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Aging and non-equilibrium phenomena in Monte Carlo simulations of the bulk and low-dimensional ferromagnets

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It is considered the non-equilibrium critical evolution of spin systems with slow dynamics which displays some features, such as aging and violation of the fluctuation-dissipation theorem. We review some results of computations that have been obtained in recent years for such quantities, as the exponents determining the scaling behavior of dynamic response and correlation functions and the fluctuation-dissipation ratio, associated with the non-equilibrium critical dynamics, with particular focus on our original Monte Carlo simulation results for the 3D pure, diluted and low-dimensional Ising-like ferromagnets.

Aging

Aging — anomalously slow down effects of non-equilibrium relaxation processes with system age increasing.

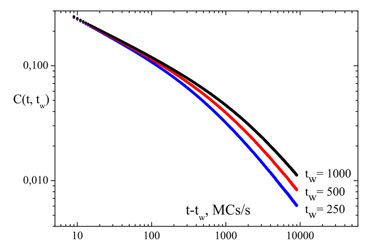

Fig. 1. Autocorrelation function $C(t, t_w)$ for 3D diluted Ising model

t_w is a waiting time ("age of system"),
$t - t_w$ is a time of observation.

Aging phenomena are characterized by two-time dependence for autocorrelation and response functions:

$$C(t,t_w) \sim (t-t_w)^{a+1-d/z}\,(t/t_w)^{\theta-1} f_C(t_w/t),$$
$$R(t,t_w) \sim (t-t_w)^{a-d/z}\,(t/t_w)^{\theta} f_R(t_w/t), \qquad (1)$$

where $f_C(t_w/t)$ and $f_R(t_w/t)$ are finite for $t_w \to 0$,

$$a = (2-\eta-z)/z,\ \theta = \theta' - (2-z-\eta)/z,$$

θ' — initial slip exponent [1]

[1]. Janssen H.K., Schaub B., Schmittmann B. Z.Phys.B, **73**, 539, 1989.

Dynamical functions

- Autocorrelation function:

$$C(t,t_w) = \frac{1}{V}\int d^dx \left[\langle S(x,t)S(0,t_w)\rangle - \langle S(x,t)\rangle\,\langle S(0,t_w)\rangle\right], \qquad (2)$$

- Response function:

$$R(t,t_w) = \frac{1}{V}\int d^dx\, \frac{\delta\langle S(x,t)\rangle}{\delta h(x,t_w)}\bigg|_{h=0}. \qquad (3)$$

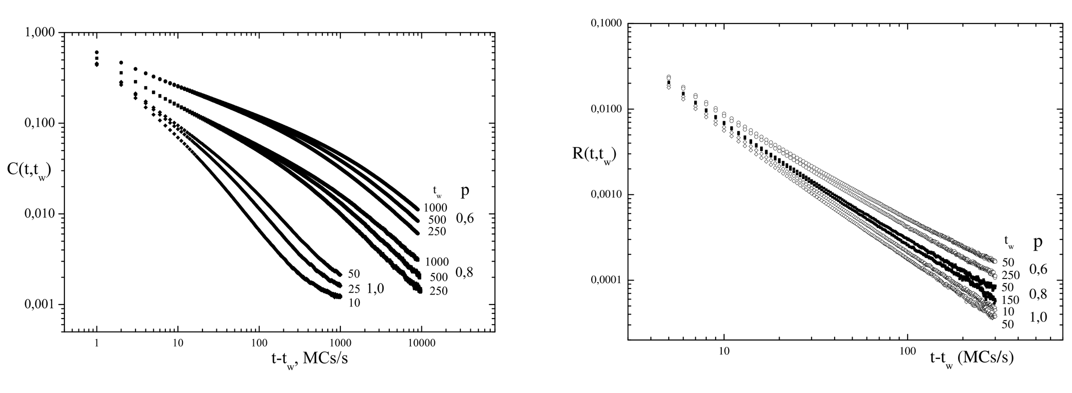

Fig. 2 Time dependencies of $C(t, t_w)$ (left) and $R(t, t_w)$ (right) as a function $(t - t_w)$ for different values of t_w

