

A local, low autocorrelation glassy model

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Some recent results by Frauke Liers, EM, Ulrike Pagacz, Federico Ricci-Tersenghi and Vera Schmitz, Köln and Rome. To be published.

Starting from the Bernasconi model, with in mind two interesting goals:

1. binary sequences with low autocorrelations;
2. structural glasses and their phenomenology. From the mean field theory down to realistic models. Many optimization problems are glassy (K-SAT, travelling salesman...).

Summary

Low autocorrelation sequences and the Bernasconi model.

Merit Factor and Statistical Mechanics.

The physics of glassy systems.

Glasses and disordered models.

Ground states, thermodynamics, replicas, dynamics in the mean field
Bernasconi model.

Realistic glassy models.

The local low autocorrelation model: definitions, methods, results.

The merit factor of long **low autocorrelation** binary sequences. M. Golay, IEEE Trans. on Information Theory, 1982.

Low autocorrelation binary sequences : **statistical mechanics** and configuration space analysis. J. Bernasconi, J. Physique 1987

Communication engineering problems. **Coding theory and secure communication**: it is useful to find binary sequences as poorly autocorrelated as possible. **Maximize merit factor F : N^2 over twice the sum of square of correlations.**

From engineering point of view merit factor is connected with the signal to self generated noise ratio of a communication system where coded pulses are transmitted and received.

Translation to Statistical Mechanics: (inverse of) the energy of a sequence.

N sites. Binary sequence:

$$\{\sigma_i\}; \quad i = 0, 1, 2, \dots, N-1; \quad \sigma_i = \pm 1 .$$

Correlation function:

$$C_d^{\text{open}} \equiv \sum_{i=0}^{V-d-1} \sigma_i \sigma_{i+d} .$$

(can be with open boundary conditions or with periodic boundary conditions)

Merit factor:

$$F_N \equiv N^2 \left(2 \sum_{d=1}^{N-1} C_d^2 \right)^{-1} .$$

A sequence whose autocorrelations are small, as measured by the sum of their squares, has a large merit factor.

Under a series of (simple) approximations Golay estimates in the open model, for $N \rightarrow \infty$:

$$F_N \sim 12.32$$

On the other side annealing and sequences that can be built with known algorithms for large N give

$$F \sim 6$$

Finding the best sequences, i.e. the ground states, is clearly very difficult.

Mertens and Bauke. Exact ground states up to $N = 60$ by an exhaustive branch and bound algorithm gives that for $N \rightarrow \infty$:

$$F_N \sim 9$$

The model, as phrased by Bernasconi in the language of Statistical Mechanics, opens an interesting direction, since a complex, deterministic Hamiltonian can be studied by **substituting it with a fiduciary disordered function**. In this way a glassy system can be analyzed by using techniques that have been developed for studying disordered systems.

J. P. Bouchaud and M. Mezard, Self induced quenched disorder: a model for the glass transition, J. Physique I 4 (1994) 1109. cond-mat/9405975; **E.M., G. Parisi and F. Ritort**, Replica field theory for deterministic models: I. Binary sequence with low autocorrelation, J. Phys. A 27 (1994) 7615, cond-mat/9405148.

The system is not random, but changing one spin to optimize some correlation functions can **make many other correlation functions increase**: this competitive effect is typical of systems that are based on disordered interactions with competing signs.

Let us start by defining the long range models.

$$H \equiv \frac{1}{N} \sum_{d=1}^{N-1} \left(C_d^{(bc)} \right)^2 ,$$

where (bc) can be for $(open)$ (the sums stop at the boundary) or for $periodic$ (we are on a ring, and indexes are taken modulo N). The ground state structure of the two systems is very different, while finite T physics is similar.

Now one defines the partition function and the free energy density as

$$Z_N(\beta) = \sum_{\{\sigma\}} e^{-\beta H[\sigma]}$$

$$f_N(\beta) = -\frac{1}{\beta N} \log (Z_N(\beta)) , \quad f = \lim_{N \rightarrow \infty} f_N(\beta) .$$

In this language optimal sequence are ground states, and good sequences are low T configurations.

Before starting a discussion of some interesting details of the [mean field Bernasconi model](#) (and eventually introducing our finite D , finite range model), I want to briefly discuss the problem of [glassy materials](#), since this is one of our two physical motivations. [For recent, excellent reviews see W. Kob, cond-mat/0212344 and A. Cavagna, arXiv:0903.4264.](#)

Typical “interesting” disordered system: spin glass.

Prototype and paradigm: Sherrington-Kirkpatrick mean field theory with dramatic phenomenology.

- [Second order phase transition to a critical spin glass phase.](#)
- [\$P\(q\)\$ has finite support in infinite volume limit.](#)

Some disordered models have a [very different phenomenology](#). For example, as far as mean field is concerned, Derrida REM, disordered p-spin model: we will come back to them. [They are reminiscent of glassy behavior.](#)

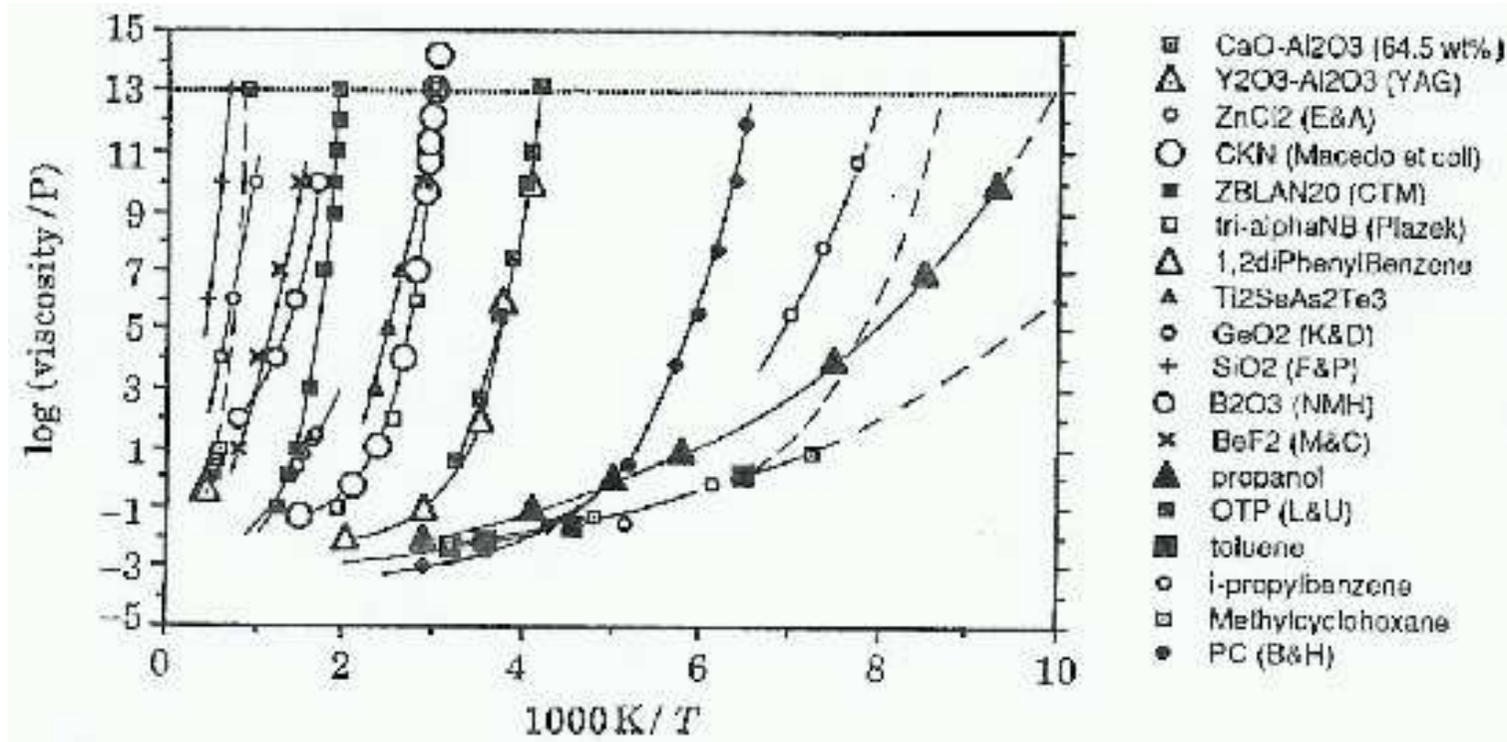
What is a glass??

