Spin-glass transition in the three-dimensional EAI model: universality and scaling corrections

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Overview

M. Hasenbusch, A. Pelissetto, E. Vicari,
J. Stat. Mech. (2008) L02001 [arXiv:cond-mat/0710.1980]

- Definition of the models and the observables
- Summary of results given in the literature
- Corrections to scaling and the Renormalization Group
- Our Monte Carlo simulations
- Conclusions

We study a simple cubic lattice with periodic boundary conditions in 3 dimensions. The Hamiltonian of the Edwards-Anderson model is given by

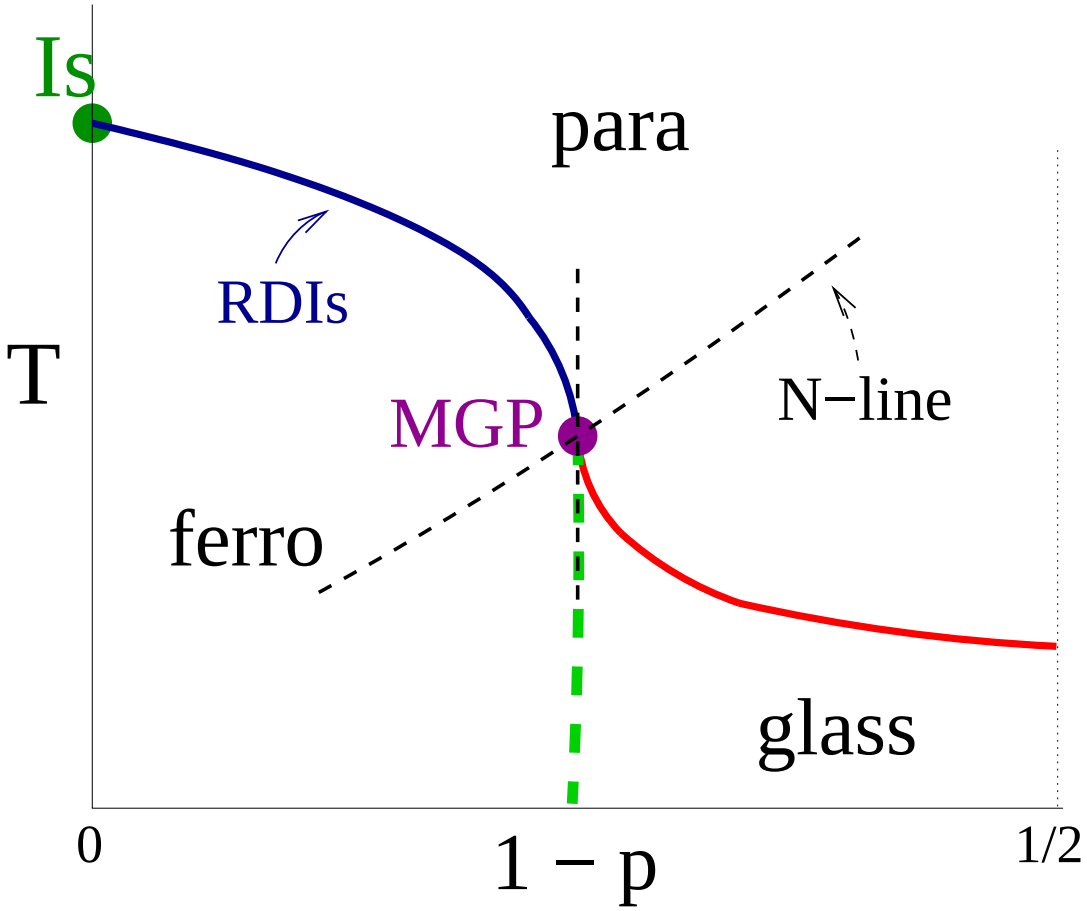
$$H = -\sum_{<xy>} J_{<xy>} s_x s_y$$

with $s_x \in \{-1, 1\}$. (As in the Ising model). Here, the coupling constants $J_{<xy>}$ are quenched uncorrelated random variables

- The $\pm J$ model: $J_{<xy>} \in \{-1, 1\}$ with $P(1) = 1 - P(-1) = p$

  We have simulated $p = 0.5$ and $p = 0.7$.
- $\pm J$ model with bond dilution: $J_{<xy>} \in \{-1, 0, 1\}$ with probabilities $P(-1) = (1-p)p_b$, $P(0) = (1-p_b)$, and $P(1) = pp_b$. We have simulated $p = 0.5$ and $p_b = 0.45$.
- Preliminary results for Gaussian distribution of $J_{<xy>}$.

