

Overlap Equivalence in the Edwards-Anderson model

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Abstract

We perform a numerical simulation (parallel tempering) to study the relative fluctuations of the link overlap and the square standard overlap in the three dimensional Gaussian Edwards-Anderson model with zero external field. We first analyze the correlation coefficient and find that the two quantities are uncorrelated above the critical temperature. Below the critical temperature we find that the link overlap has vanishing fluctuations for fixed values of the square standard overlap and large volumes. We identify the functional relation among the two using the method of the least squares which turn out to be a monotonically increasing function and we approximate it up to the third order. Our results show that the two overlaps are completely equivalent in the description of the low temperature phase of the Edwards-Anderson model and by consequence the TNT picture should be rejected.

1 Introduction

The low temperature phase of short-range spin-glasses is among the most unsettled problems in condensed matter physics [1, 2]. To detect its nature it was originally proposed an order parameter by Edwards and Anderson [3], the disorder average of the local squared magnetization

$$q_{EA} = \text{Av}(\omega_i^2) = \text{Av} \left(\left[\frac{\sum_{\sigma} \sigma_i e^{-\beta H_{\sigma}}}{\sum_{\sigma} e^{-\beta H_{\sigma}}} \right]^2 \right) \quad (1.1)$$

which coincides with the quenched expectation of the local *standard* overlap of two spin configurations drawn according to two copies of the equilibrium state carrying identical disorder

$$\text{Av}(\omega_i^2) = \langle q_i \rangle = \text{Av} \left(\frac{\sum_{\sigma, \tau} \sigma_i \tau_i e^{-\beta(H_{\sigma} + H_{\tau})}}{\sum_{\sigma, \tau} e^{-\beta(H_{\sigma} + H_{\tau})}} \right) \quad (1.2)$$

The previous parameter should reveal the presence of frozen spins in random directions at low temperatures. While that choice of the local observable is quite natural it is far to be unique; one can consider for instance the two point function $\text{Av}(\omega_{ij}^2)$. In the case of nearest neighbour correlation function this yields to the quenched average of the local *link* overlap.

When summed over the whole volume link overlap and standard overlap give rise to a priori different global order parameters. In the mean field case the two have a very simple relation: in the Sherrington-Kirkpatrick (SK) model for instance it turns out that the link overlap coincides with the square power of the standard overlap up to thermodynamically irrelevant terms. But in general, especially in the finite dimensional case of nearest neighbor interaction like the Edwards-Anderson (EA) model, the two previous quantities have a different behavior with respect to spin flips: when summed over regions the first undergoes changes of volume sizes after spin-flips, while the second is affected only by surface terms.

From the mathematical point of view their role is also quite different. The square of the standard overlap represents in fact the covariance of the Hamiltonian function for the SK model, while the link overlap is the covariance for the EA model. Two different overlap definitions are naturally related to two different notions of distance among spin configurations. It is an interesting question to establish if two distances are equivalent for the equilibrium measure in the large volume limit and if yes to what extent (see [4] for a broad discussion on *overlap equivalence* and its relation with ultrametricity). They could in fact be simply equivalent in preserving

L	Therm	Equil	Nreal	n_β	δT	T_{min}	T_{max}
3 – 6	50000	50000	2048	19	0.1	0.5	2.3
8	50000	50000	2680	19	0.1	0.5	2.3
10	70000	70000	2048	37	0.05	0.5	2.3
12	70000	70000	2048	37	0.05	0.5	2.3

Table 1: Parameters of the simulations: system size, number of sweeps used for thermalization, number of sweeps for measurement of the observables, number of disorder realizations, number of temperature values allowed in the PT procedure, temperature increment, minimum and maximum temperature values.

neighborhoods (topological equivalence) or they could preserve order among distances (metric equivalence).

In this paper we consider the EA model in $d=3$, with Gaussian couplings and zero external magnetic field in periodic boundary conditions. We study the relative fluctuations of the link overlap with respect to the square of standard overlap. We use the parallel tempering algorithm (PT) to investigate lattice sizes from $L = 3$ to $L = 12$. For every size we simulate at least 2048 disorder realizations. For the larger sizes we used 37 temperature values in the range $0.5 \leq T \leq 2.3$. The thermalization in the PT procedure is tested by checking the symmetry of the probability distribution for the standard overlap q (see Sec. 2) under the transformation $q \rightarrow -q$. Moreover for the Gaussian coupling case it is available another thermalization test: the internal energy can be calculated both as the temporal mean of the Hamiltonian and - by exploiting integration by parts - as expectation of a simple function of the link overlap [5]. We checked that with our thermalization steps both measurements converge to the same value. All the parameters used in the simulations are reported in Tab.1.