- Analytic understanding.
- Computer simulations.
- Role of models.

Liquid state, high T . Viscosity, η small. Diffusion constant, D , high. Typical relaxation time τ , microscopic ($\geq 1ps$).

Lower T : would expect crystallization, but instead enter the metastable supercooled regime.

1. In this regime structural properties only show a weak T dependence.
2. Most dynamic properties, like the viscosity η and the diffusion constant D , change, on the contrary, dramatically.

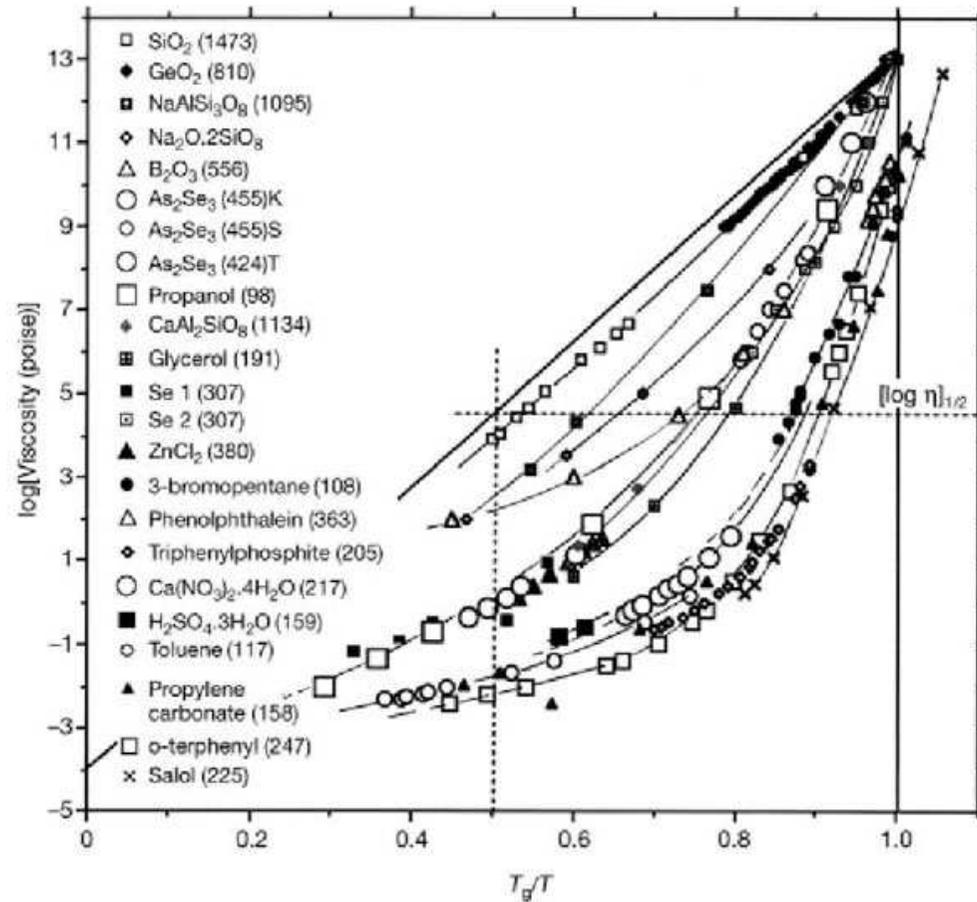


Very strong T -dependence: Arrhenius plot of the viscosity η .

A small change in T leads to an increase of η of up to 14 decades.

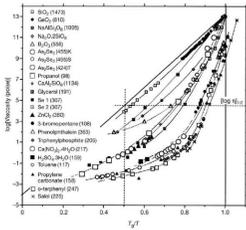
Many different materials: oxides like SiO_2 , molecular liquids as toluene, polymeric systems.

Very slow dynamics is a very general phenomenon.



Angell plot.

Define $T_G|\eta = 10^{13}\text{Poise}$ and use the reduced temperature scale T_G/T .



In Angell plot one can distinguish two types of systems.

1. $\log(\eta) \sim T_G/T$, Arrhenius with good approximation. Upper curves, close to straight lines. For example SiO_2 . Activation energy is constant. “Strong” glass-formers.
2. Lower curves: bending and strong curvature at $T_G/T \sim 0.8$. Can be parametrized with T -dependent activation energy. “Fragile” glass former.

Can characterize fragile and strong by slope of $\log(\eta)$ at T_G : large slope is fragile, small slope is strong.

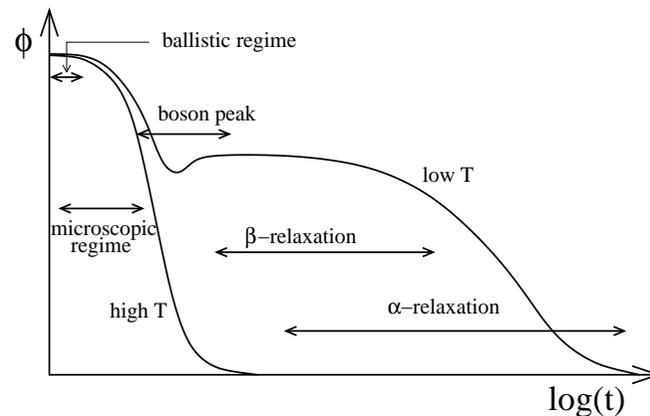
A correlation between fragility and other properties exists: it is a relevant concept.

A further remark: Arrhenius is a special case, with $T_0 = 0$, of the Vogel-Fulcher law

$$\eta(T) = \eta_0 \exp(A/(T - T_0)) .$$

Good fit of data, but no theoretical foundations. $T_0 < T_G^{exp}$ implies that no experiment can detect if T_0 exists.

Decay of time correlation functions. Two curves for high T (liquid) and low T .



From Walter Kob Les Houches course, cond-mat/0212344

Thermodynamical quantities.