Phase diagram of the $\pm J$ model



$p_{MGP} = 0.76820(4)$, $2p - 1 = \tanh(J/T)$

The observables

Expectation value for a given set of coupling constants:

$$\langle A \rangle_{\{J\}} := \frac{\sum_{\{s\}} \exp\left(-\beta H(\{J\},\{s\})\right)\ A(\{J\},\{s\})}{\sum_{\{s\}} \exp\left(-\beta H(\{J\},\{s\})\right)}$$

Overlapp variables are needed for the study of the glass transition:

$$q_x = s_x^{(1)} s_x^{(2)}$$

$s_x^{(1)}$ and $s_x^{(2)}$ are the spins of two statistically independent configurations for the same set of coupling constants $J_{<xy>}$.

Expectation value of overlapp observables for a given set of coupling constants:

$$\langle B \rangle_{\{J\}} :=$$

$$\frac{\sum_{\{s^{(1)}\},\{s^{(2)}\}} \exp\left(-\beta[H(\{J\},\{s^{(1)}\}) + H(\{J\},\{s^{(2)}\})]\right)\ B(\{J\},\{q\})}{\sum_{\{s^{(1)}\},\{s^{(2)}\}} \exp\left(-\beta[H(\{J\},\{s^{(1)}\} + H(\{J\},\{s^{(2)}\}])\right)}$$

Average over all sets of couplings:

$$[F(\langle A \rangle_{\{J\}}, \langle B \rangle_{\{J\}}, \ldots)] := \frac{\sum_{\{J\}} [\prod_{<xy>} p(J_{<xy>})] F(\langle A \rangle_{\{J\}}, \langle B \rangle_{\{J\}}, \ldots)}{\sum_{\{J\}} \prod_{<xy>} p(J_{<xy>})}$$

Very useful for Finite Size Scaling (FFS):
Renormalization Group invariant quantities

Cumulants:

$$U_4 = \frac{[\mu_4]}{[\mu_2]^2} \qquad U_{22} = \frac{[\mu_2^2] - [\mu_2]^2}{[\mu_2]^2}$$

with $\mu_k = \langle \left(\sum_x q_x\right)^k \rangle$

Second moment correlation length over the linear lattice size L:

$$R_\xi = \xi_{2nd}/L$$

Overlapp susceptibility

$$\chi = \frac{1}{V}[\mu_2]$$

Fourier transform of the correlation function at lowest non-vanishing momentum

$$F = \frac{1}{V}\sum_{x,y}\langle q_x q_y\rangle \cos(2\pi(y_1 - x_1)/L)$$

$$\xi_{2nd} = \frac{1}{2\sin(\pi/L)}\left(\frac{\chi}{F} - 1\right)^{1/2}$$

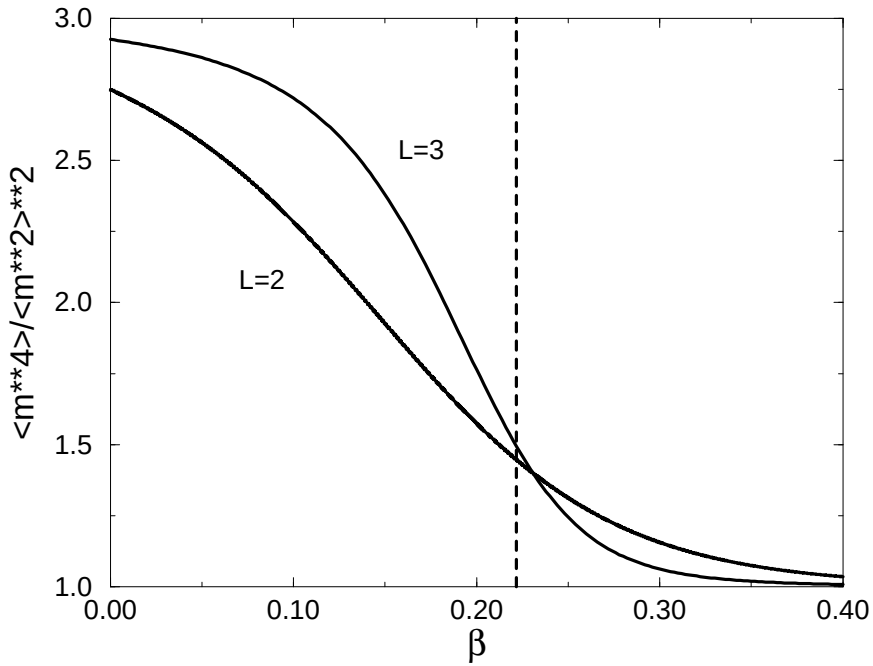
RG invariant quantities like U_4 or R_ξ behave close to T_c as