Dynamical regimes

- $t - t_w < t_w$: $R = R(t - t_w)$ quasi-equilibrium regime;
- $t - t_w \sim t_w$: $R \approx t_w^{-2\beta/\nu z - 1} F_R(t/t_w)$ **aging** regime;
- $t - t_w \gg t_w$: $R \sim (t/t_w)^{\theta}$ short-time dynamics regime [2],

$$1 \ll t_w < t \ll t_{equil} \sim |T - T_c|^{-z\nu}$$

[2]. Prudnikov, Pospelov, et al. Phys. Rev. E, 81, 011130, 2010.

Violation of FDT

- Fluctuation-dissipation theorem (FDT) $t \gg t_{equil}$

$$R(t,t_w) = \frac{1}{T}\frac{\partial C(t,t_w)}{\partial t_w} \qquad (4)$$

- Fluctuation-dissipation ratio (FDR) $t < t_{equil}$

$$X(t,t_w) = \frac{T R(t,t_w)}{\partial C(t,t_w)/\partial t_w} \qquad (5)$$

$$X^\infty = \lim_{t_w\to\infty}\lim_{t\to\infty} X(t,t_w) \qquad (6)$$

- The asymptotic value of the FDR is new universal characteristic of non-equilibrium behavior [3]

$$T_{eff} = T/X^\infty \qquad (7)$$

[3]. Calabrese and Gambassi, J. Phys. A, **38**, R133, 2005.

Aging

- $T < T_c$:

$$X(t,t_w) \simeq t_w^{-a} f_X(t/t_w), \qquad (8)$$

where $\lim_{x\to\infty} f_X(x) = \mathrm{const}$.

- $T = T_c$:
  - aging regime $t - t_w \sim t_w$

$$C(t,t_w) \approx t_w^{-2\beta/\nu z} F_C(t/t_w),\quad R(t,t_w) \approx t_w^{-2\beta/\nu z - 1} F_R(t/t_w), \qquad (9)$$

where $2\beta/\nu z = (d - 2 + \eta)/z$.

  - short-time regime $t - t_w \gg t_w$

$$F_C(t/t_w) \sim (t/t_w)^{-c_a},\quad F_R(t/t_w) \sim (t/t_w)^{-c_r}, \qquad (10)$$

where $c_a = c_r = d/z - \theta'$.

Dynamical scaling

$$C(t,t_w) \sim t_w^{-2\beta\nu/z} F_C(t/t_w),\quad R(t,t_w) \sim t_w^{-2\beta\nu/z-1} F_R(t/t_w),$$
$$(d - 2 + \eta)/z \equiv 2\beta\nu/z$$

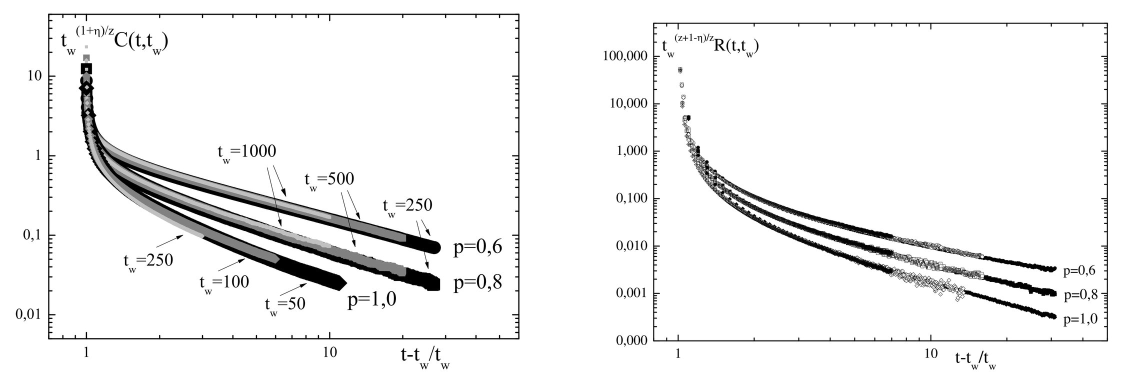

Fig. 3 Data collapse for $C(t, t_w)$ (left) $R(t, t_w)$ (right)