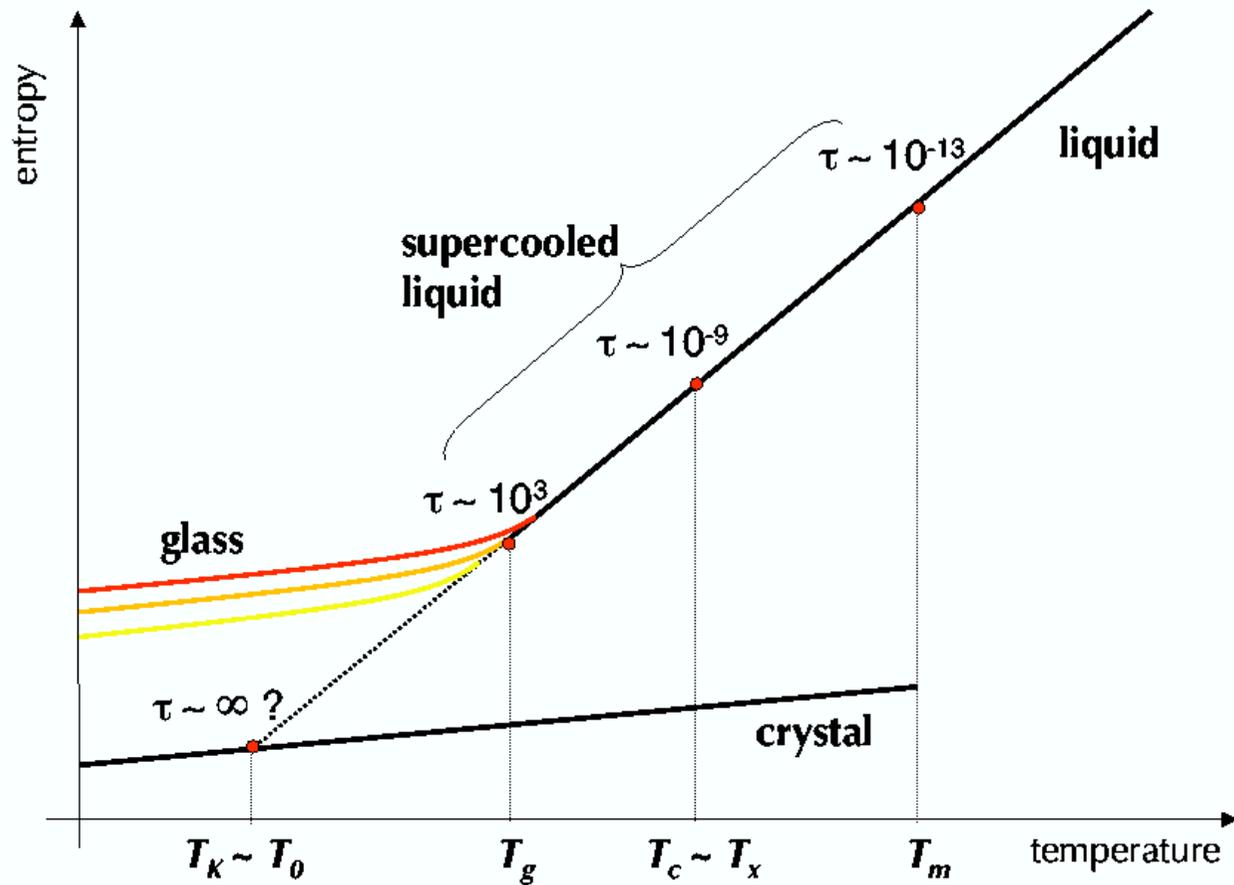
- Smooth behavior of pressure, specific heat, ...
- So it is surprising that the behavior of the entropy of supercooled systems hints the existence of a phase transition at low T (Kauzmann 1948).

From experimental data for the specific heat one can compute the entropy difference $\Delta S \equiv S_{liquid} - S_{crystal}$.

Fragile systems: $\Delta S \rightarrow 0$ at $T = T_K$, Kauzmann temperature, finite.

(This cannot really happen, Stillinger: at least very close to T_c things have to change).

Empirical again: T_K is very close to T_0 .



To wrap up critical points and time scales: from A. Cavagna review, [arXiv:0903.4264](https://arxiv.org/abs/0903.4264).

Spin glasses have quenched disorder, so at first sight one would not connect them to glasses, but the behavior of a class of them has much in common with the behavior of supercooled liquids (Kirkpatrick and Wolynes). Typical of this class is the mean field p -spin:

$$H_{(p)} \equiv - \sum_{i_1 i_2 \dots i_p}^N J_{i_1 i_2 \dots i_p} \sigma_{i_1} \sigma_{i_2} \dots \sigma_{i_p} .$$

(also REM, $q \geq 3$ Potts spin glass).

Dynamical equations obtained in the mean field p -spin model are identical to the ones of the Mode Coupling approximation.

At low T dynamical correlation functions have a two step decay.

The height of the plateau is discontinuous, as it is in super-cooled liquids.

Mean field p -spin.

Metastable states are precisely defined: local minima of f . f depends on T , and minima are different for different T values.

Mean field: free energy barriers are infinite, and the phase space can be divided in basins of attraction of the metastable states.

In the mean field p -spin everything can be computed exactly.

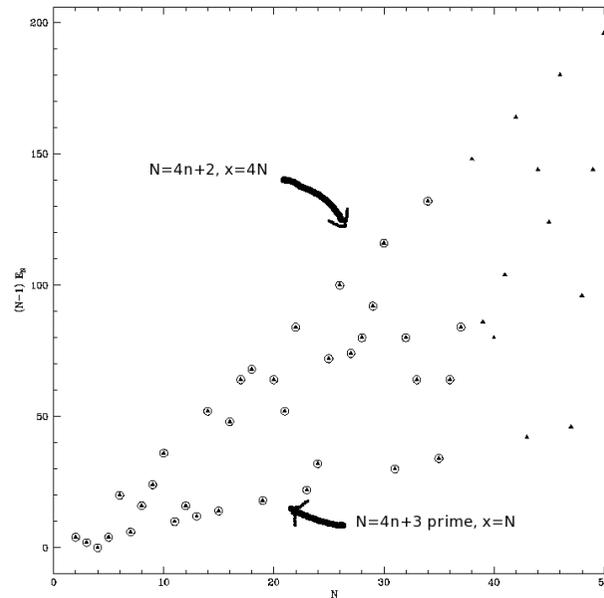
Not clear at all how to generalize all this out of mean field. (Biroli and Kurchan, Phys Rev. E 64 (2001) 016101)

Role of real space.

Find relevant length scale.

... and now, back to the infinite range Bernasconi model...

Ground states of these models can be very peculiar, and this has not much of an effect on thermodynamics. This point is very clear in the **mean field Bernasconi model** with **periodic boundary conditions**.



EM, G. Parisi and F. Ritort 1994; S. Mertens and C. Bessenrodt 1998.

Energy density of the ground state is zero in the infinite volume limit (different from open boundary conditions).

Fact: N prime of the form $4n + 3$: $E = 1$.

Fact: one can also find exact ground states in other cases, for example for N of the form $2^p - 1$ by using Galois fields.

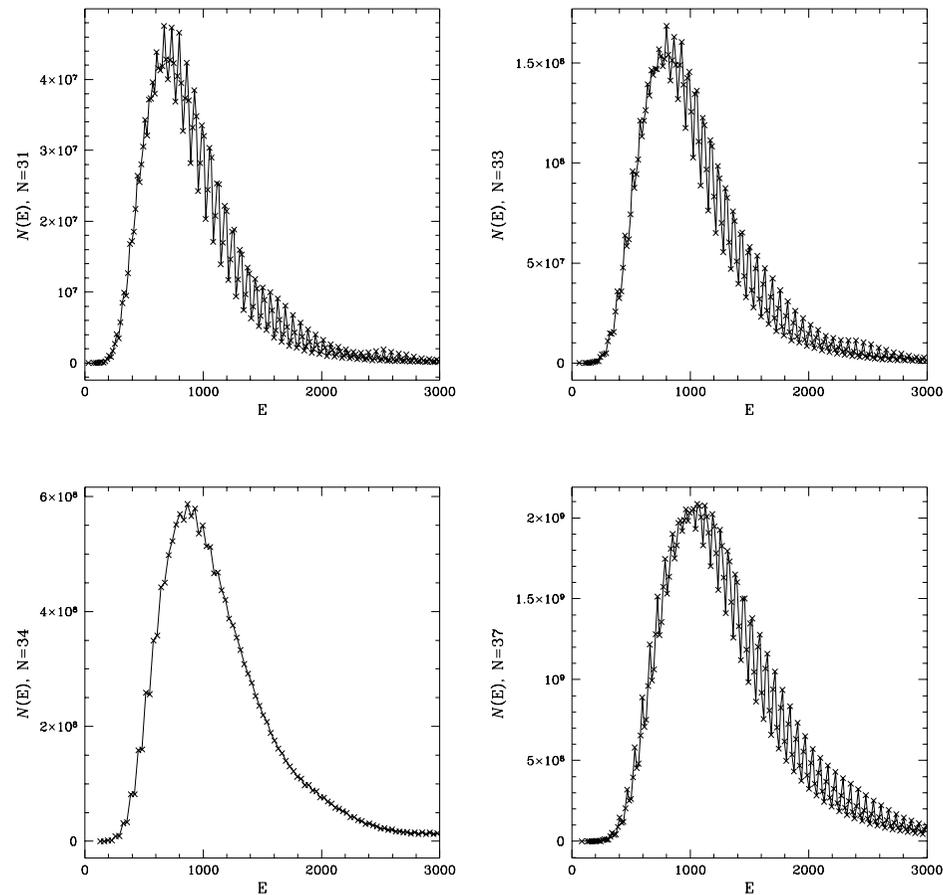
If $p = 57$ and $N = 2^{57} - 1$ the sequence defined by $\sigma_j = \sigma_{j-24}\sigma_{j-57}$ is a ground state. **This is a random number generator!** In some sense this is not completely surprising, since in a random number generator one wants small autocorrelations.