$$R = R^* + a(\beta - \beta_c)L^{1/\nu} + cL^{-\omega} + \ldots$$

$\longrightarrow$ Binder crossing method to find T_c

$\longrightarrow$ determine ν from slope at T_c

Example: 3D Ising model
simple cubic lattice



Our implementation of FSS:

$$R_\xi(L, \beta_f(L)) = R_{\xi,f}$$

with $R_{\xi,f} \approx R_\xi^*$ defines $\beta_f(L)$. Quantities are analysed at $\beta_f(L)$:

$$\beta_f = \beta_c + a^{-1}(R_{\xi,f} - R_\xi^* - cL^{-\omega})L^{-1/\nu} + ...$$

$$U_4(R_f) = U_4^* + \frac{a_U}{a_R}(R_{\xi,f} - R_\xi^*) + (c_u - \frac{a_U}{a_R}c_R)L^{-\omega} + ...$$
$$= \bar{U}_4^* + \bar{c}_u L^{-\omega} + ...$$

$$\left.\frac{\partial R}{\partial \beta}\right|_{\beta=\beta_f} = \bar{a}L^{1/\nu} \times (1 + \bar{c}L^{-\omega} + ...) \qquad \chi(\beta_f) = \bar{b}L^{2-\eta}(1 + ...)$$

Results for $\pm J$ model at $p = 0.5$ taken from H. Katzgraber, M. Körner, and A. P. Young, Phys. Rev. B **73**, 224432 (2006).

authors	year	T_c	ν	η
Ogielski, Morgenstern	1985	1.20(5)	1.2(1)	
Ogielski	1985	1.175(25)	1.3(1)	-0.22(5)
Singh, Chakravarty	1986	1.2(1)	1.3(2)	
Bhatt, Young	1985	1.2(2)	1.3(3)	-0.3(2)
Kawashima, Young	1996	1.11(4)	1.7(3)	-0.35(5)
Bernardi et al	1996	1.165(10)		-0.245(20)
Berg, Janke	1998	1.12(1)		-0.37(4)
Palassini, Caracciolo	1999	1.156(15)	1.8(2)	-0.26(4)
Mari, Campbell	1999	1.20(1)		-0.21(2)
Ballesteros et al.	2000	1.138(10)	2.15(15)	-0.337(15)
Mari, Campbell	2001	1.190(15)		-0.20(2)
Mari, Campbell	2002	1.195(15)	1.35(10)	-0.225(25)
Nakamura et al	2003	1.17(4)	1.5(3)	-0.4(1)
Pleimling, Campbell	2005	1.19(1)		-0.22(2)
Katzgraber et al.	2006	1.120(4)	2.39(5)	-0.395(17)
our result	2007	1.101(5)	2.53(8)	-0.384(9)

Estimates for ν from different quantities differ quite a lot:

E.g. FSS (finite size scaling), Katzgraber et al.
(Using power law ansätze without corrections):

- 2.39(5) from ξ/L
- 2.79(11) from the Binder Cumulant
- 1.57(3) from the slope of χ

