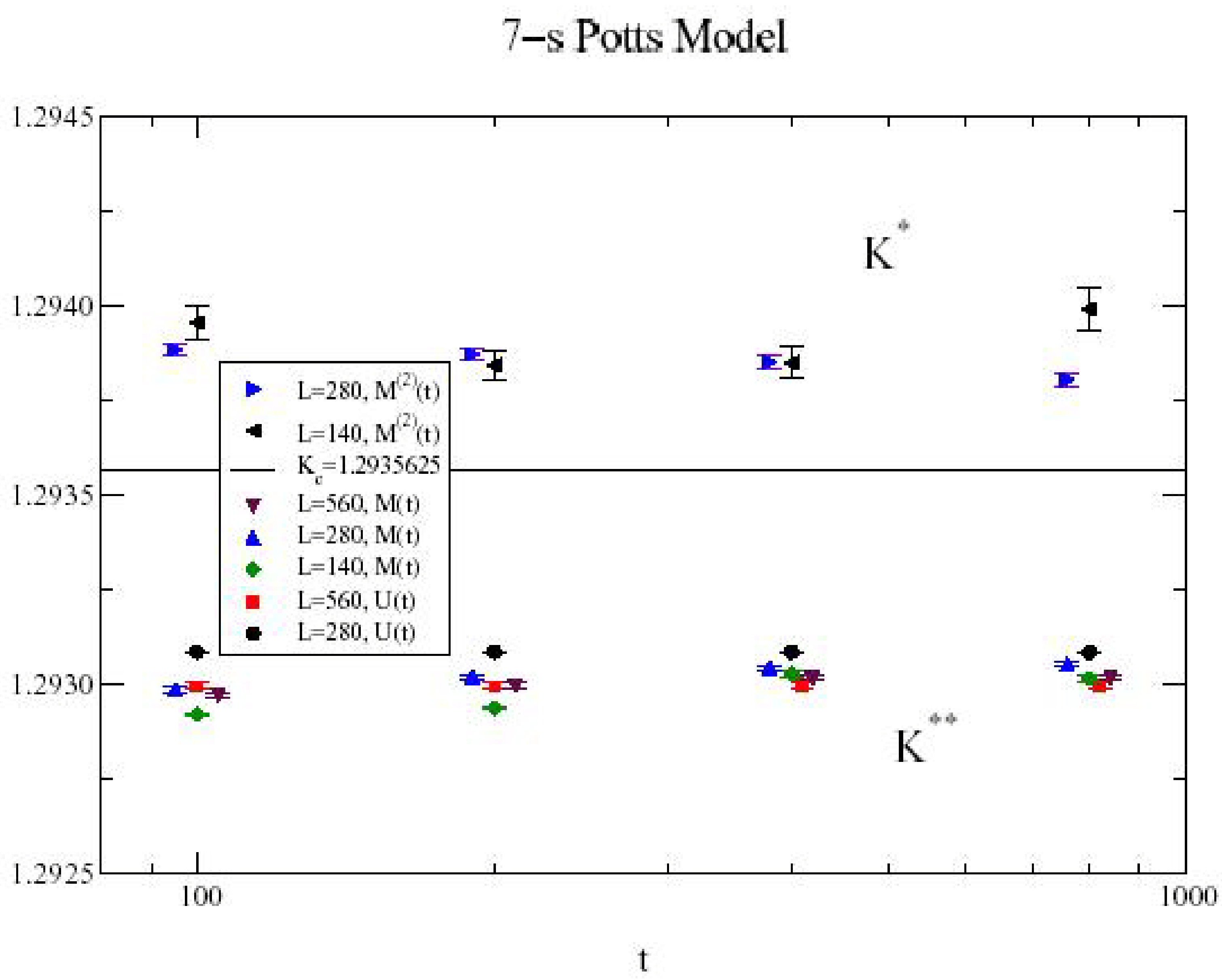
Kc

2D 7-state Potts model, heat-bath algorithm

M(0)=1



K**



7-s Potts Model
1.2945
1.2940
1.2935
1.2930
1.2925
100
1000
t
K*
K**
L=280, M(2)(t)
L=140, M(2)(t)
Kc=1.2935625
L=560, M(t)
L=280, M(t)
L=140, M(t)
L=560, U(t)
L=280, U(t)

2D Potts models

Schulke, Zheng, PRE(2000)

	K^{**}	K_c	K^*
$q = 5$	1.174322(2)	1.174359	1.174404(7)
$q = 7$	1.293008(7)	1.293562	1.293854(29)

The random-bond Potts model

(Yin and Zheng, PRE 2004, 05)

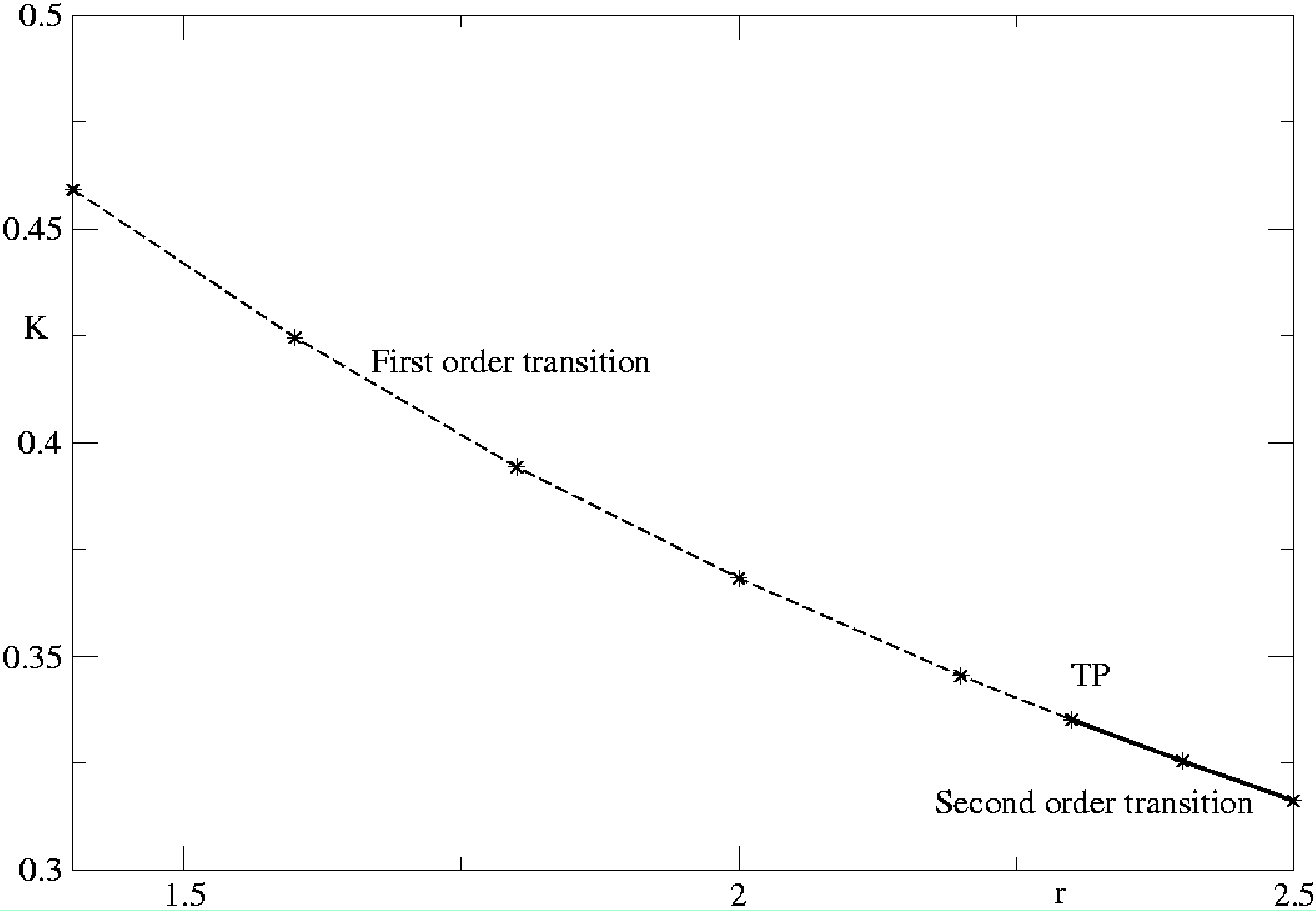
$$-\frac{1}{kT}H = \sum_{<i,j>} K_{ij}\ \delta_{\sigma i,\sigma j} \qquad K_{ij} > 0$$