Calculation of FDR $X^\infty(t_w)$

$$X^\infty(t_w) = -\lim_{C\to 0}\frac{\partial(T\chi(t,t_w))}{\partial C(t,t_w)} \qquad X^\infty(t_w) = \lim_{t\to\infty} X(t,t_w)$$

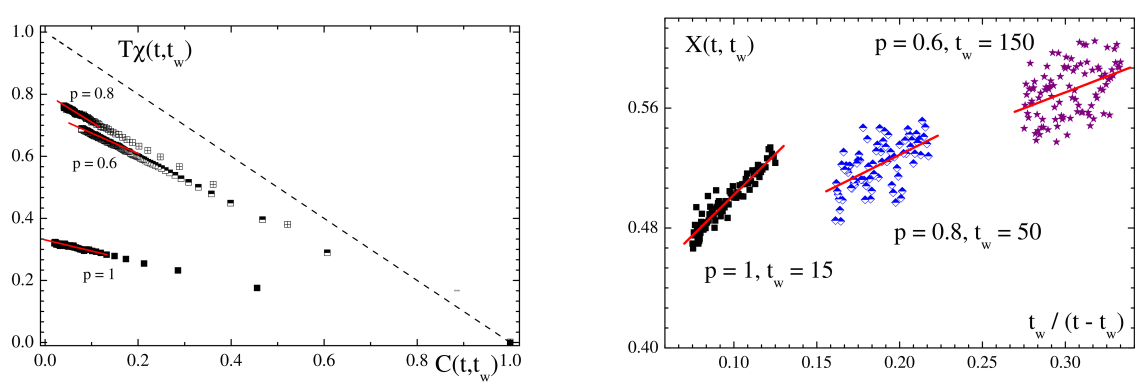

Fig. 4 FDR $X^\infty(t_w)$ for probing field (left) and heat-bath dynamic (right)

Calculation of asymptotic FDR X^∞

$$X^\infty = \lim_{1/t_w\to 0} X^\infty(t_w)$$

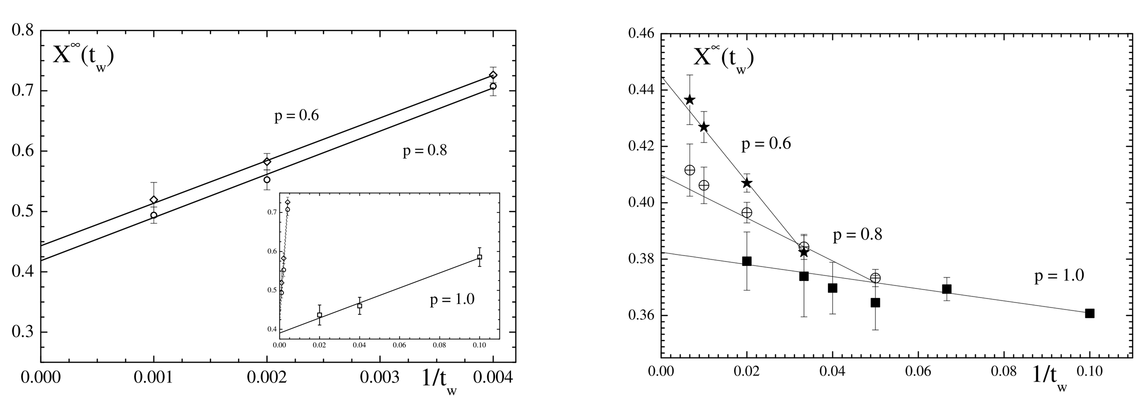

Fig. 5 Asymptotic FDR $X^\infty = \lim_{t_w\to\infty} X^\infty(t_w)$ for probing field (left) and heat-bath dynamic (right)