$\Rightarrow$ Have to understand corrections to scaling

The singular part of the free energy

$$f(\beta, h, L) = L^{-d} f_s(u_t L^{y_t}, u_h L^{y_h}, u_3 L^{y_3}) + f_{ns}(\beta, h)$$

where u_t, u_h and u_3 are non-linear scaling fields:
$u_t = t + ah^2 + \ldots$ and $u_h = h + bth + \ldots$ where $t = \beta - \beta_c$.
For $h = 0$:

$$\chi = \frac{\partial^2 f}{\partial h^2} = L^{-d}(f_s^{(0,2)} L^{2y_h}(1 + 2bt + \ldots) + \ldots)) + f_{ns}^{(0,2)}$$

$$\frac{\partial \chi}{\partial \beta} = L^{-d}(f^{(1,2)} L^{2y_h + y_t}(1 + \ldots) + 2bf^{(0,2)} L^{2y_h}(1 + \ldots) + \ldots) + f_{ns}^{(1,2)}$$

$$\propto L^{2y_h + y_t - d}(1 + cL^{-y_t} + \ldots)$$

The derivatives of ξ/L and the Binder cumulant with respect to β at β_c do not suffer from corrections $\propto L^{-y_t}$

The simulation

- Local Metropolis updates
- Multispin coding implementation
  (64 systems run in parallel, same random number for all systems)
- Random exchange method (Parallel tempering)
- Avoid bias in quantities like $[\langle A \rangle \langle B \rangle]$ ...
- Careful check of equilibration: double lenght of the equilibration time until results are consistent within errors
- We compute the Taylor expansion of the observables up to 2^{nd} order

In total about 30 years of a single core 2.4 GHz Opteron CPU.

Compute a table with two entries:

```
for(ite=0;ite<NTEMP;ite++)
  {
  pp[ite][0]=exp(-4.*beta[ite]);
  pp[ite][1]=exp(-8.*beta[ite]);
  }

/*  metropolis routine for 2D system */
void metro(int l1,int l2)
{
  long int p1,p2,p3,p4;
  long int jj1,jj2,ii1,ii2,ido;
  int i0,is0,iq0,i1,is1,iq1;

  double xxrr;
```

```
for(i0=0;i0 < L0;i0++)
  {
  iq0=i0-1; if(i0==0) iq0=L0-1; is0=i0+1; if(is0==L0) is0=(
  for(i1=0;i1 < L1;i1++)
    {
    iq1=i1-1; if(i1==0) iq1=L1-1; is1=i1+1; if(is1==L1) is1

    xxrr=genrand_res53();

    if(xxrr<pp[l1][1]) {spins[l1][l2][i0][i1]=~spins[l1][l2
    else
      {
      p1=link[iq0][i1][0]^spins[l1][l2][i0][i1]^spins[l1][l
      p2=link[i0][i1][0]^spins[l1][l2][i0][i1]^spins[l1][l2
      p3=link[i0][iq1][1]^spins[l1][l2][i0][i1]^spins[l1][l
      p4=link[i0][i1][1]^spins[l1][l2][i0][i1]^spins[l1][l2
```

```
    if(xxrr<pp[l1][0])
      {
      /* check that at least one bond is not satisfied */
      ido=p1|p2|p3|p4;
      spins[l1][l2][i0][i1]=ido^spins[l1][l2][i0][i1];
      }
    else
      {
      /* check that at least two bonds are not satisfied
      ii2=p1&p2; ii1=p1^p2;
      jj2=p3&p4; jj1=p3^p4;
      ido=ii2|jj2|(ii1&jj1);
      spins[l1][l2][i0][i1]=ido^spins[l1][l2][i0][i1];
      }
    }
}
```

```
    }
}
```

Avoiding bias

$$\bar{A}_{N,j} \approx \frac{1}{N} \sum_{i=1}^{N} A_{i,j}$$

Problem

$$\lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} \bar{A}_{N,j} \bar{B}_{N,j} \neq [< A >< B >]$$

Solution:

$$\bar{A}_{N/2,1,j} \approx \frac{1}{N} \sum_{i=1}^{N/2} A_{i,j} \qquad \bar{B}_{N/2,2,j} \approx \frac{1}{N} \sum_{i=N/2+1}^{N} B_{i,j}$$

then

$$\lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} \bar{A}_{N/2,1,j} \bar{B}_{N/2,2,j} = [< A >< B >]$$

Fixed ratio for length of thermalization, measurement and decorrelation: $N_t = 20N_m$, $N_d = N_m$;