$$P(K) = p\delta(K - K_1) + (1 - p)\delta(K - K_2)$$

$$r = K_2 / K_1$$

***p*=1/2, in TWO dimensions**

$$(e^{K_{1c}} - 1)(e^{K_{2c}} - 1) = q$$


0.5
0.45
0.4
0.35
0.3
K
1.5
2
r
2.5
First order transition
TP
Second order transition

Contents

Kosterlitz-thouless transitions

e.g. 2D Clock model, 2D XY model, 2D FFXY model, …

2D Josephson junction array,…

2D Hard disk model,…

Logarithmic divergence of correlation length above *Tc*

$$\xi(\tau) = a \ \exp(b\tau^{-\nu})$$

Remains critical below *Tc*

Critical slowing down is severer!

Non-equilibrium dynamics

Logarithmic corrections to the scaling for a random start **Bray PRL(00)**

Auto-correlation

$$A(t) \sim [t / \ln(t / t_0)]^{-d/z+\theta}$$

Second moment

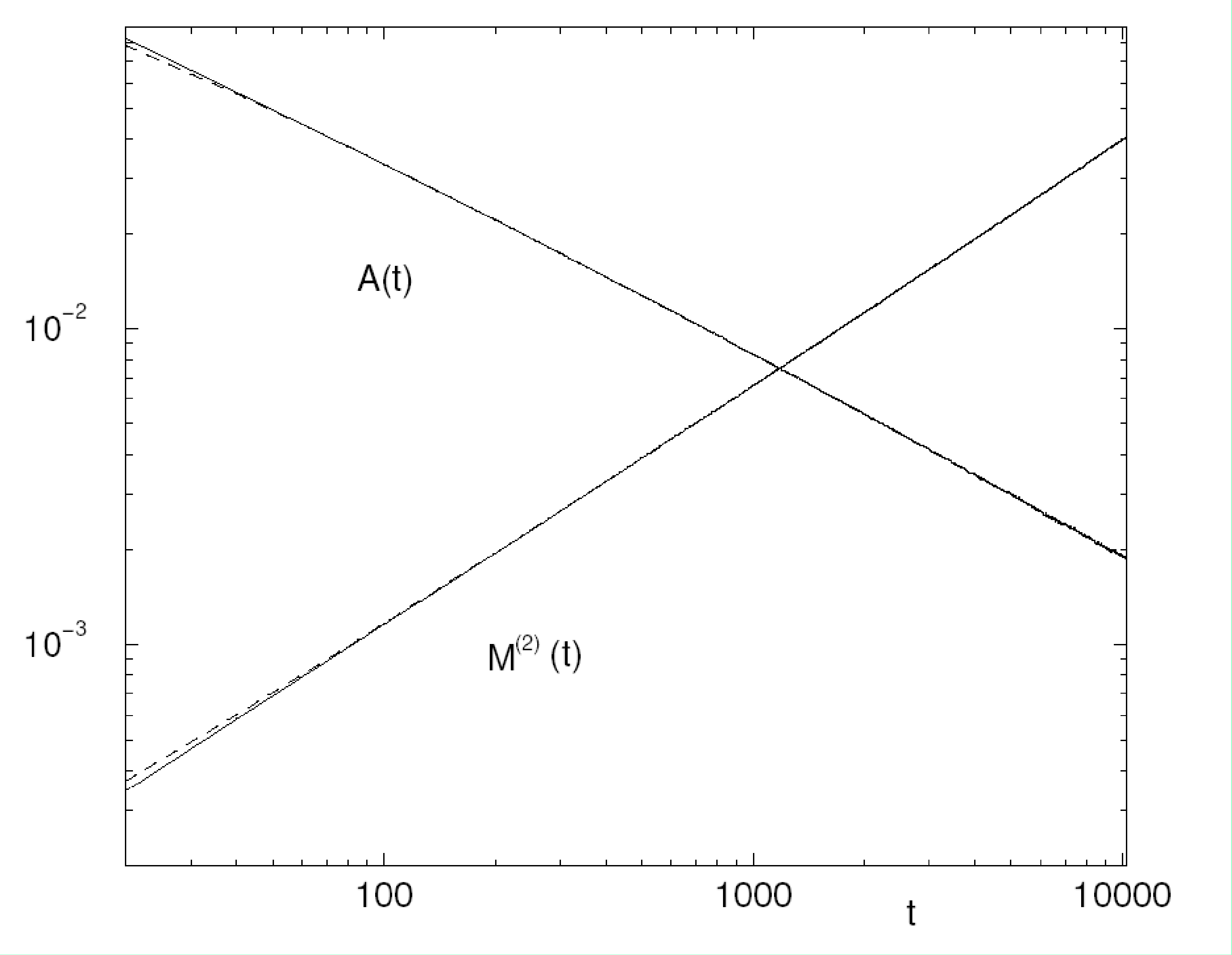
$$M^{(2)}(t) \sim [t / \ln(t / t_0)]^{C}$$

Only power law corrections for an ordered start

Zheng, Ren PRE (2003)

2D XY model, random initial state,

Ying, Zheng et al PRE(01)