2 Definitions

We recall the basic definitions. For a 3-dimensional lattice Λ of volume $N = L^3$, the *square of the standard overlap* among two spin configurations $\sigma, \tau \in \{+1, -1\}^N$ is

$$q^2(\sigma, \tau) = \left(\frac{1}{N} \sum_i \sigma_i \tau_i \right)^2 \quad (2.3)$$

The *link overlap* is instead obtained from the nearest neighbor spins, namely for $b = (i, j)$ with $i, j \in \Lambda$, $|i - j| = 1$ and $\sigma_b = \sigma_i \sigma_j$

$$Q(\sigma, \tau) = \frac{1}{3N} \sum_b \sigma_b \tau_b \quad (2.4)$$

Firs we investigate the behavior of the correlation coefficient between q^2 and Q

$$\rho(q^2, Q) = \frac{\langle (q^2 - \langle q^2 \rangle)(Q - \langle Q \rangle) \rangle}{\sqrt{\langle (q^2 - \langle q^2 \rangle)^2 \rangle \langle (Q - \langle Q \rangle)^2 \rangle}} \quad (2.5)$$

This quantity will tell us in which range of temperatures the two random variables are correlated. In that range we further investigate the nature of the mutual correlation by studying their joint distribution and, in particular, the conditional distribution for instance of Q at fixed values of q^2 . We are interested in understanding if a functional relation among the two quantities exists i.e. if the variance of the conditional distribution shrink to zero at large volumes and around what curve $Q = G(q^2)$ the conditional distribution is peaked.

Namely:

$$P(Q|q^2) = \frac{P(Q, q^2)}{P(q^2)} = \frac{\text{Av} \left(\frac{\sum_{\sigma, \tau} \delta(Q - Q_{\sigma, \tau}) \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}} \right)}{\text{Av} \left(\frac{\sum_{\sigma, \tau} \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}} \right)} \quad (2.6)$$

For this conditional distribution we compute the mean and the variance:

$$G(q^2) = \langle Q|q^2 \rangle = \frac{\text{Av} \frac{\sum_{\sigma, \tau} Q_{\sigma, \tau} \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}}}{\text{Av} \frac{\sum_{\sigma, \tau} \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}}} \quad (2.7)$$

$$\langle Q^2|q^2 \rangle = \frac{\text{Av} \frac{\sum_{\sigma, \tau} Q_{\sigma, \tau}^2 \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}}}{\text{Av} \frac{\sum_{\sigma, \tau} \delta(q^2 - q_{\sigma, \tau}^2) e^{-\beta[H_\sigma + H_\tau]}}{\sum_{\sigma, \tau} e^{-\beta[H_\sigma + H_\tau]}}} \quad (2.8)$$

$$\text{Var}(Q|q^2) = \langle Q^2|q^2 \rangle - \langle Q|q^2 \rangle^2 \quad (2.9)$$

The method of the least squares immediately entails that $G(q^2)$ is the best estimator for the functional dependence of Q in terms of q^2 . In fact, given any function $g(q^2)$, the mean of $(Q - g(q^2))^2$ according to the joint distribution $P(Q, q^2)$ is $\sum_{i,j} (Q_i - g(q_j^2))^2 P(Q_i, q_j^2) = \sum_j P(q_j^2) \sum_i (Q_i - g(q_j^2))^2 P(Q_i|q_j^2)$, where the sums run over all possible values of the random

variables Q, q^2 , which are finitely many on the finite system we simulated. Therefore, to minimize the mean it suffices to minimize the inner sum, i.e. to choose $g(q^2)$ as the mean $G(q^2)$ of Q with respect to the conditional distribution (2.6). The variance, on the other hand, measures how precise it is the estimate.

3 Results

Fig. (1) shows the correlation between the square standard overlap and the link overlap. The plot of Eq.(2.5) is done for different sizes of the system as a function of the temperature.

For a given temperature, we did a fit of the data to the infinite volume limit. For every temperature value there is monotonicity in the system size L , even if in the low temperature region $T \leq 1.0$ the data are very slowly decreasing as the system size increases. We tried different scaling for the data, both exponential $\rho_L(T) = \rho_\infty(T) + a(T)e^{b(T)L}$ and power law $\rho_L(T) = \rho_\infty(T) + \alpha(T)L^{\beta(T)}$. The interesting information is contained in the asymptotic value $\rho_\infty(T)$. We measured the χ^2 for different values of $\rho_\infty(T)$ in the range $[0, \min_L \rho_L(T)]$ and keeping $a(T)$ and $b(T)$ (or $\alpha(T)$ and $\beta(T)$) as free parameters. In the region $T \in [1.8, 2.3]$ both the exponential and power law follows the data in a qualitative way. They have the minimum value of the normalized χ^2 for $\rho_\infty(T) = 0$. The power law fit seems to work better, for example at $T = 2.0$ we found χ_{exp}^2 is $O(10^{-2})$ and χ_{power}^2 is $O(10^{-4})$. In the range $T \in [1.1, 1.7]$ the two fit have a minimum χ^2 again at $\rho_\infty(T) = 0$, but the exponential fit is preferable because it has a smaller χ^2 and better confidence intervals. Finally for $T \leq 1.0$ the χ^2 develops a sharp minimum corresponding to values $\rho_\infty(T) \neq 0$ and the exponential fit performs better than the power law fit, which actually is not even able to reproduce the behaviour of the data. The whole plot of the curve $\rho_\infty(T)$ as obtained from the best fit is represented in Fig. (2).