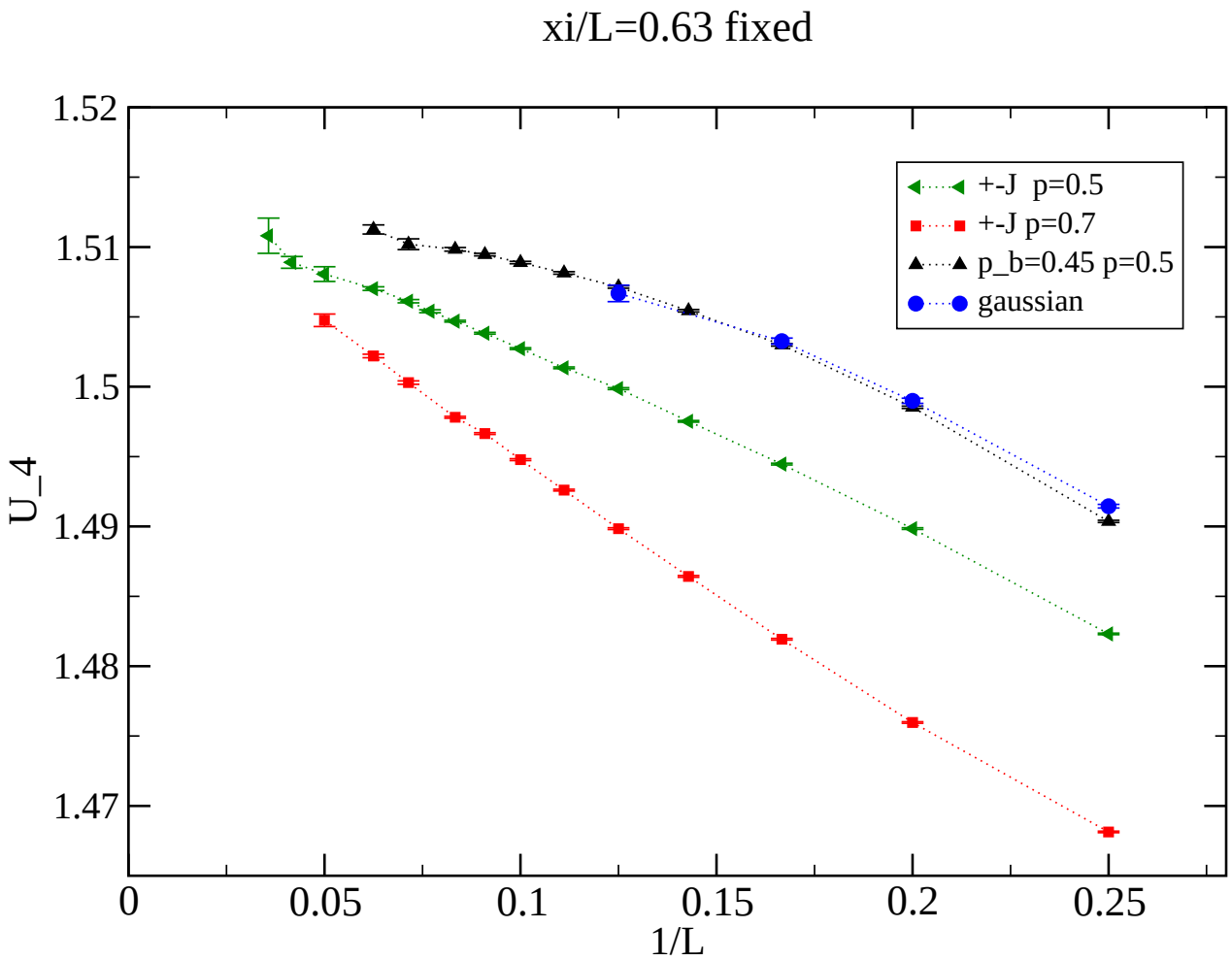
In our simulation: 12 measurement intervals to compute ... $[< A >< E >< E >]$ up to $[< A >< B >< E >< E >]$

Thermalization and Decorrelation errors are simultaneously checked by doubling N_m until all observables studied are independent of N_m (within stat. errors)

