Numerical Simulations of a Glassy Potts Model

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Schematic Summary

- Systems with Frustration and Quenched Disorder: Spin Glasses;
- Mean Field Properties of the Potts Model;
- Numerical Simulations: Parallel Tempering, an Improved Monte Carlo Method;
- Numerical Study of the Glassy Potts Model;

The Model

Ising spin-glass: $\mathcal{H} = -\sum_{<i,j>} s_i J_{ij} s_j$, gauge invariant under the transformation:
$s_i \to -s_i$, $J_{ij} \to -J_{ij}$, i, j first neighbouring sites.

This kind of symmetry does not permit the system to enter a low temperature ferromagnetic phase

Glassy Potts Model: mantains the same kind of gauge invariance:

$$\mathcal{H} = -\sum_{<i,j>} \delta_{s_i \Pi_{ij}(s_j)},$$

spin variables q with values $(0, \ldots, q-1)$, and Π_{ij} quenched random permutations of the group of q elements.

The model allows a comparison between 1RSB systems and real amourphus systems: same structure of the glassy phase, same dynamic evolution equations.

Spin Glasses: almost total understanding, open questions concerning the corrections of mean field results in short range models.

Sherrington-Kirkpatrick (SK) model:

$$\mathcal{H}_J[s] = -\sum_{<ij>} J_{ij} s_i s_j - \sum_i H_i s_i$$

$\{J_{ij}\}$ quenched random variables distributed according to a given $P(J_{ij})$ (first and second order moments scaling respectively as $1/N$ and $1/\sqrt{N}$)

- Frustration: no configuration of spins satisfies all dynamical links;
- Quenched Disorder: to obtain the correct free energy it is necessary to average over the J_{ij} only after the usual thermal average.

Free Energy Landscape: hill-valley structure with a lot of nearly degenerate minima. The system in the glassy phase is a kind of quenched paramagnet, with $< s_i > \neq 0$ and $M = \frac{1}{N} \sum_i < s_i > = 0$

Replica Theory

Free Energy Density in the presence of quenched variables:

$$f = \overline{f_J} = \lim_{N\to\infty} -\frac{1}{\beta N}\overline{\ln \mathcal{Z}_J}$$

The solution is found using the identity:

$$\ln \mathcal{Z} = \lim_{n\to 0} \frac{\mathcal{Z}^n - 1}{n}$$

The $n \times n$ symmetric overlap matrix $\mathcal{Q}$, introduced by computing $\overline{\mathcal{Z}^n}$:

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} s_i^\alpha s_i^\beta$$

The mean field Free Energy Density is related to the saddle point solution of:

$$\int \prod_{\alpha<\beta} dq_{\alpha\beta} \exp(-\beta N A[Q]) \propto \overline{\mathcal{Z}_J^n}$$

Spontaneous Replica Symmetry Breaking

1RSB scheme: the saddle point solution gives two different values of the overlap. The order parameter is a two step function $q(x)$.

$$P(q) = m\delta(q - q_0) + (1 - m)\delta(q - q_1)$$

FRSB scheme: $q(x)$ turns out to be a continuous function in $[0, x_M]$, with a plateau corresponding to the maximum allowed overlap q_{EA} in $[x_M, 1]$.

$$P(q) = \tilde{P}(q) + (1 - x_M)\delta(q - q_{EA})$$

Order Parameter Function and Equilibrium Order Parameter:

$$q = \int_{-1}^{1} \mathcal{P}(q) q \, dq = \int_{0}^{1} q(x) dx$$

$x(q)$ is the probability of finding an overlap less than q.

Potts Hamiltonian:

$$\mathcal{H}[s] = -\sum_{i<j} J_{ij}(p\delta_{s_i s_j} - 1) + h_l \sum_i (p\delta_{l s_i} - 1)$$

the local variables take a discrete set of values $s_i = 1, \ldots p$
(analogies with orientational glasses).

Exchange Variables Distribution:

$$P(J_{ij}) = \sqrt{\frac{N}{2\pi J^2}} \exp[-N(J_{ij} - J_0/N)^2/2J^2]$$

(moments of J scaling exactly as in the SK case)

Lack of spin inversion symmetry: feature shared by several physical systems, not present in spin-glass type models.

Replica Method: the solution of the model is a generalization of the Parisi *ansatz* (1981, Sompolinsky).

It follows a 1RSB scheme, a kind of transition which turns out to be suitable to describe the glassy phase in a large class of systems (e.g. p-spin glass).