In the high temperature phase the two random variables are asymptotically uncorrelated while in the low temperature one they display a non-vanishing correlation which suggests further investigation concerning the functional relation among them. Within our available temperature values the temperature at which the correlation coefficient starts to be different from zero is in good agreement with the estimated critical value of the model $T_c \sim 1$.

We consider then the problem of studying the functional dependence (if any) between the two random variables Q and q^2 in the low temperature region. The points in the Fig. (3) show the function $G(q^2)$ of Eq.(2.7) for different

system sizes at $T = 0.5$. Also we studied a third order approximation of the form $Q = g(q^2) = a + bq^2 + cq^4 + dq^6$. Since we must have $Q = 1$ for $q^2 = 1$, this actually implies $d = 1 - a - b - c$. The coefficients $a_{L,T}, b_{L,T}, c_{L,T}$ have been obtained by the least square method and then fitted to the infinite volume limit. The result is shown as continuous lines in Fig (3). The good superposition of the curves to the data for $G(q^2)$ indicates that the functional dependence between the two overlaps is well approximated already at the third order.

Finally Fig (4) shows the normalized variance at low temperature for different sizes of the system. It shows that the distribution is concentrating for large volumes around its mean value. The trend toward a vanishing variance for infinite system sizes is very clear. The best fit (in terms of the χ^2) of the data is obtained by a power law of the form $aL^{-b} + c$ and it gives $c = 0$ for every value of q^2 . We also investigated how the non-normalized variance scales to zero and found that the coefficient b stays in the range [1.4,1.6] which indicate that the variance could scale to zero as the inverse power of the square root of the volume.

4 Comments

It is interesting to compare our result with previous work. Marinari and Parisi [6] have studied the relation $Q = (1 - A(L)) + (A(L) - B(L))q^2 + B(L)q^4$ among the two overlaps at zero temperature, by ground state perturbation. We have extrapolated our data in the low temperature regime to zero temperature by a polynomial fit and then to the infinite volume limit ($L = \infty$). The best fit for $L = \infty$ (i.e. the one with smaller χ^2) is quadratic in L^{-1} . It gives $A = 0.30 \pm 0.05$ ($\chi^2 = 0.21$), which is in agreement with the independent measure of Marinari and Parisi ($A = 0.30 \pm 0.01, \chi^2 = 0.6$). Note that their results are obtained with a complete different method than Montecarlo simulations, namely exact ground states. Sourlas [7] studied the same problem in a different setting called soft constraint model. Although a direct quantitative comparison is not possible with our method his results are qualitatively similar.

In conclusion, our result shows quite clearly that the study of the two order parameters, the square of the standard overlap and the link overlap, are equivalent as far as the quenched equilibrium state is concerned. In view of our result the proposed pictures which assign different behaviour to the two overlap distributions, in particular the TNT [8] picture, should be rejected. It is interesting to point out that since the present analysis deals

only with the distribution of $P(q^2, Q)$ and not with the higher order ones like for instance $P(q_{1,2}^2, q_{2,3}^2, Q_{1,2}, Q_{2,3})$ our results are compatible with different factorization properties of the two overlaps like those illustrated in [9].

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References

- [1] M. Mezard, G. Parisi, M.A. Virasoro, *Spin Glass Theory and Beyond* World Scientific, Singapore (1987).
- [2] C.M. Newman and D.L. Stein, “Short-Range Spin Glasses: Results and Speculations”, *cond-mat/0503345*.
- [3] S.F. Edwards and P.W.Anderson, “Theory of spin glasses” *Jou. Phys. F.*, **5**, 965, (1975).
- [4] G. Parisi, F. Ricci-Tersenghi, “On the origin of ultrametricity”, *J. Phys. A: Math. Gen.* **33**, 113, (2000).
- [5] P. Contucci, “Replica Equivalence in the Edwards-Anderson Model” *J. Phys. A: Math. Gen.* **36**, 10961, (2003).
- [6] E. Marinari, G. Parisi, “Effects of a Bulk Perturbation on the Ground State of 3D Ising Spin Glasses” *Phys. Rev. Lett.* **86**, 3887, (2001).
- [7] N. Sourlas, “Soft annealing: A new approach to difficult computational problems”, *Phys. Rev. Lett.* **94**, 70601, (2005).
- [8] M.Palassini, A.P.Young, “Nature of the Spin Glass State” *Phys, Rev. Lett.* **85**, 3017, (2000).
- [9] P.Contucci, C.Giardina, “Factorization properties in the 3D Edwards-Anderson model”, *Phys. Rev. B* **72**, 14456, (2005).