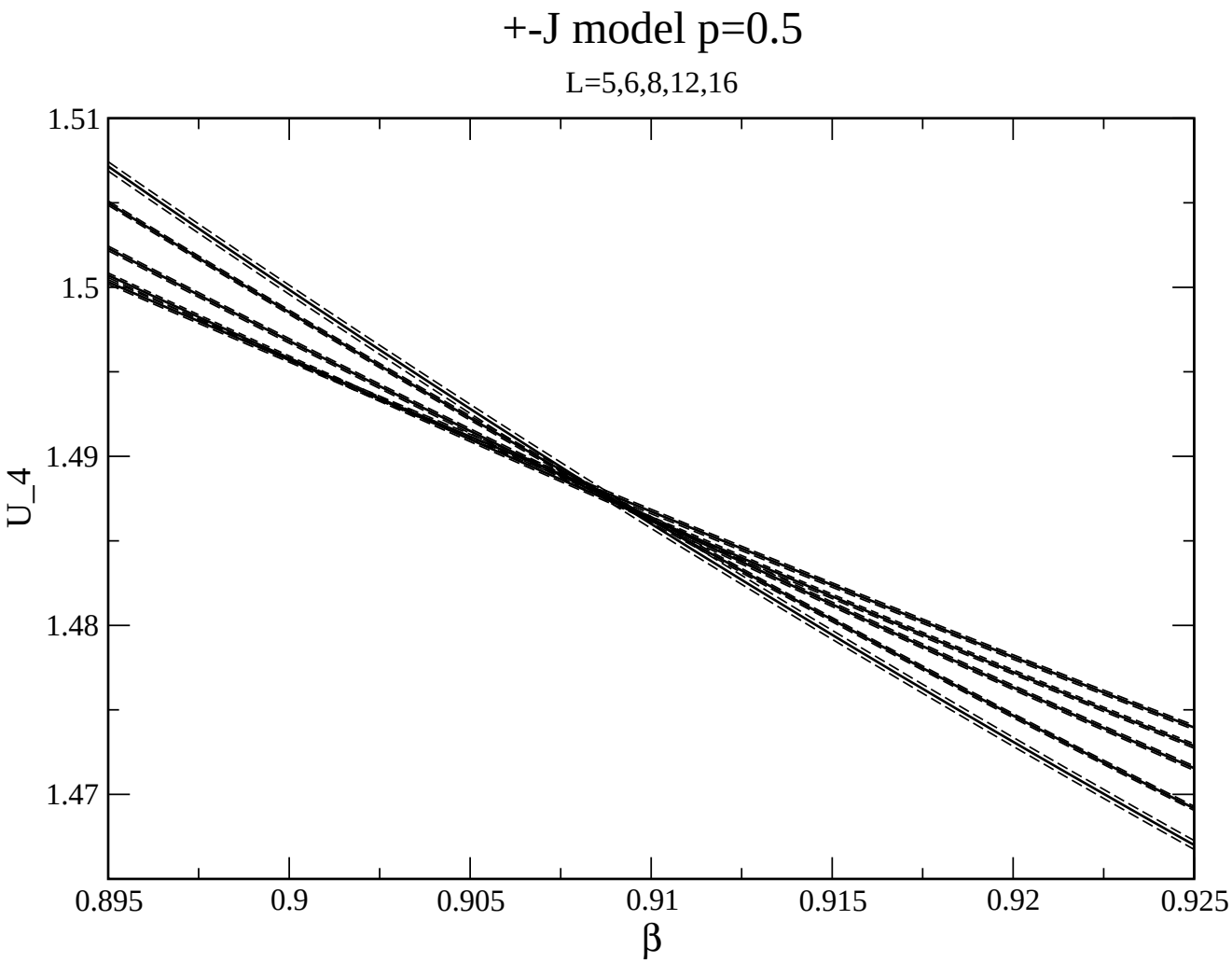
L	samples/64	MC sweeps	N_t	CPU-time/days
8	100000	19200	5	4
9	110850	48000	8	27
10	100681	72000	8	50
11	109779	144000	10	183
12	106812	192000	10	308
13	38282	288000	10	210
14	31600	480000	10	361
16	24331	480000	20	831
20	1542	1920000	32	658
24	717	3000000	32	826
28	285	7200000	20	782