Conclusions

- The non-equilibrium critical dynamics of the diluted Ising model is characterized by new universal FDRs with $X^\infty_{\text{pure}} < X^\infty_{\text{weak diluted}} < X^\infty_{\text{strong diluted}}$;

Model and Simulations

- disordered 3D Ising model

$$H = -J\sum_{i,j} p_i p_j S_i S_j, \qquad (11)$$

where $J > 0$ is the ferromagnets interaction constant,
$S_i = \pm 1$ – Ising spins,
p_i are quenched, uncorrelated random variables described by the following distribution function:

$$P(p_i) = p\,\delta(p_i - 1) + (1-p)\,\delta(p_i), \qquad (12)$$

where p – spin concentration.

- Influence of initial non-equilibrium states:
  - high-temperature initial state with magnetization $m_0 \ll 1$;
  - low-temperature initial state with magnetization $m_0 = 1$;
- Influence of quenched disorder:
  - weakly disordered system $p = 0.8$;
  - strong disordered system $p = 0.6$.

Experimental FDT violation

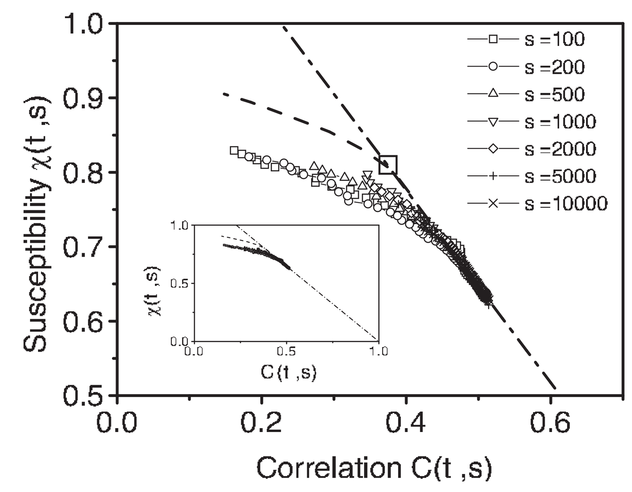

Fig. 4 FDT violation in spin-glass $CdCr_{1.7}In_{0.3}S_4$, $T = 13.3K = 0.8\,T_c$ [4]

[4]. D.Hérisson, M.Ocio. Phys. Rev. Lett. **88**, 257202, 2002; Eur. Phys. J. B **40**, 283, 2004.

Scaling critical exponents

$$t - t_w \gg t_w,\quad F_R(t/t_w) \sim (t/t_w)^{-c_r};\quad F_C(t/t_w) \sim (t/t_w)^{-c_a};$$

Tab. 1 Scaling critical exponents $t - t_w \gg t_w$

	$p = 1.0$	$p = 0.8$	$p = 0.6$
c_r	1.357(18)	1.251(24)	0.950(8)
c_a	1.333(40)	1.237(22)	0.982(30)
Jaster, et al., 1999 [5]	1.362(19)		
Prudnikov, et. al, 2010 [2]		1.242(10)	
Prudnikov, et. al, 2014 [6]			0.993(60)

[5]. Jaster, Mainville, Schülke, Zheng, J. Phys. A, 32, 1395, 1999;
[6]. Prudnikov, Prudnikov, and Vakilov, Theoretical Description Methods of Non-Equilibrium Critical Behavior of Structurally Disordered Systems (Fizmatlit, Moscow, 2014) [in Russian].