Landau expansion for the free energy, $T \sim T_c$:

$$\begin{aligned} F(n) &= -\tfrac{(p-1)}{2}\Big\{(1-\tfrac{T}{J})Trq^2 + \tfrac{1}{3}Trq^3 \\ &\quad + \tfrac{p-2}{6}\textstyle\sum_{\alpha\neq\beta} q^3_{\alpha\beta} - \tfrac{y}{12}\textstyle\sum_{\alpha\neq\beta} q^4_{\alpha\beta}\Big\} \end{aligned}$$

other fourth-order terms are omitted since they do not add anything new.

The y term changes sign for $p = p^* \sim 2.8$, and is positive for larger p:

$s < s^*$ Parisi-like solution with continuous $q(x)$

$s > s^*$ 1RSB, $q(x)$ with a discontinous jump

Main Findings

$p < p^*$ SK-like solution with zero minimum overlap: many phases uncorrelated;

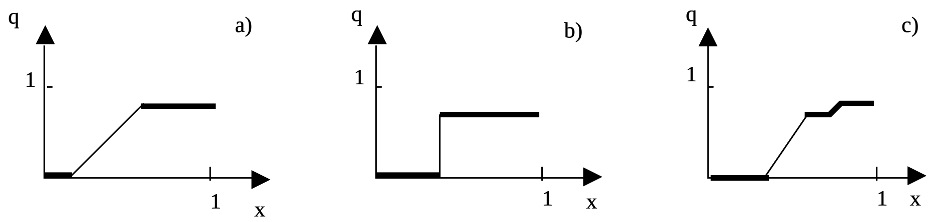
$p^* < p < 4$ 1RSB-like solution (REM and p-spin): discontinuous $q(x)$

$$\begin{cases} q_{EA} & \propto & \frac{T_c - T}{4-p} < 1 \\ \overline{x} & = & \frac{p-2}{2} \end{cases}$$

As $p \to 4$, $\overline{x}(T \sim T_c) \to 1$, the transition becomes discontinuous;

$p > 4$ perturbative expansion around $p \sim 4$. It is found that $q(1, T_c) \propto (p-4)$

For $p > p^*$ there is a second transition at $T_2 < T_c$, with a continuous Parisi function with positive slope for $x > \overline{x}$

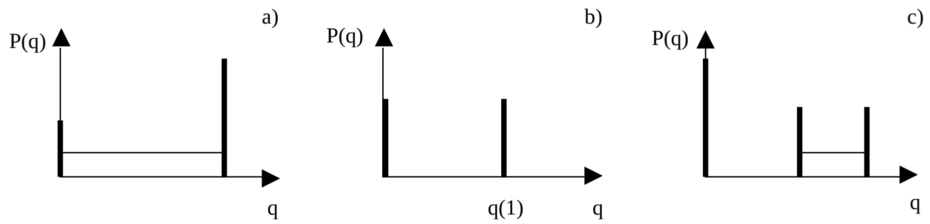


$q(x)$ in the Potts glass:

a) for $p < p^*$

b) for $p > p^*$, $T_2 < T < T_c$

c) for $p > p^*$, $T < T_2$



$P(q)$ in the Potts glass:

a) for $p < p^*$

b) for $p > p^*$, $T_2 < T < T_c$

c) for $p > p^*$, $T < T_2$

Monte Carlo Method (MC)

Gibbs average value of an observable $\mathcal{O}$

$$\langle \mathcal{O} \rangle = \int d[C]\mathcal{O}(C)\exp(-\beta\mathcal{H}[C])$$

The system configuration evolves according to an ergodic Markovian transition matrix $\mathcal{W}$, whose elements satisfy the detailed balance condition:

$$p_\alpha \mathcal{W}(\alpha \to \alpha') = p_{\alpha'} \mathcal{W}(\alpha' \to \alpha)$$

The frequency of occurence of each state at equilibrium is proportional to the correct Gibbs-Boltzmann weight $p_\alpha \propto \exp(-\beta\mathcal{H}[C])$, then it follows that:

$$\langle \mathcal{O} \rangle = \frac{1}{\tau}\sum_t \mathcal{O}(t)$$

Metropolis algorithm for the Markov process:

- Generate a new configuration (single spin flip);
- Calculate the energy change $\Delta E = E_{\alpha'} - E_\alpha$;
- Calculate $\mathcal{W} = \min(1, \exp(-\beta \Delta E))$;
- Generate random number $r \in [0, 1]$;
- Accept move if $r \leq \mathcal{W}$;

Parallel Tempering Method (PT)

Glassy systems with a "hill-valley" structure landscape need improved MC methods in order to explore the whole phase space in reasonable time.