Different N sequences have different behavior for N large. Further patterns:

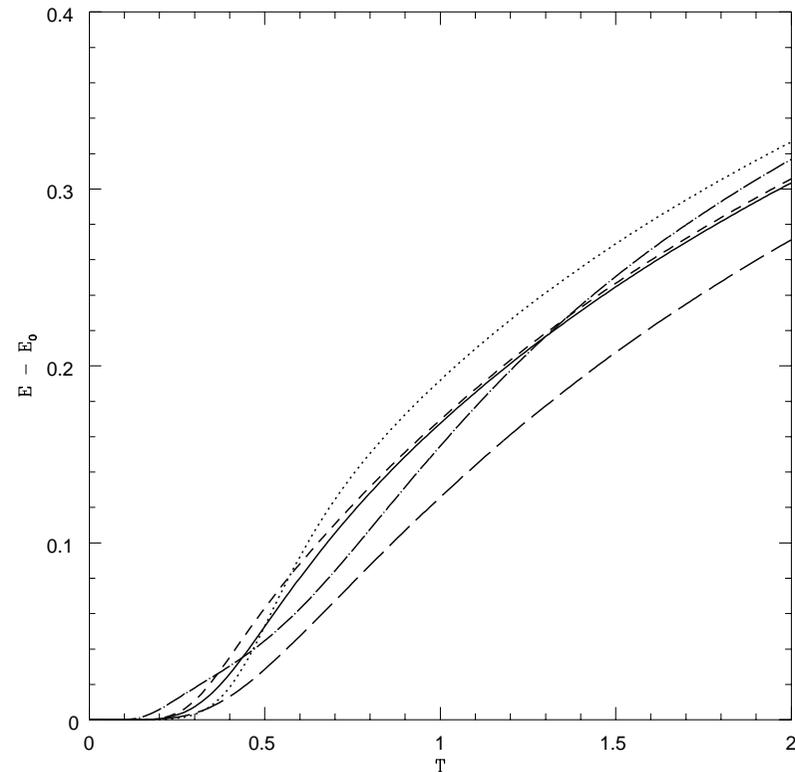
$N = 4n + 2$, conjecture that $E = 4$.

$N = 4n + 1$, conjecture that $E = 5 - c/N$.

It is plausible that the ground state density energy of the Bernasconi model is zero in the thermodynamic limit. Different N sequences have different corrections.



$\mathcal{N}(E)$ for different N values: differences in the details and similar overall shape.



$E(T) - E(T = 0)$ as a function of T , respectively for $N = 19$ and $N = 31$ (good primes, respectively dots-dashes and dots), 33 (of the form $4n + 1$, non prime, short dashes), 34 (of the form $4n + 2$, long dashes) and 37 (of the form $4n + 1$, prime, continuous line)

Peak in the specific heat: **phase transition** in the infinite volume limit.

First excited levels are typically not similar to the ground states.

Typically first excited states are not single spin flips from ground states (for some N values none is).

Few configurations with small energy start to dominate the partition function at low $T < T_c$. The situation is very reminiscent of Derrida REM.

It is easy to obtain an approximate solution of the finite T model, assuming that the correlation functions are independent: **this coincides with Golay computation.**

Replica treatment. The Bernasconi mean field Hamiltonian can be substituted with a random Hamiltonian:

$$\frac{1}{N} \sum_{d=1}^{N-1} (C_d)^2 \longrightarrow \frac{1}{N} \sum_{d=1}^{N-1} (\tilde{C}_d)^2 ,$$

where

$$\tilde{C}_d \equiv \sum_{m,j} J_{m,j}^k \sigma_m \sigma_j$$

and where the coupling are equal to one with probability $1/N$ and are zero otherwise.

The replica symmetric solution coincides with the Gola approximation.

One can obtain the one step, replica symmetry broken solution, and obtain a phenomenology of the REM type.

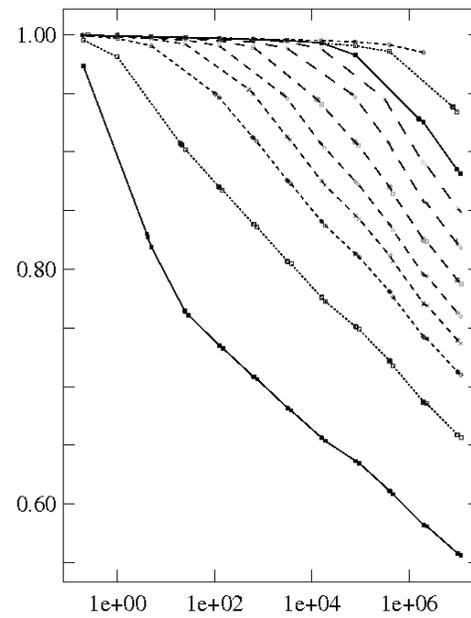
The dynamical behavior of the model.

(Krauth and Mezard, cond-mat/9407029; Migliorini and Ritort, cond-mat/9407105)

Single spin flip dynamics. Usual Metropolis very uneffective. Very low acceptance rate for small T .

Bortz, Kalos, Lebowitz: compute transition probabilities to all neighbors. Always move to one neighbor, and compute τ . More expensive, but look-up tables are useful. Becomes advantageous when acceptance is of order $1/N$.

Dynamics is very slow...



Aging in the mean field Bernasconi model.

The quest for (realistic) glassy models

Realistic: finite D , finite range.

Correlation length.

Heterogeneities.

Destiny of metastable states.

Two directions: **models with disorder** (even if in glasses you do not have quenched disorder, see the points we have discussed before) or **non-disordered, “complex”** models.

In the following we will propose to start from mean field Bernasconi to try this second path.

Models with disorder

The p -state random Potts model

$$H \equiv - \sum J_{ij} (p\delta_{\sigma_i\sigma_j} - 1) ,$$

where $\sigma = (1, 2, \dots, p)$ [Elderfield-Sherrington 1983](#).

At low T this model can undergo an inconvenient ferromagnetic phase transition.

Maybe more convenient the random permutation glassy Potts Model ([EM, Mossa and Parisi 1998](#))

$$H \equiv - \sum \delta_{\sigma_i \Pi\{\sigma_j\}} ,$$

where $\sigma = (1, 2, \dots, p)$ and Π is a link attached, random quenched permutation of $(1, 2, \dots, p)$.

The plaquette random model:

$$H \equiv - \sum_{\square} J_{\square} \prod_{i \in \square} \sigma_i ,$$

\square : plaquettes of a D -dimensional cubic lattice. [Kisker, Rieger and Schreckenberg, 1994](#); [Alvarez, Franz and Ritort, 1996](#)

Models without disorder

[Shore, Holzer and Sethna 1992](#) Competition in interactions:

$$-J_1 \sum_{nn} \sigma_i \sigma_j + J \sum_{nnn} \sigma_i \sigma_j ,$$

and a tiling model.