2D XY model

Zheng, Ren PRE (2003)

		T=0.90	0.89	0.80	0.70
m0=1					
U(t)	d/z	1.000(10)	0.995(5)	0.999(4)	0.995(5)
	z1	2.00(2)	2.01(1)	2.00(1)	2.01(1)
M(t)	$\eta/2z$	0.0614(4)	0.0581(2)	0.0441(3)	0.0358(2)
	η	0.246(3)	0.234(2)	0.176(2)	0.144(1)
Gup92	η	0.239	0.229	0.179	0.146
m0=0					
M2(t)	z2	2.04(3)	2.01(2)	2.03(2)	2.02(2)
A(t)	z3	2.01(2)	2.02(2)	2.05(2)	2.05(2)

Extracting correlation length, for *T>Tc*

The scaling form

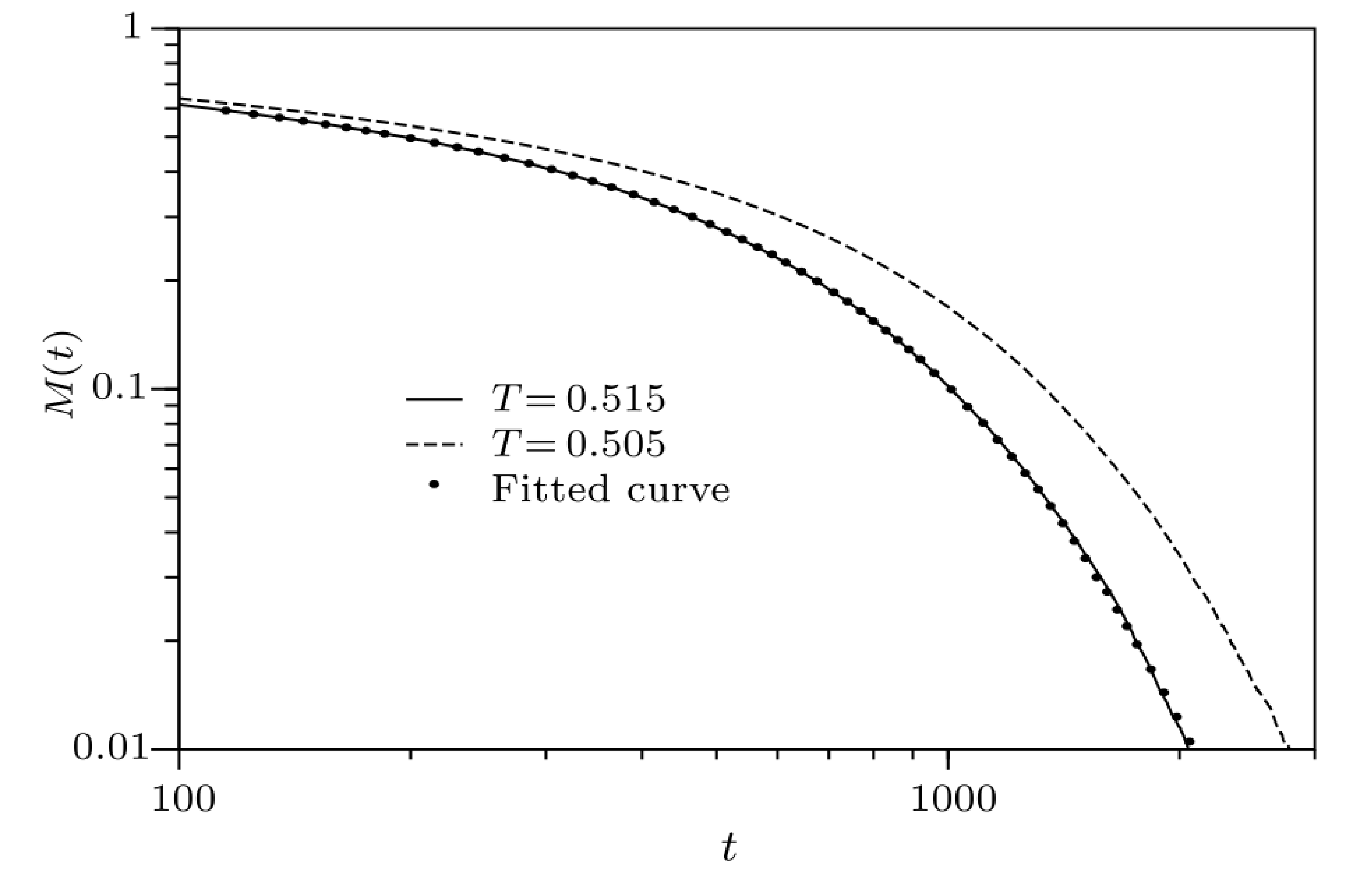
$$M^{(k)}(t,\xi) = b^{-k\eta/2} M^{(k)}(b^{-z}t, b^{-1}\xi), \quad k = 1, 2$$