Generally it is a hard task both to reach and to identify thermal equilibrium.

The "trick": add a second Markov chain to usual Metropolis and let the temperature vary in order to make easier for the system to cross the free energy barriers.

PT: N_β replicas of the system, with different β values assigned *a priori*, evolve in parallel.

$$\begin{aligned} \mathcal{Z}_{ext} &= \prod_i \mathcal{Z}(\beta_i) \\ \mathcal{P}(\{x,\beta\}) &= \prod_i \mathcal{P}_{eq}(x_i,\beta_i) \end{aligned}$$

Transition Probability Matrix (TPM)
(Metropolis-like test):

$$W(x,\beta_m|x',\beta_n) = \begin{cases} 1, & \Delta < 0 \\ \exp(-\Delta), & \Delta > 0 \end{cases}$$

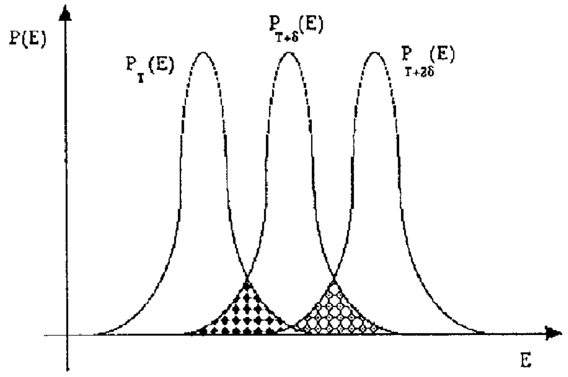
with

$$\Delta = (\beta_n - \beta_m)(\mathcal{H}(x) - \mathcal{H}(x')).$$

PT step:

- update independently the replicas with a standard MC method;
- try to swap the configurations with two neighbouring temperatures, according to the TPM.

How to select the β values: the overlap of each two probability distributions has to be non negligible (the larger the system, the more the replicas).



$P(E)$ for different values of T.

The method works for continuous phase transitions.

Thermalization check:

- no observable drift in time
- good acceptance ratio for the proposed β swaps
- each configuration must visit all the allowed β values

Numerical Study

Overlap parameter: difficult to check thermal equilibrium.

$$\overline{<q_{\sigma\tau}>} = \overline{\frac{1}{V}\sum_{i}^{V}\delta_{\sigma,\tau} - \frac{1}{4}}.$$

$\mathcal{M}_{co}$ model: the Hamiltonian contains only permutation Π that commute with $R = (0,1,2,3) \rightarrow (2,3,0,1)$, $[\Pi, R] = 0$.

Modified overlap w: defined so that its probability distribution $P(w)$ is symmetric at equilibrium under $w \rightarrow -w$

$$\overline{<w_{\sigma,\tau}>} = \overline{\frac{1}{V}\sum_{i}^{V}(\delta_{\sigma\tau} - \delta_{\sigma R(\tau)})}.$$

The two models turn out to be equivalent †.

† E. Marinari, S. Mossa and G. Parisi, *The Glassy Potts Model* (cond-mat/9805300).

Numerical study of the $\mathcal{M}_{co}$ model with $q = 4$ states in 4 spatial dimensions d (PT method).

Simulation Parameters

L	Samples	N_β	δT	T_{min}	T_{max}
4	10	13	0.8	1.0	2.0
5	10	26	0.4	1.0	2.0
6	10	34	0.3	1.0	2.0

We average over ten configurations of the disorder. We perform long thermal runs to reach the thermalization of the samples (400000 PT full sweeps of the lattice).