[M. Newman and C. Moore 1999](#): on a $2D$ triangular lattice

$$\frac{1}{2} \sum_{i,j,k \in \nabla} \sigma_i \sigma_j \sigma_k$$

only on downward pointing triangles. Exactly soluble.

The local low autocorrelation model.

Finite range, finite D , no quenched disorder.

D dimensional lattice, $V = L^D$.

$\mathcal{R}_{(i)}$ is a hypercube of size R^D , centered around site i .

$$H \equiv \mathcal{N} \sum_{i \in V} \left[\begin{array}{c} \text{max distance in } \mathcal{R}_{(i)} \\ \sum_{d=1} \\ \left(\sum_{\substack{\text{all couples in } \mathcal{R}_{(i)} \\ \text{at distance } d}} \sigma_j \sigma_k \right)^2 \end{array} \right].$$

The free model is defined with free boundary conditions, periodic model with periodic boundary conditions.

We analyze here the case of $D = 1$, free boundary conditions. We define:

$$H_R \equiv \frac{V}{R(R-1)(V-R+1)} \sum_{i=0}^{V-R} \sum_{d=1}^{R-1} \left(\sum_{j=i}^{i+R-d-1} \sigma_j \sigma_{j+d} \right)^2 .$$

The normalization can be easily understood: when $R = V$ it coincides with the correct one for the long range Bernasconi model with free boundary conditions.

Let us start looking at simple cases. $R = 2$ is too simple, since we only get V constant contributions of the form $(\sigma_i \sigma_{i+1})^2 = 1$.

The first non trivial case is for $R = 3$. Here we get two contributions. For distance one we get

$$(\sigma_i \sigma_{i+1} + \sigma_{i+1} \sigma_{i+2})^2 = 2 + 2\sigma_i \sigma_{i+2} ,$$

and for distance two only the constant term

$$(\sigma_i \sigma_{i+2})^2 = 1 ,$$

In other terms, but for constant, irrelevant additive terms:

$$H_2^{(D=1)} = \sum_i \sigma_i \sigma_{i+2} .$$

This is a decoupled set of two antiferromagnets, one on even sites and one on odd sites. There are four bi-staggered ground states...

Now let us look at $R = 4$. Here $d = 1$ gives a quartic contribution.

Let us look at $i = 1$:

$$(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4)^2 = 2(\sigma_1\sigma_3 + \sigma_2\sigma_4 + \sigma_1\sigma_2\sigma_3\sigma_4) + \text{const} .$$

$d = 2$ gives only the same quartic contribution

$$2\sigma_1\sigma_2\sigma_3\sigma_4 ,$$

while $d = 3$ gives a trivial additive constant. All together we have that

$$H_3^{(D=1)} = \frac{4}{3} \sum_i [\sigma_i\sigma_{i+2} + \sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3}] .$$

This model is already frustrated. The quadratic term is like before, but the quartic term is, for ground states of $H_3^{(D=1)}$, always positive.

Methods, T=0 and finite T.

T=0 exact enumeration

Easily all ground states up to $R = N = 36$.

T=0 branch and bound

We use **branch-and-bound (BB)**, to determine **all** exact ground states (and also local optima at most at distance δ away from the ground states) for our local glassy model, up to $N \leq 54$, for small and medium R .

In a BB approach, the problem is solved using **recursion**. In the **branching step**, one of the $\sigma_i \in \sigma_1, \dots, \sigma_n$ is chosen. **Two sub problems** are created: in one we set $\sigma_i = +1$, in the other $\sigma_i = -1$.

The sub problems are solved recursively. In each sub problem, an upper and a lower bound on the value of the optimum solution are determined.

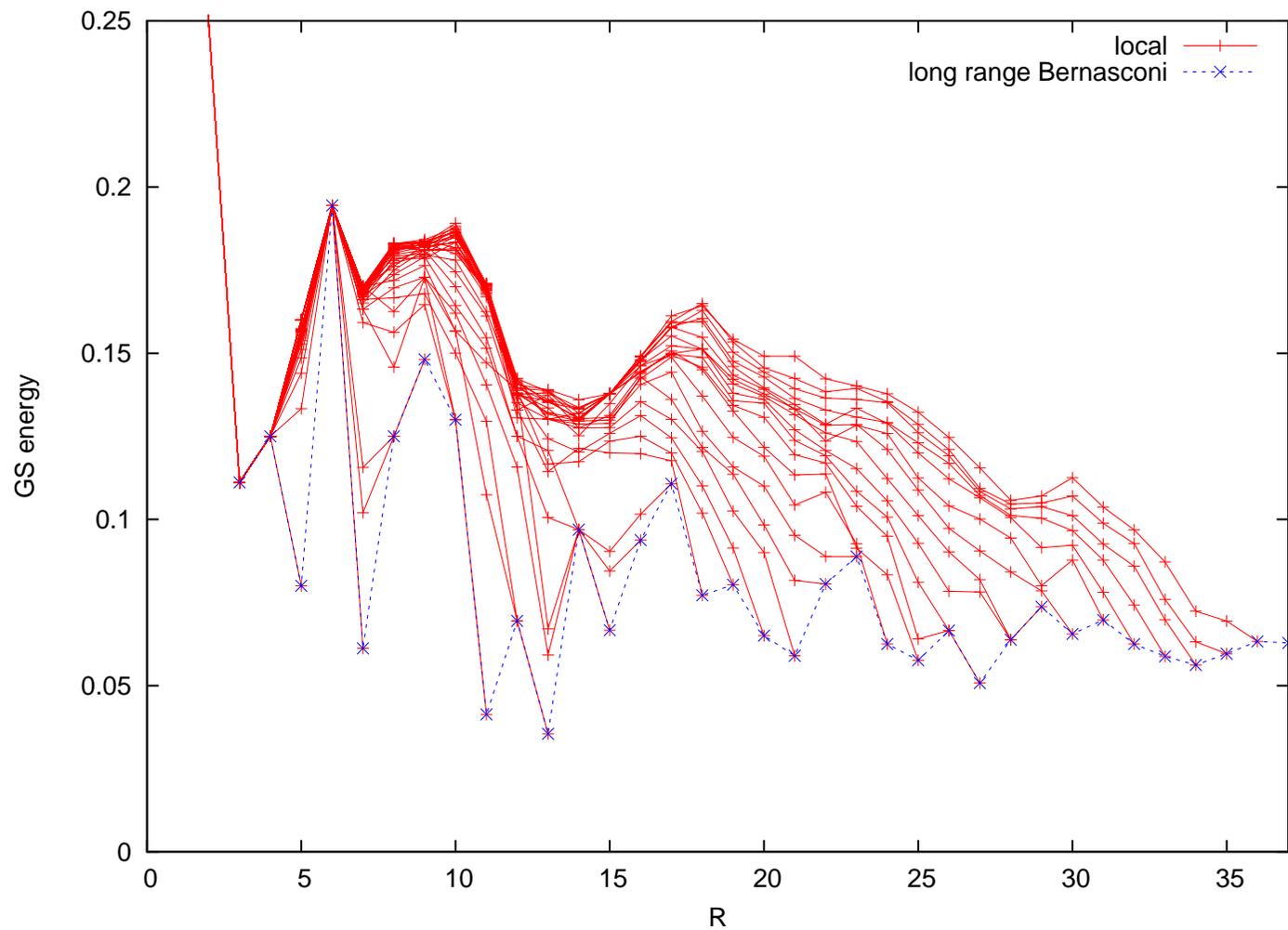
If in a sub problem the lower bound attains a higher value than the upper bound, no solution better than the upper bound can be contained in the corresponding sub problem, and it can be dropped.