$$\xi^{z}(\tau) = a \ \exp(b\tau^{-\nu})$$

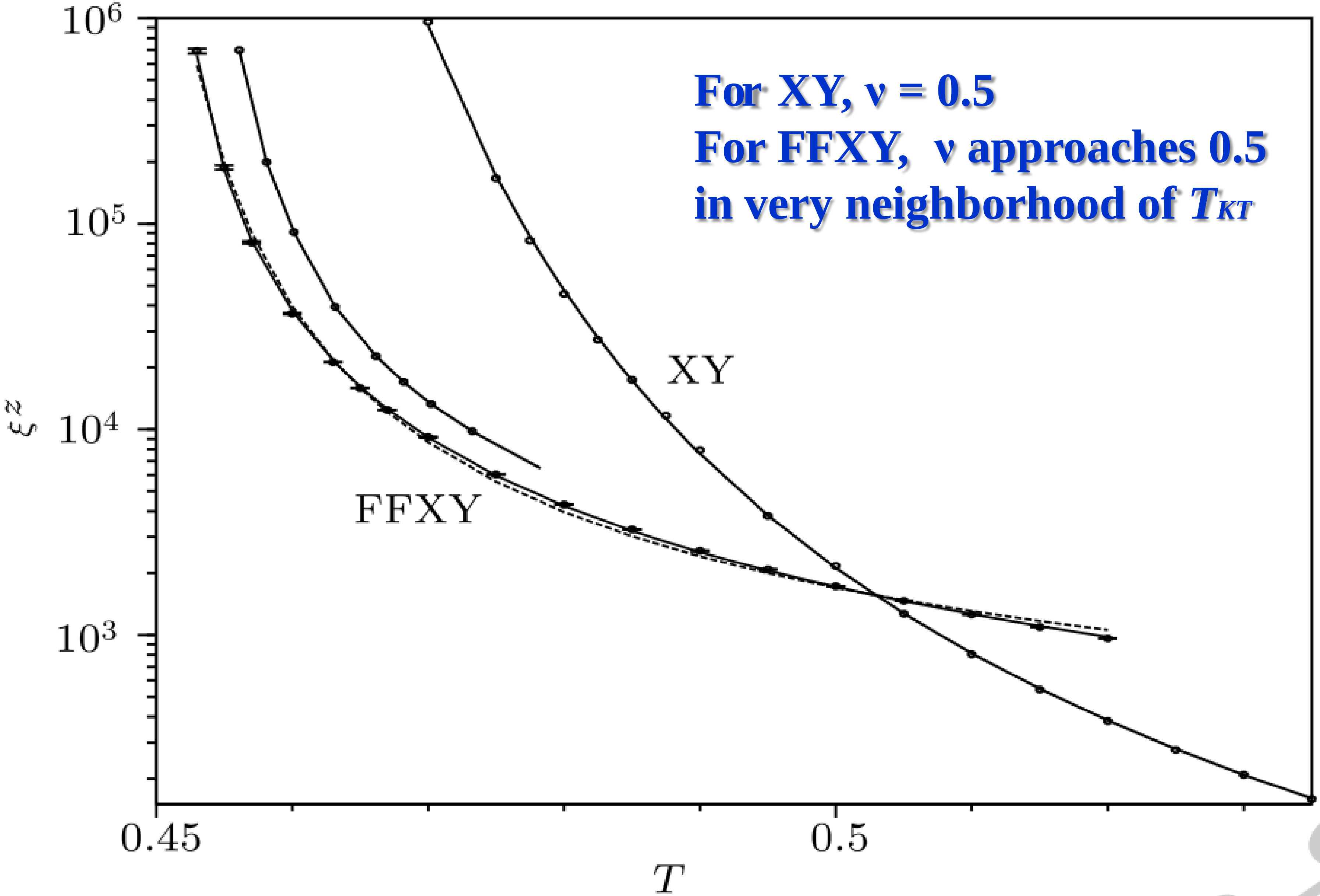
$$U(t,\xi) = b^{d} U(b^{-z}t, b^{-1}\xi)$$

From *M(t)*, we obtain ξ^{z} and $\eta / 2z$

From *U(t)*, we obtain ξ and z



1
0.1
0.01
M(t)
100
1000
t
T = 0.515
T = 0.505
Fitted curve


For XY, ν = 0.5
For FFXY, ν approaches 0.5
in very neighborhood of T_{KT}
XY
FFXY
10^6
10^5
10^4
10^3
ξ^z
0.45
0.5
T

Ageing phenomena in 2D XY model

Disordered initial state

logarithmic corrections to scaling

Ordered initial state

power-law corrections to scaling

Two-time correlation function at *Tc*

$$A(t',t) \equiv < \vec{S}_i(t') \cdot \vec{S}(t) >$$

$$= \xi(t')^{-\eta} F(\xi(t)/\xi(t'))$$

$\xi(t)$ **is the non-equilibrium spatial correlation length.**

The spatial unit $\xi(t')$ **changes with time *t'***

For the Ising model

$$\xi(t) \propto t^{1/z}$$

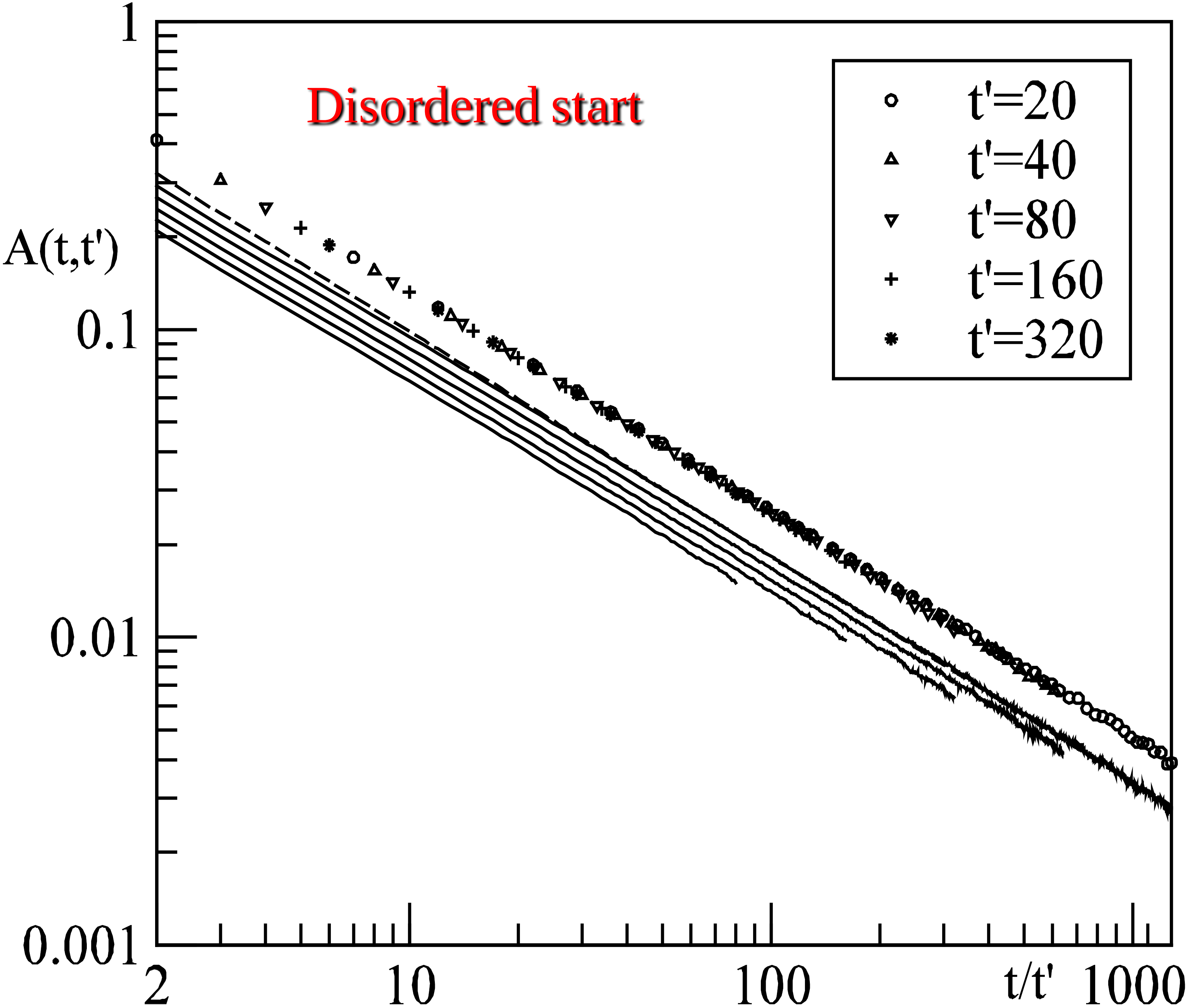
When $\xi(t)/\xi(t') \to \infty$

Disordered initial state

$$F(x) \to x^{-\lambda}$$

Ordered initial state

$$F(x) \to x^{-\eta/2}$$



Disordered start
A(t,t')
t'=20
t'=40
t'=80
t'=160
t'=320
1
0.1
0.01
0.001
2
10
100
t/t'
1000