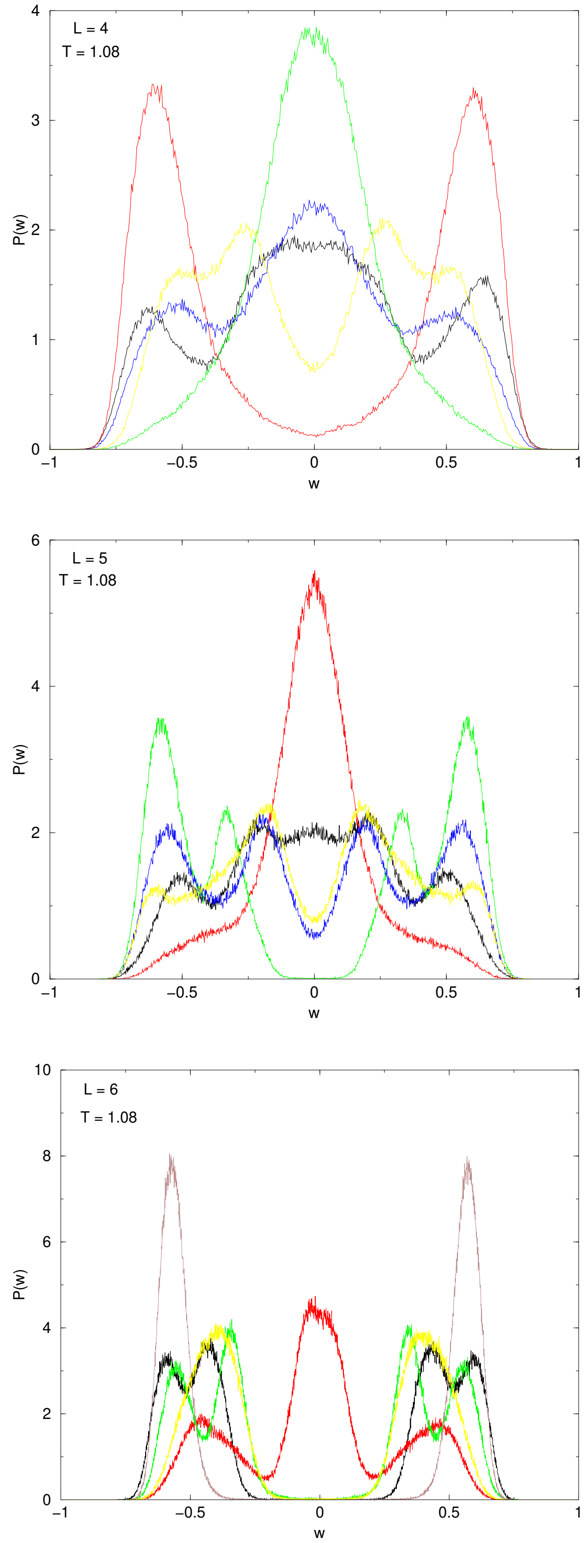
Thermalization steps: one third of the total time.

Thermalization checks:

- no time drift of observables on logarithmic time scales;
- probability of swapping temperature ~ 0.5;
- fairly flat histogram counting the time that each system spends at each temperature;
- single sample $P_J(q)$ symmetric within statistical errors;

L	4	5	6
Probability of swapping temperature	0.68	0.59	0.56

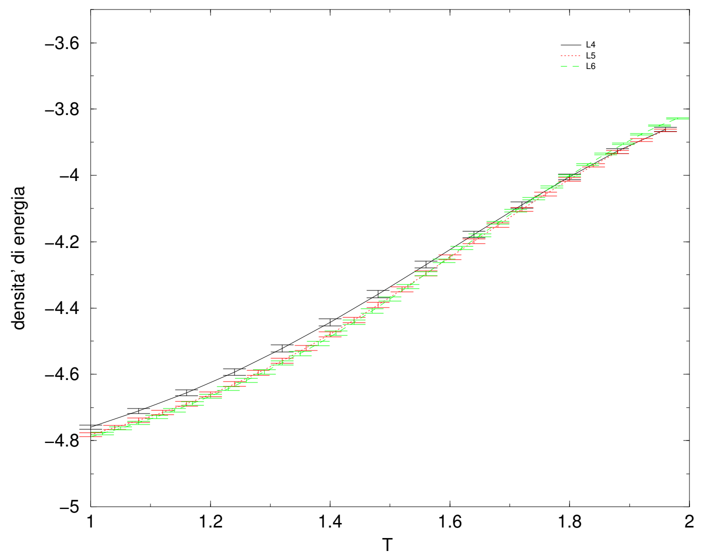
Minimum value of the swapping temperature probability