Following Mertens BB approach for the mean field Bernasconi model we first narrow the search space exploiting some of the model symmetries. E.g., having a ground state configuration $\sigma_1 \dots \sigma_n$ at hand, also its reversal $\sigma_n \dots \sigma_1$ is optimum. Furthermore, both multiplying each spin by -1 or multiplying only each second spin by -1 also yields a ground state. Therefore we can restrict ourselves to the enumeration of representatives of these symmetry classes.

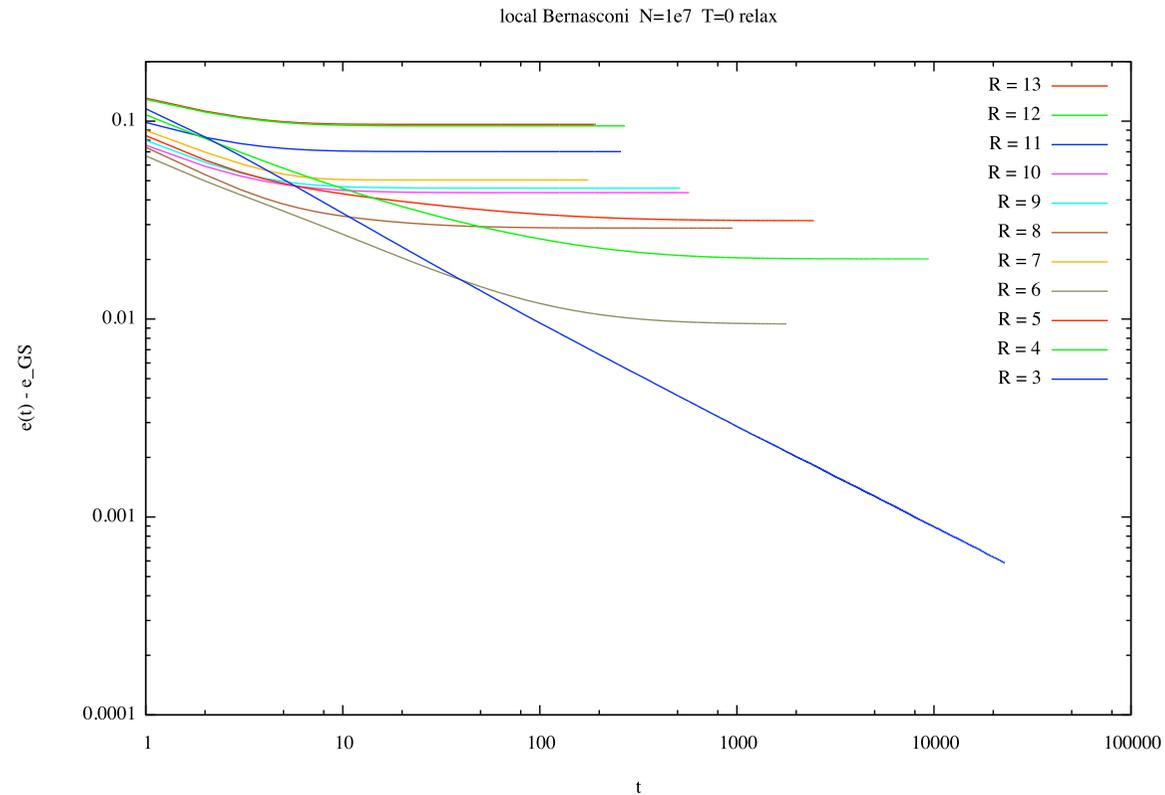
Each spin configuration can serve as an upper bound. The determination of the lower bound is trickier and crucial for the performance of the algorithm.

T=0 relaxation: steepest descent dynamics

Finite T simple Glauber dynamics



Blue is Mertens for long range, open mean field Bernasconi. Red is the local glass, open chain, for different N values. $R = 6$ is a trivial model.

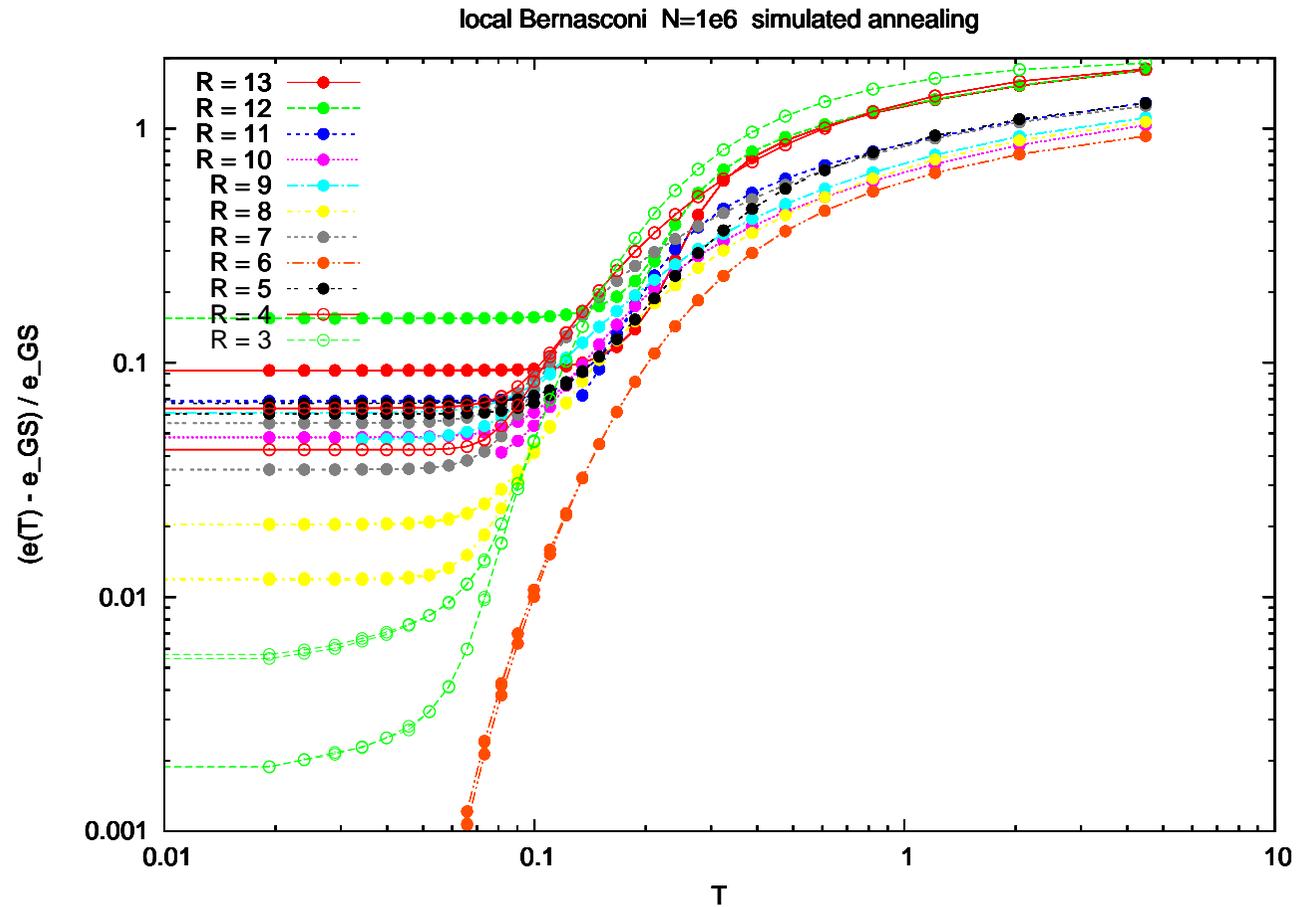


$T = 0$ relaxation: distance from the Ground State energy.

$R = 3$, staggered anti-ferromagnet $1D$ Ising: decay.

$R > 3$, slowing down (but $R = 6$ has fastest decay).