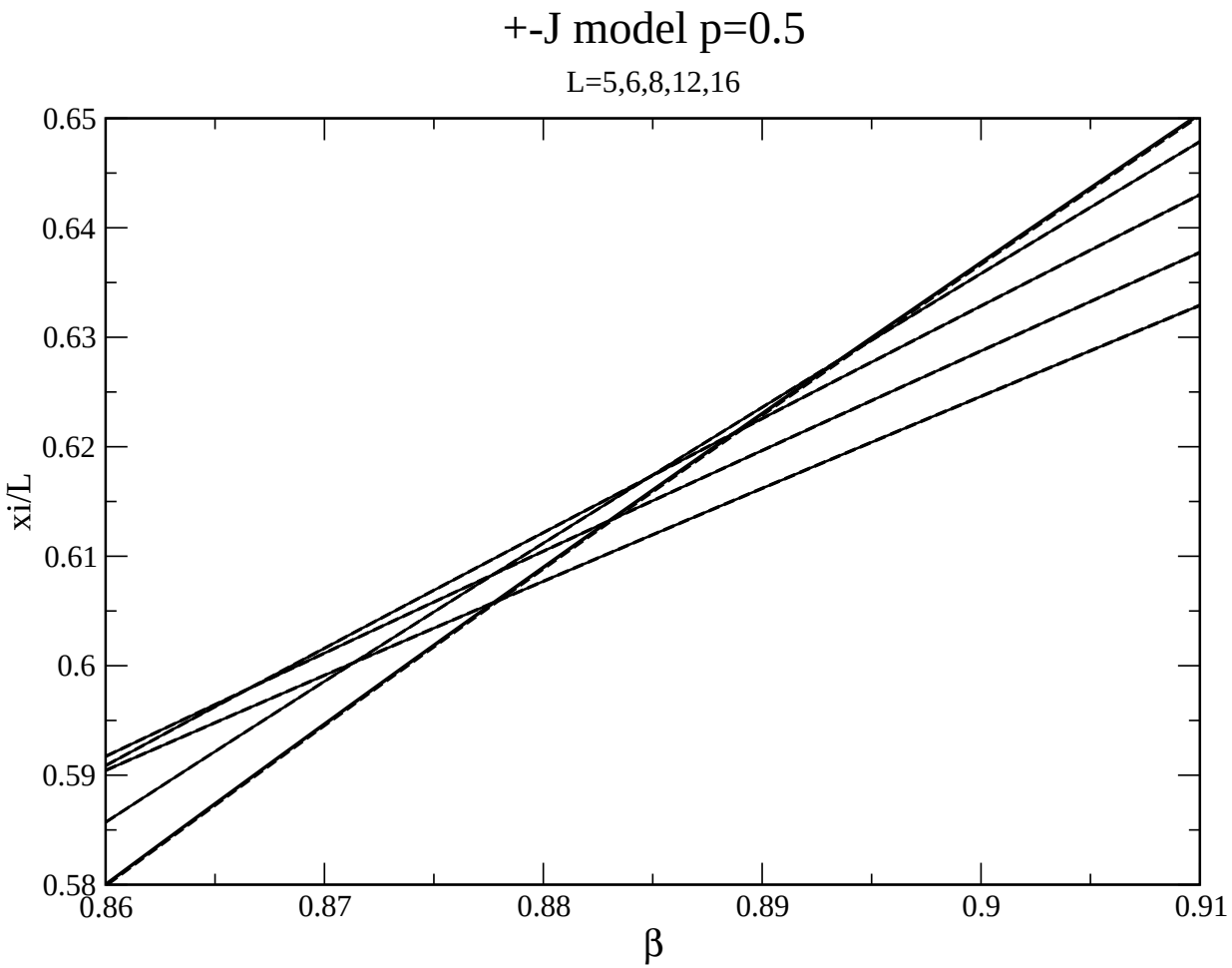
Effort grows roughly $\propto L^9$.

Compare with Katzgraber et al: Number of samples: 30000,15807,11360,9408,8416 for $L = 8, 12, 16, 20, 24$ respectively.



Conclusion from various fits: $\omega = 1.0(1)$


+-J model p=0.5
L=5,6,8,12,16
1.51
1.5
1.49
1.48
1.47
U_4
0.895
0.9
0.905
0.91
0.915
0.92
0.925
β