Aging for $m_0 = 1$

$$X^\chi_\infty = -\lim_{C\to 0}\frac{d(T\chi)}{dC}, \qquad (13)$$

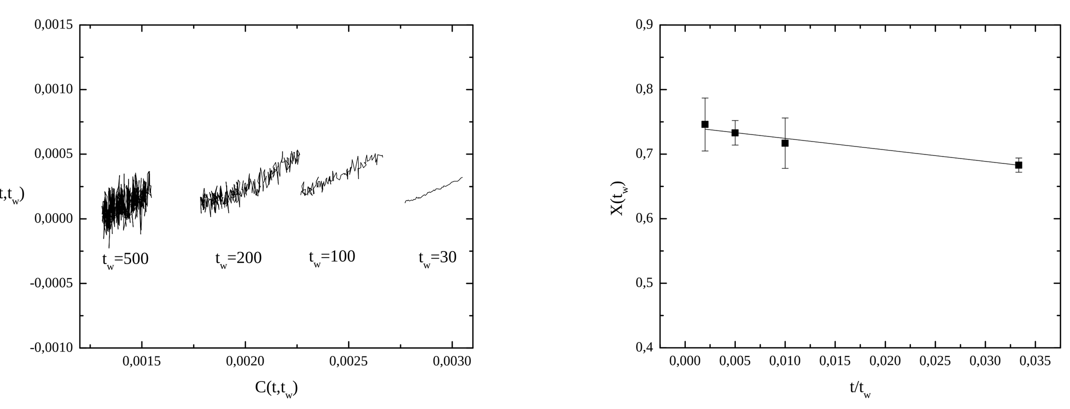

Fig. 5 $T\chi(t, t_w)$ versus $C(t, t_w)$ (left) and FDR X^∞ (right) for $m_0 = 1$ and $p = 0.95$

FDR for high-temperature initial state $m_0 \ll 1$

Tab. 2 Values of FDR X^∞ for $p = 1.0, 0.8$ and 0.6

	X^∞		
	$p = 1.0$	$p = 0.8$	$p = 0.6$
$m_0 \ll 1$ heat-bath dynamics [7]	0.380(13)	0.413(11)	0.446(8)
$m_0 \ll 1$ probing field [8]	0.390(12)	0.415(18)	0.443(6)

- Pure 3D Ising model [9]

$$\frac{(X^\infty)^{-1}}{2} = 1 + \frac{n+2}{4(n+8)}\epsilon + \epsilon^2\frac{n+2}{(n+8)^2}\left[\frac{n+2}{8} + \frac{3(3n+14)}{4(n+8)}\right] + O(\epsilon^3),$$

where $\epsilon = 4 - d$. Padé summation: $n = 1 \to X^\infty = 0.429(6)$

- Diluted 3d Ising model [10]

$$\frac{(X^\infty)^{-1}}{2} = 1 + \frac{1}{2}\sqrt{\frac{6\epsilon}{53}} + O(\epsilon^2),\quad n = 1 \to X^\infty = 0.416$$

[7]. Prudnikov, Prudnikov, Pospelov, JETP Letters, **98**, 619, 2013;
[8]. Prudnikov, Prudnikov, Pospelov, JETP, **118**, 401, 2014;
[9]. Calabrese and Gambassi, Phys. Rev. E, **66**, 066101, 2002;
[10]. Calabrese and Gambassi, Phys. Rev. E, **66**, 212407, 2002.

FDR for low-temperature initial state $m_0 = 1$

Tab. 3 Values of FDR X^∞ for $p = 1.0, 0.95$

	X^∞		
	$p = 1.0$	$p = 0.95$	$p = 0.8$
$m_0 = 1$ heat-bath dynamics	0.77(6)	0.74(3)	0.73(2)

- RG calculation for pure system [11]

$$X^\infty = \frac{4}{5} - \left(\frac{73}{600} - \frac{\pi^2}{100}\right)\epsilon + O(\epsilon^2), \qquad (14)$$

for $d = 3$ $X^\infty = 0.78$

[11]. Calabrese, Gambassi and Krzakala, J. Stat. Mech., P06016, 2006.

Acknowledgements

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