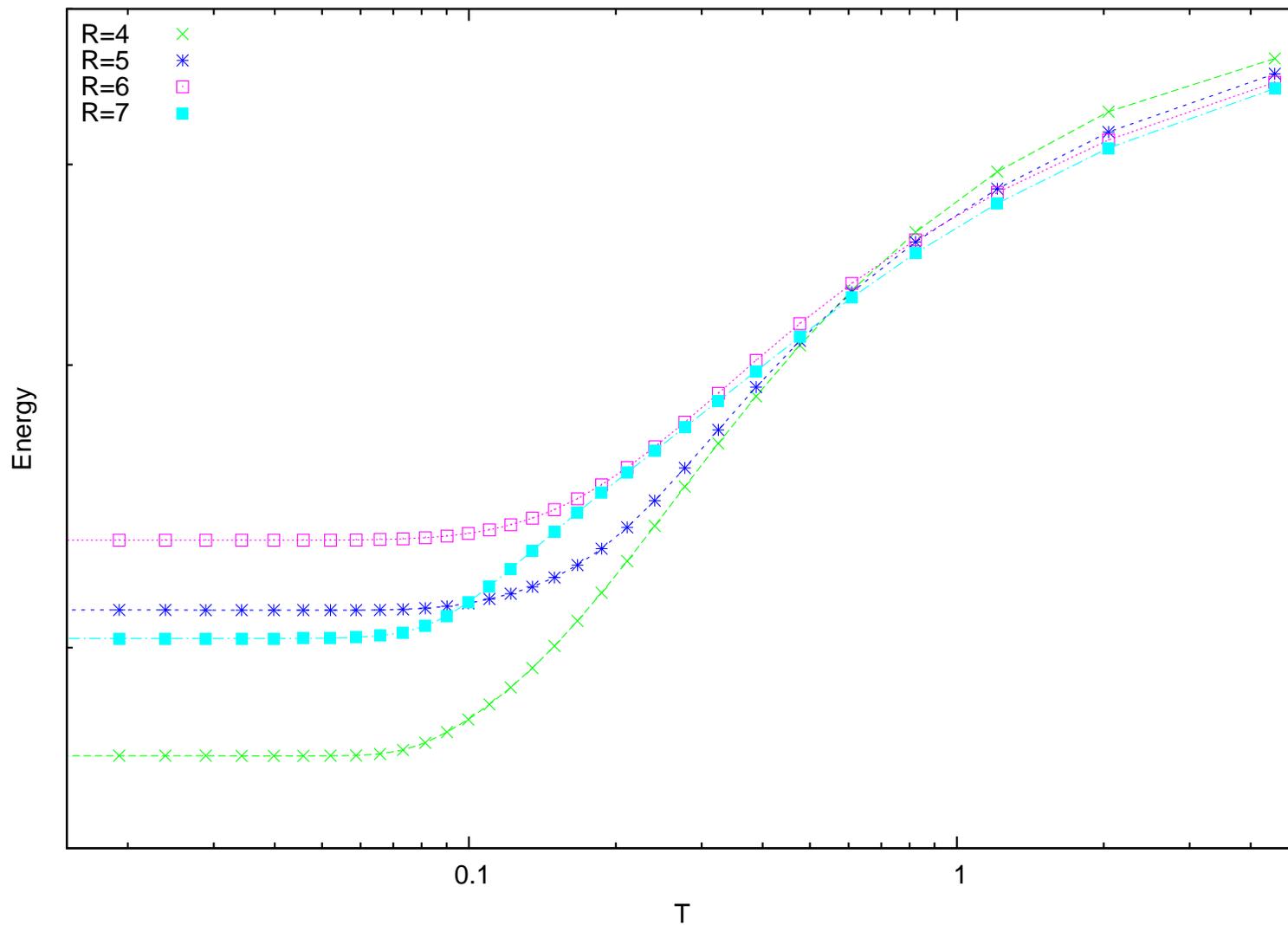
Some R values much slower than others: see $R = 5$.



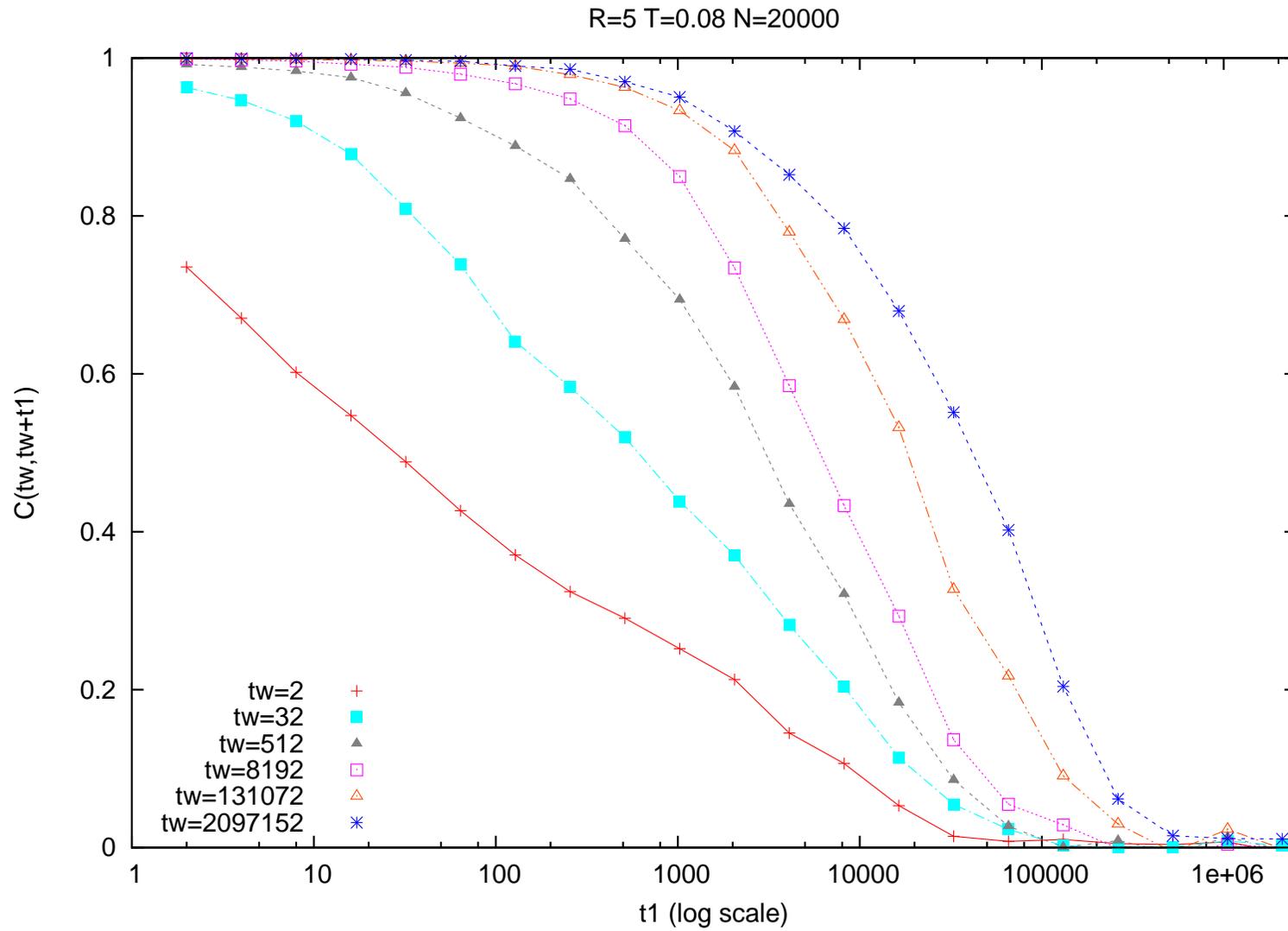
Distance from ground state energy.