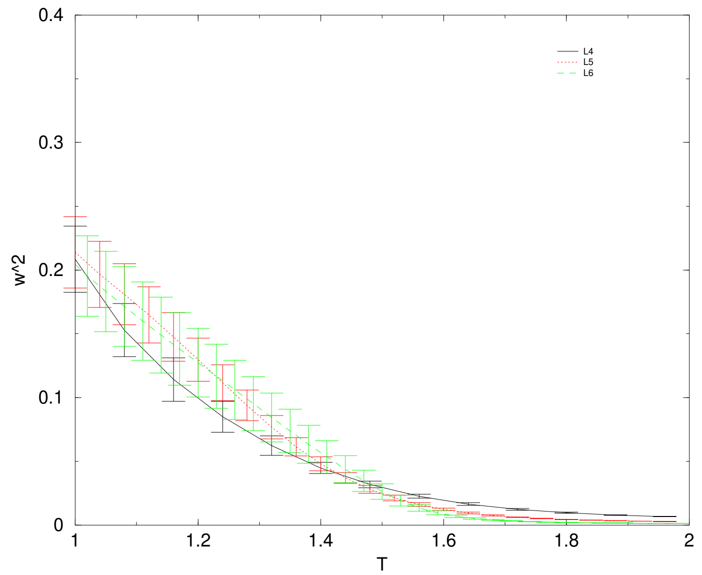
Probability distribution of the overlap order parameter w for different samples, lattice size $L = 4$, $L = 5$, $L = 6$

Behaviour at equilibrium

Energy density versus T for the different sizes considered



Squared overlap parameter w versus T



Small finite size effects evident for $L = 4$

High temperature expansion

Partition function of two neighbouring sites:

$$\mathcal{Z}_{link} = \sum_{link} e^{-\beta \mathcal{H}_{link}} = e^{2\beta} + 3$$

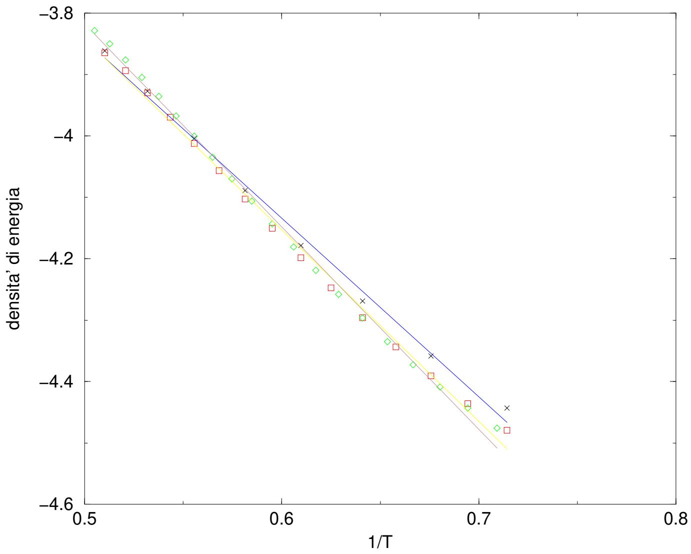
Energy density:

$$u_{link} = -(2 + 3\beta)$$

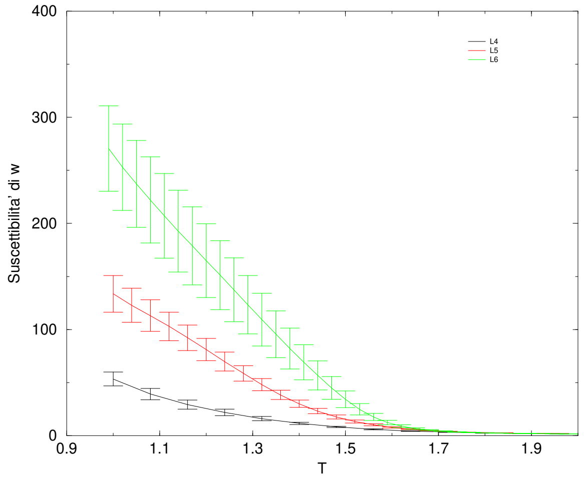
Fit parameters $u = a + b\beta$

L	4	5	6
a	-2.39 $\pm$ 0.04	-2.28 $\pm$ 0.03	-2.16 $\pm$ 0.03
b	-2.91 $\pm$ 0.08	-3.10 $\pm$ 0.06	-3.30 $\pm$ 0.05

Energy density in the high temperature regime



The spin glass susceptibility $\chi_w \equiv V \left\langle w^2 \right\rangle$ exhibits second order thermodinamical transition at a $T_c \neq 0$.