For the 2D XY model

Disordered initial state

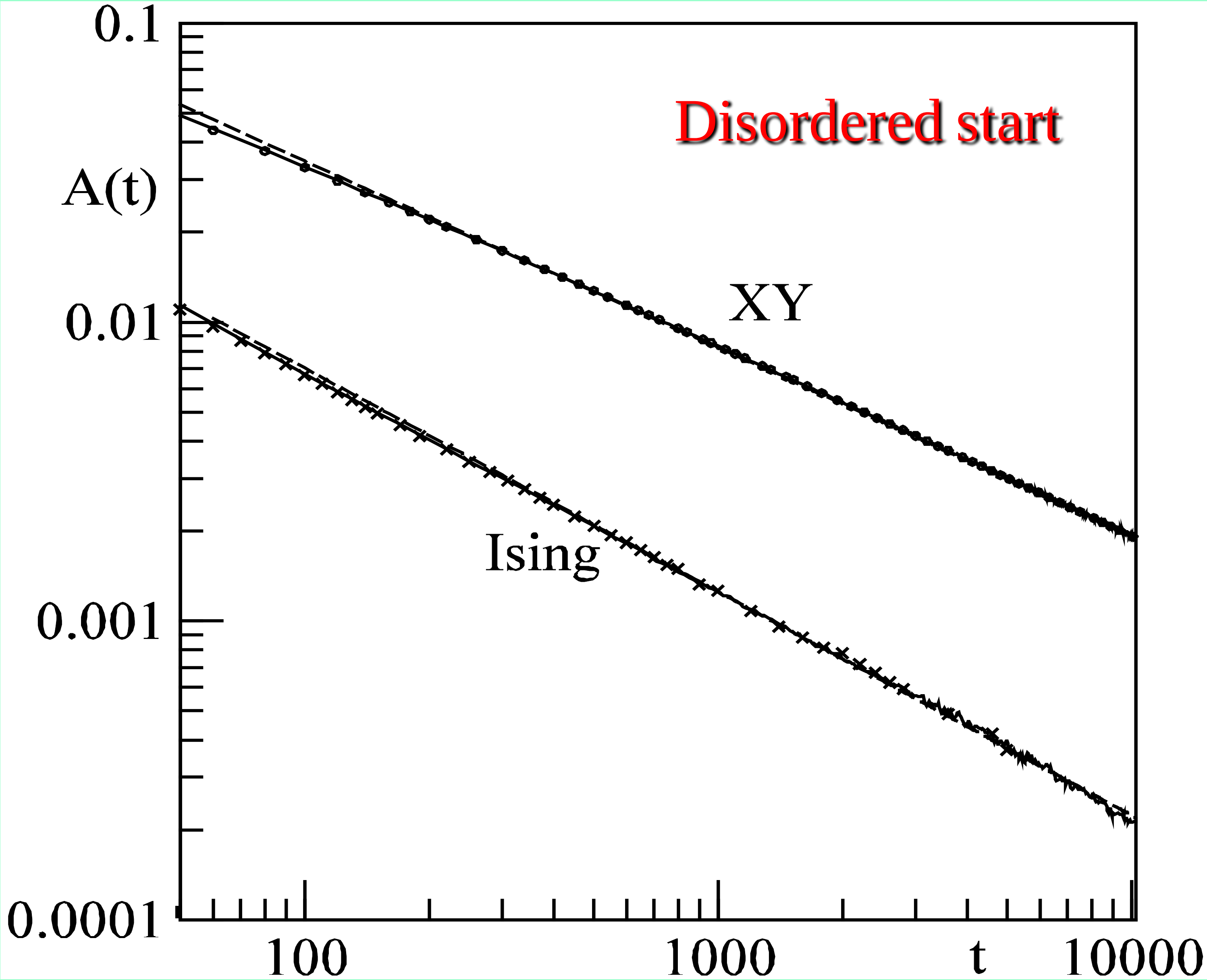
$$\xi(t) \propto (t / \ln(t / t_0))^{1/z}$$

Ordered initial state

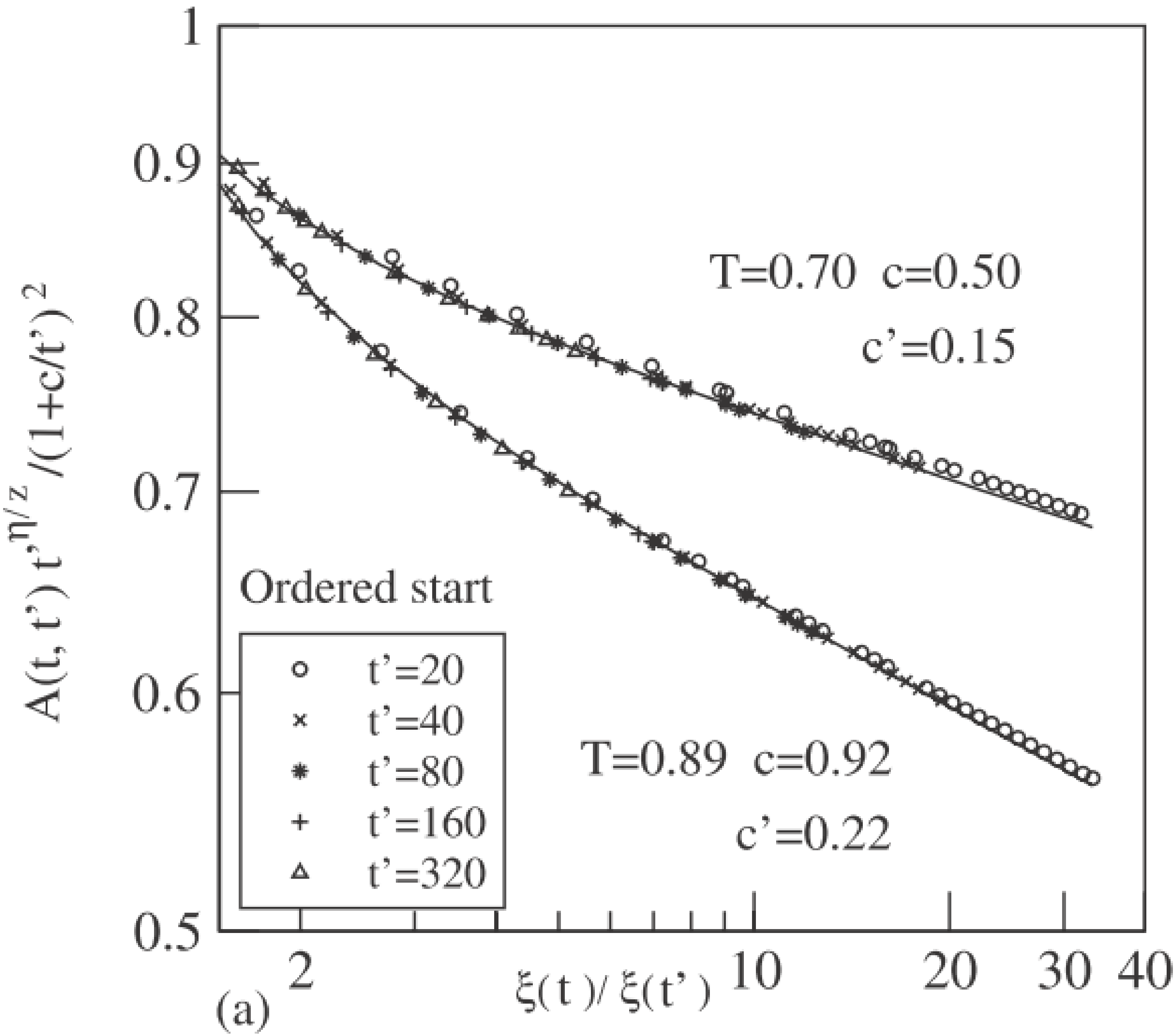
$$\xi(t) \propto (t /(1 + c / t^b))^{1/z}$$