Two different cooling schedules for each R value.

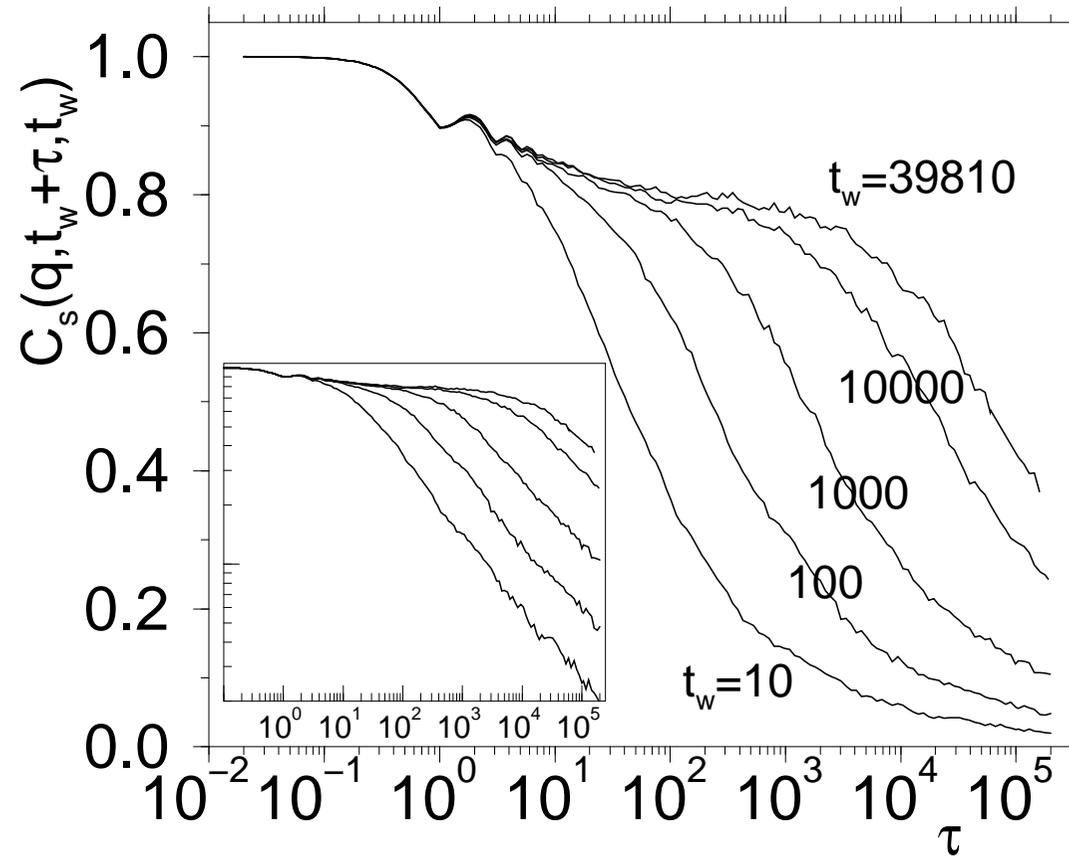
$R = 6$ decays fast. $R = 5$ stops early and high.



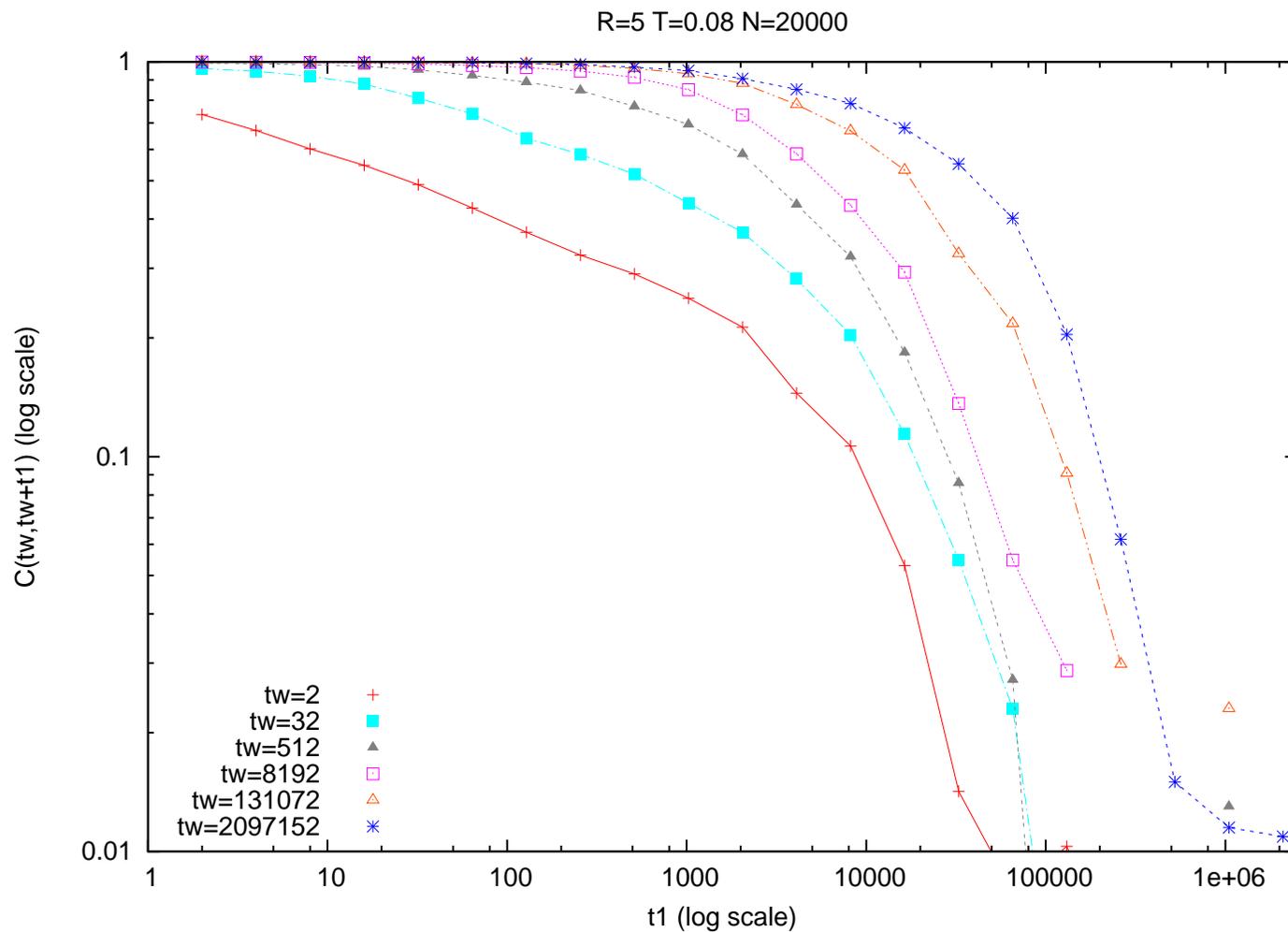
Energy versus T , fixed annealing schedule.



Aging on long time scales.



Time dependence of the correlation function in a Lennard-Jones mixture (Kob and Barrat, *Phys. Rev. Lett.* 78 (1997) 4581).



C on logarithmic time scale.

$R = 5$: we have aging on very long time scales. This is remarkable: already with a very small range of the interaction we have an interesting behavior.

By changing the value of R (in $D = 1, 2$ or $3\dots$) we can generate models without quenched disorder with a very slow dynamics, that becomes slower as the range increases.

Many things should be investigated.

Detailed properties of ground states, of low energies states and of the full partition function.

Use the Bortz, Kalos, Lebowitz dynamics.

$D > 1$: here we will have real phase transitions, and we can study their nature.

Do we have an interesting “primology” also in our finite range, periodic system?