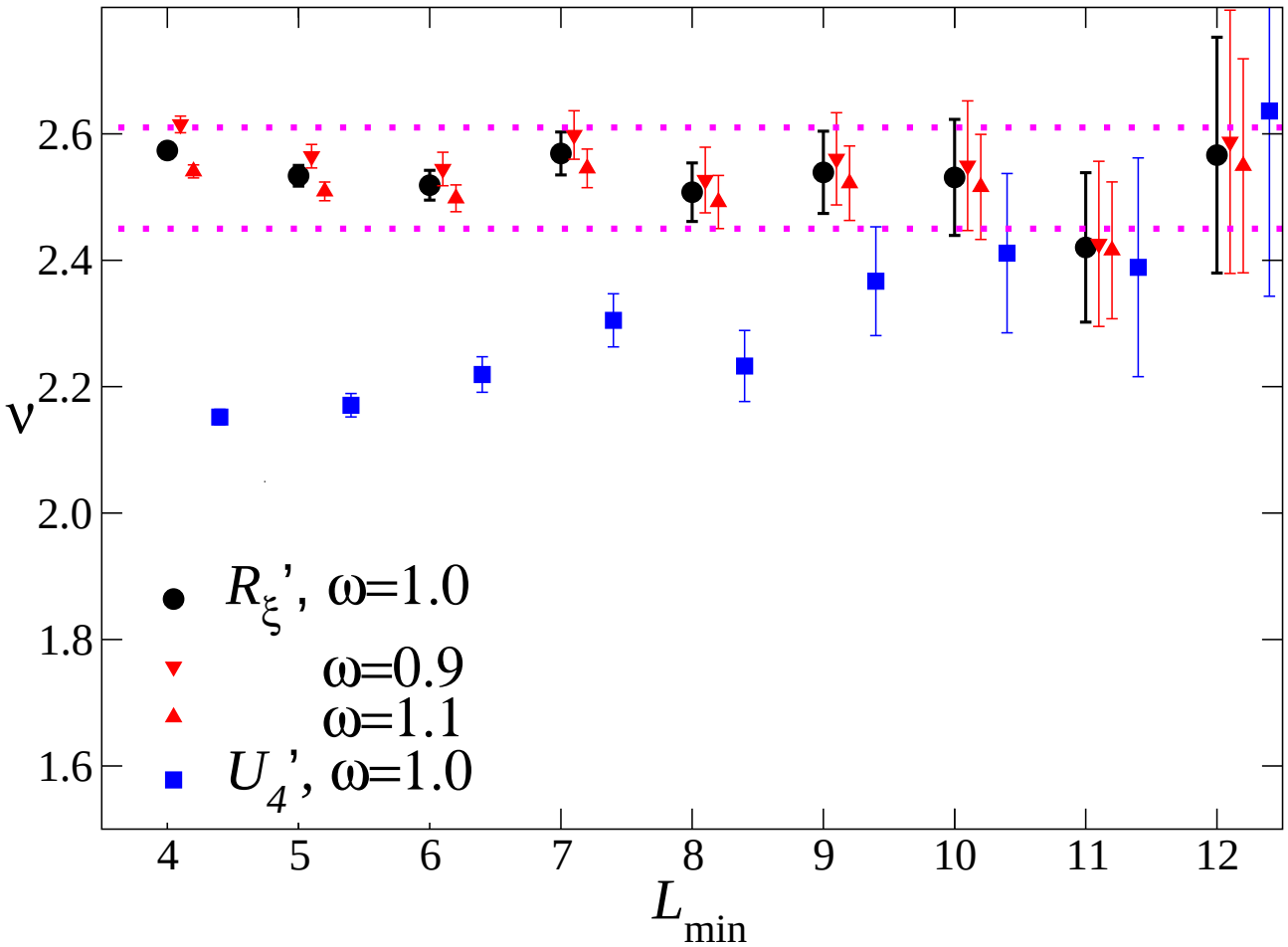

+-J model p=0.5
L=5,6,8,12,16
xi/L
β
0.65
0.64
0.63
0.62
0.61
0.6
0.59
0.58
0.86
0.87
0.88
0.89
0.9
0.91

- Very small corrections in the case of U_4
- Strong corrections in the case of ξ/L;
  crossing points move to larger values of β and ξ/L
  as L increases
  Including corrections with $\omega = 1$ we get β_c consistent
  with that obtained from U_4

Our final results (From data with $L \geq 8$):

$U_4^* = 1.490(7)$, $\xi/L^* = 0.654(7)$, $\beta_c = 0.908(4)$ for $p = 0.5$.

Ansatz: $R' = L^{1/\nu}\,(1 + cL^{-\omega})$



Conclusions

- In some quantities $1/\nu$ corrections are leading!
- U_4 at ξ/L fixed is the same for all three models
- $\omega = 1.0(1)$
- $\nu = 2.53(8)$, $\eta = -0.384(9)$