Data agree well with the finite size scaling law:

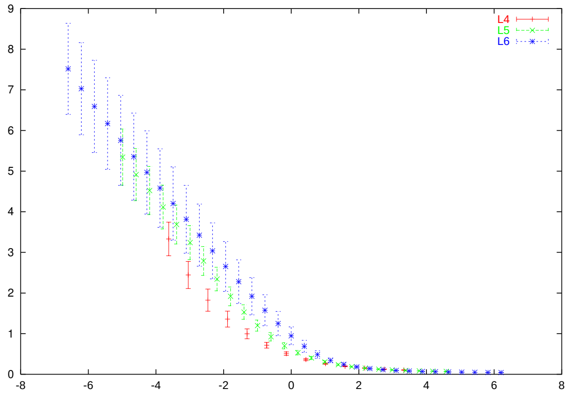
$$\chi_w(L,T)/L^{2-\eta} = \tilde{\chi}_w(L^{1/\nu}(T - T_c))$$

according with a previous estimate † of the γ value $(1.3 \div 1.5)$, we estimate T_c between 1.5 and 1.7, for $\nu \sim 0.7$.

† E. Marinari, S. Mossa and G. Parisi, *The Glassy Potts Model* (cond-mat/9805300).

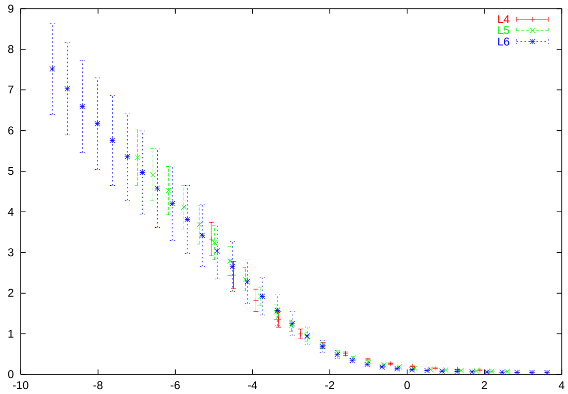
Overlap susceptibility $\chi_w/L^{2-\eta}$ versus $L^{1/\nu}(T-T_c)$, with

$T_c = 1.5$, $\nu = 0.7$ and $\eta = 0$



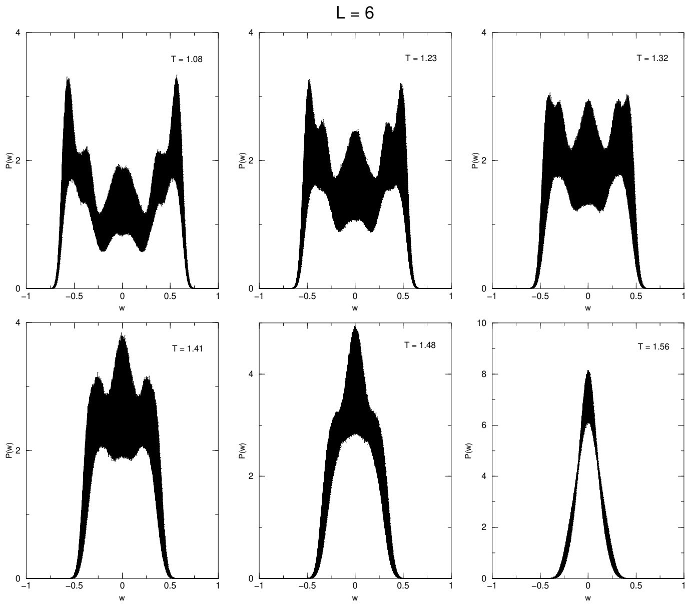
Overlap susceptibility $\chi_w/L^{2-\eta}$ versus $L^{1/\nu}(T-T_c)$, with

$T_c = 1.7$, $\nu = 0.7$ and $\eta = 0$



Results on $P(w)$

$P(w)$ becomes clearly non-Gaussian approaching T_c, with the formation of a three peaks structure.



$P(w)$ greater than zero for intermediate q values: possible finite size effect (presence of metastable states).

Non-trivial $P_J(w)$: the system explores in a "jumpy manner" the phase space.

Conclusions

Preliminary study of a 4 states, 4 dimensions disordered Potts model:

- The transition appears to be of second order, characterized by a diverging correlation lenght;
- The overlap probability distribution is not trivial at low temperature: appearance of a glassy phase similar to that of 1RSB systems;
- the phase space is characterized by a complex dynamics, the role of metastable states seems to be crucial;