Two kinds of corrections mix up!

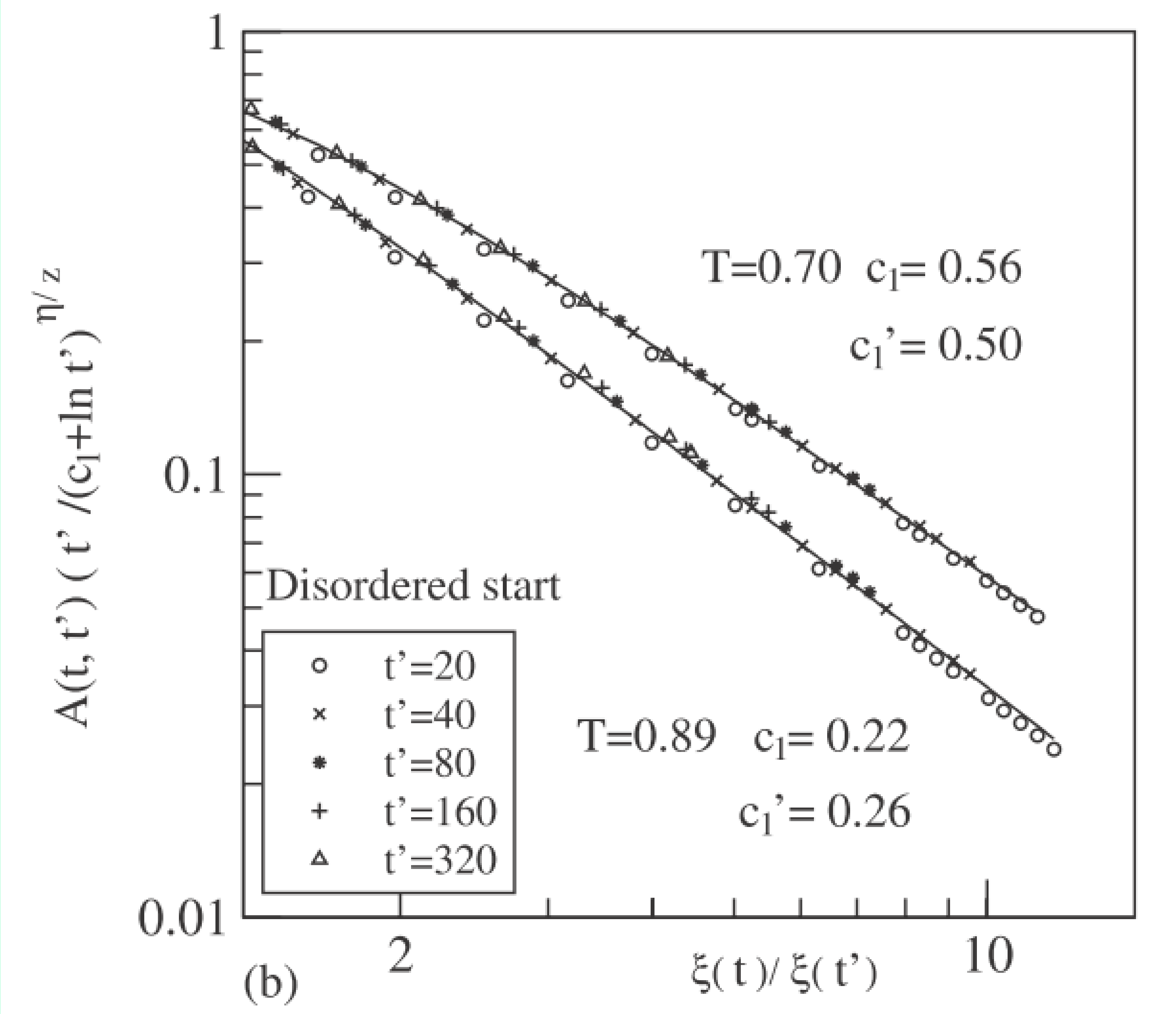
When $\xi(t)/\xi(t') \to \infty$ **,** ***F(x)*** **is dominated by power laws as for the Ising model. Therefore, corrections to scaling can be determined from** ***A(t',t)*** **with** ***t'=0, or 1*****.**



Disordered start
A(t)
0.1
0.01
0.001
0.0001
XY
Ising
100
1000
t
10000



A(t, t') t'^{η/z} /(1+c/t')^2
ξ(t)/ ξ(t')
T=0.70 c=0.50
c'=0.15
T=0.89 c=0.92
c'=0.22
Ordered start
t'=20
t'=40
t'=80
t'=160
t'=320
1
0.9
0.8
0.7
0.6
0.5
2
10
20
30
40
(a)



1
0.1
0.01
2
10
A(t, t') (t' /(c1+ln t'))^η/z
ξ(t)/ ξ(t')
T=0.70 c1= 0.56
c1'= 0.50
T=0.89 c1= 0.22
c1'= 0.26
Disordered start
t'=20
t'=40
t'=80
t'=160
t'=320
(b)

To explore *F(x)*, we assume $x = \xi(t)/\xi(t')$ **is large, but not too large.**