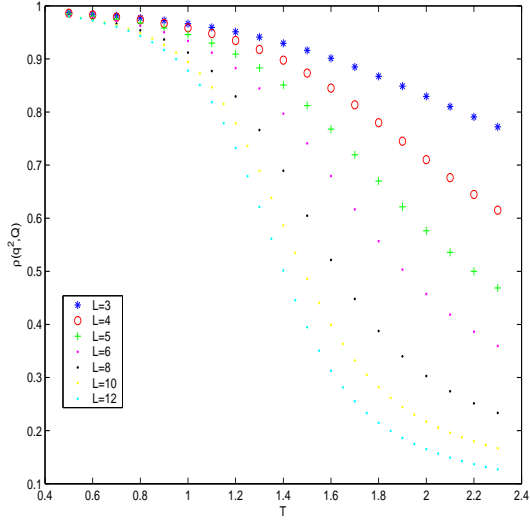


Figure 1: $\rho(q^2, Q)$ as a function of the temperature T for different sizes L of the system.

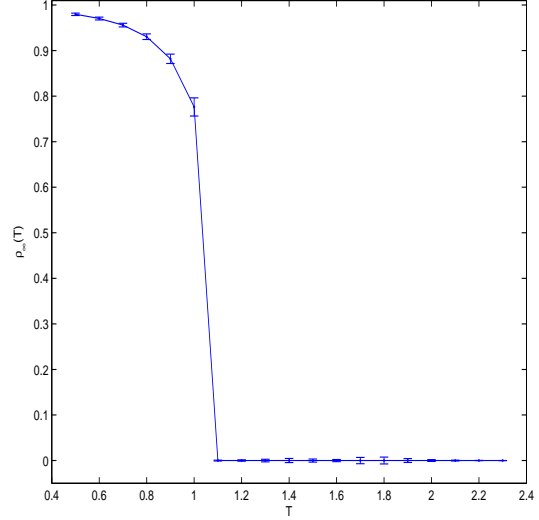


Figure 2: $\rho_\infty(T)$ as a function of the temperature T .

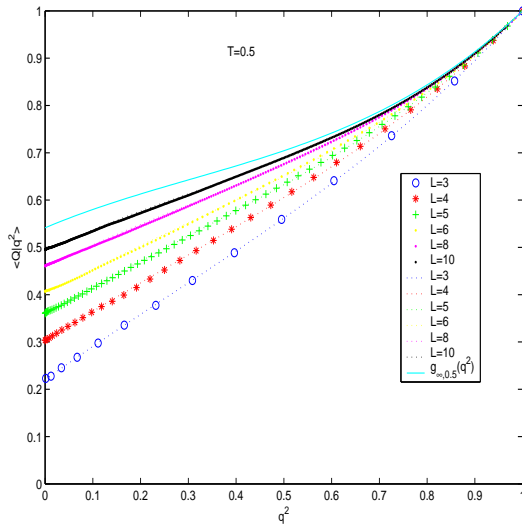


Figure 3: Plot of the curves $g_{L,T}(q^2)$ (continuous lines) and of $\langle Q|q^2 \rangle_{L,T}$ (dotted lines) together with the infinite volume limit curve $g_T(q)$ (upper continuous line) for $T = 0.5$.

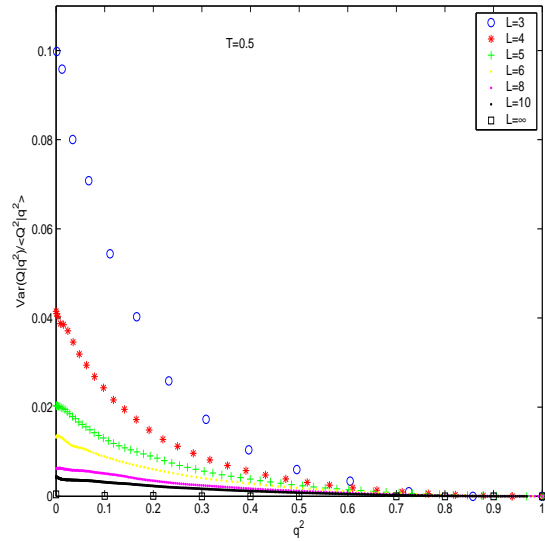


Figure 4: $Var(Q|q^2)_{L,T} / \langle Q^2|q^2 \rangle$ as a function of q^2 for the temperature $T = 0.5$ and for different sizes L together with the infinite volume limit.