Ordered initial state $F(x) \to x^{-\eta/2}(1 + c'/x^{b'})$

$$A(t,t') = t'^{-\eta/z} \cdot (1 + c/t'^{b})^2 \cdot \frac{t^{-\eta/2z} \cdot (1 + c/t^{b})}{t'^{-\eta/2z} \cdot (1 + c/t'^{b})} (1 + c'/(t/t')^{b'})$$

$$= t'^{-\eta/z} \cdot (1 + c/t'^{b})(t/t')^{-\eta/2z} \cdot (1 + c/t^{b} + c'/(t/t')^{b'})$$

。

Usually, b=1, b'=1,

$$A(t,t') = t'^{-\eta/z} \cdot (1 + c/t')(t/t')^{-\eta/2z} \cdot (1 + (c/t' + c')/(t/t'))$$

Disordered initial state, $F(x) \to (x(1+c'/\ln x))^{-\lambda}$

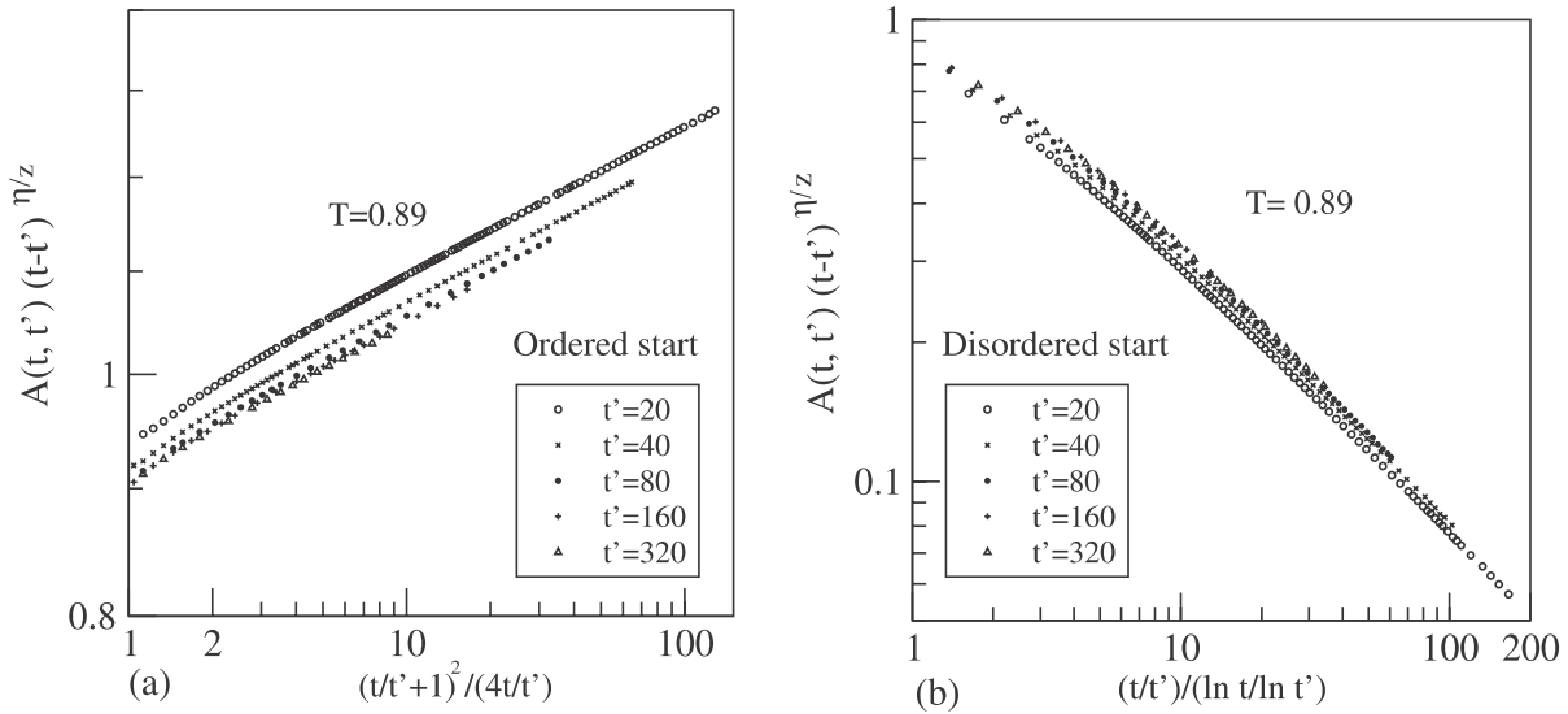
$$A(t,t') = (t'/(1+c\ln t'))^{-\eta/z}\,\frac{(t/(1+c\ln t))^{-\lambda}}{(t'/(1+c\ln t'))^{-\lambda}}(1+c'/\ln(t/t'))^{-\lambda}$$

$$= (t'/(1+c\ln t'))^{-\eta/z}\cdot[(t/t')/(1+(\tilde{c}+\tilde{c}')\ln(t/t')]^{-\lambda}$$

$\tilde{c} = c/(1+c\ln t')$ $\tilde{c}'$ is const， related to c’

In literature, some forms of *F(x)* are derived with spin-wave approximations, but not valid at higher temperatures

Data collapse from literature



Melting transition

In 2D, it is not of first order, but two KT transitions

Positional symmetry breaks first then orientational symmetry

Experiments: Phys.Rev.Lett. 82 (1999) 2721, 85 (2000) 3656

Methods: dynamic approach (but in equilibrium)

Molecular dynamics simulations with dipole-dipole interactions

SZ Lin, B. Zheng and S. Trimper, PRE(2006)

Bond orientational order parameter

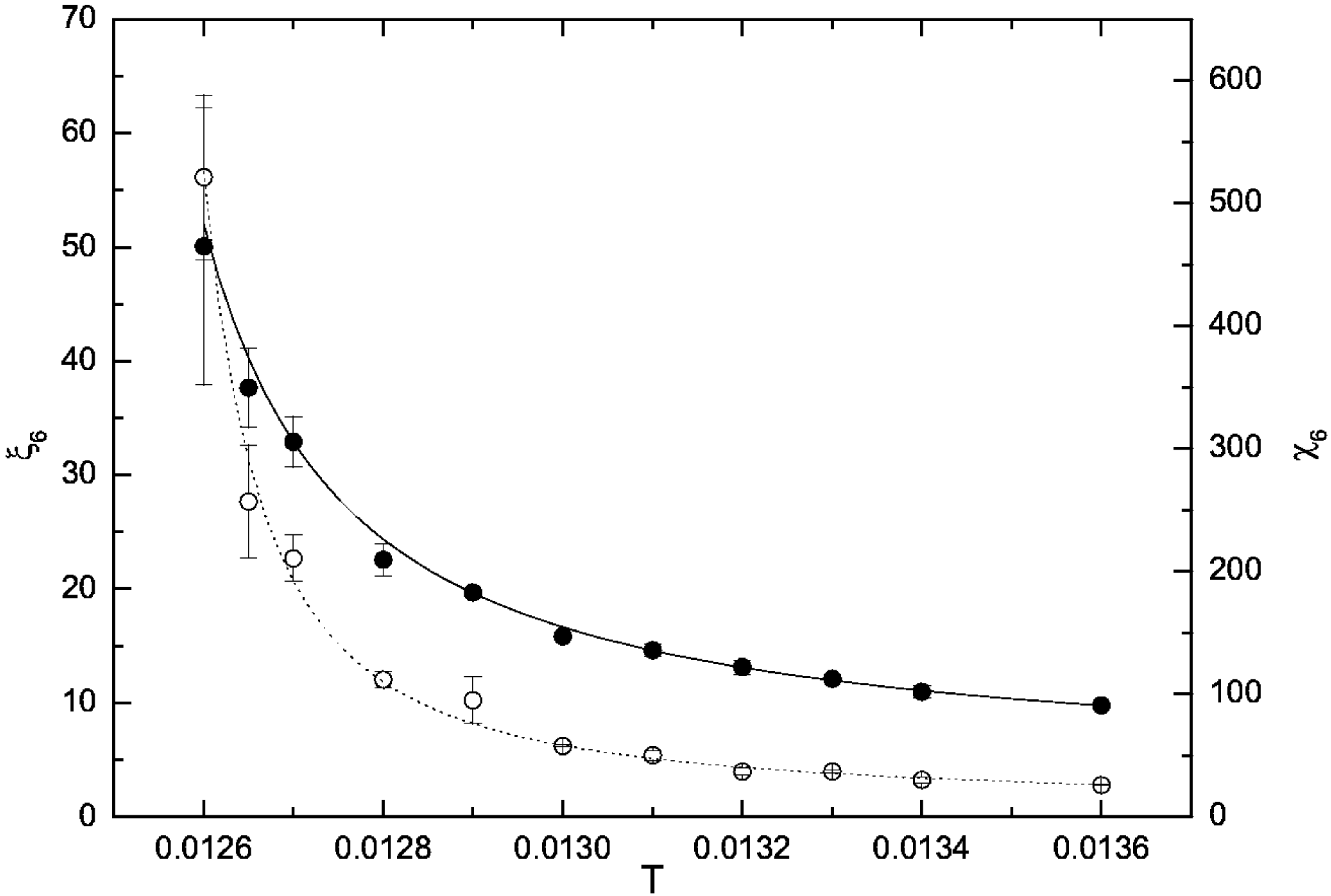
$$\Psi_6 = \left\langle \left| \frac{1}{N} \sum_{k=1}^{N} \psi_{6,k} \right| \right\rangle, \qquad \psi_{6,k} = \frac{1}{N_k} \sum_{j} \exp(i6\theta_{kj}).$$

Bond orientational correlation function

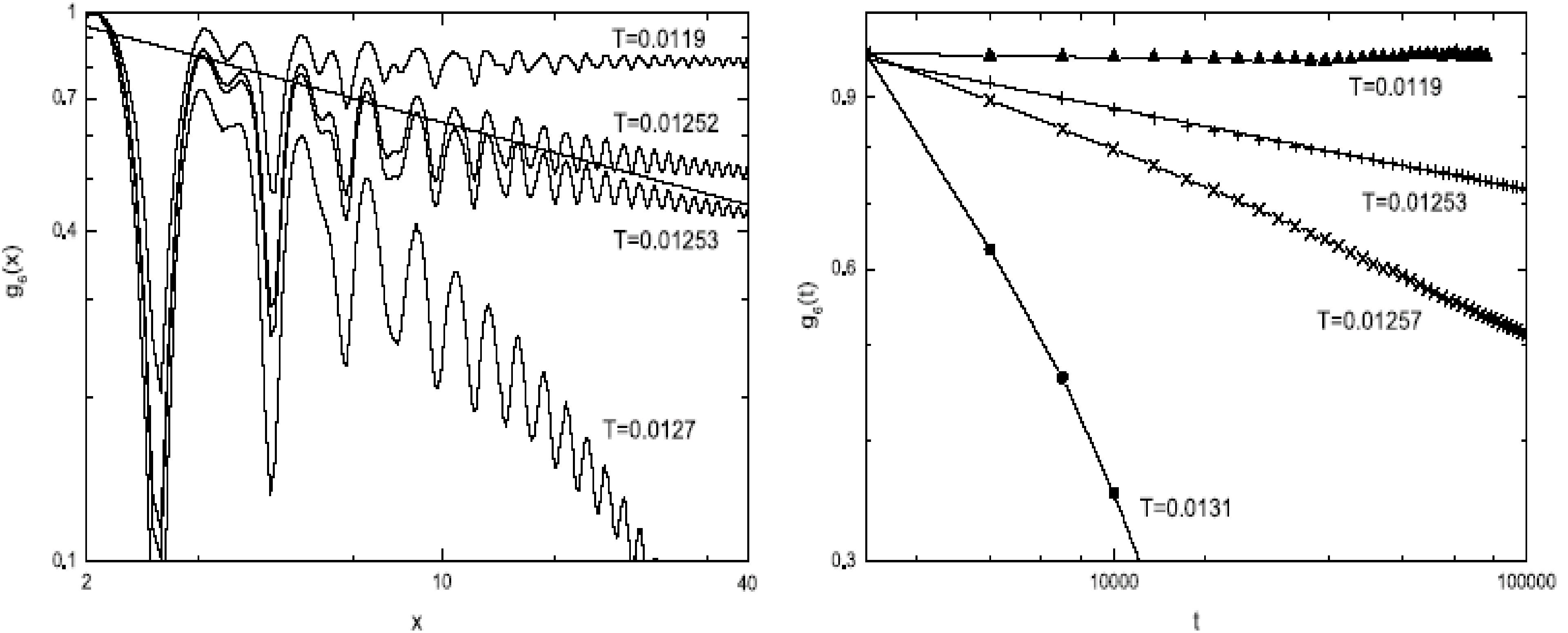
$$g_6(\vec{r_1} - \vec{r_2}) = \langle \psi_{6,k}^{*}(\vec{r_1}) \psi_{6,k}(\vec{r_2}) \rangle.$$

Time correlation of bond orientational order

$$g_6(t) = \langle \psi_{6,k}^{*}(t_0) \psi_{6,k}(t_0 + t) \rangle$$



70
60
50
40
30
20
10
0
600
500
400
300
200
100
0
ξ_6
χ_6
0.0126
0.0128
0.0130
0.0132
0.0134
0.0136
T



The finite size effects and coexistence phase is excluded

Concluding remarks

With Monte Carlo simulations and molecular dynamics simulations, we reveal the universal scaling behavior in critical dynamics far from equilibrium, in addition, we report

*** Application to weak first order transitions**

*** Ageing phenomena around phase transitions**