Overlap Equivalence in the Edwards-Anderson model

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We 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. Our data show that the conditional variance scales to zero in the thermodynamic limit. This implies that, if one of the two random variables tends to a trivial one (i.e. delta-like distributed), then also the other does and, by consequence, the TNT picture should be dismissed. We identify the functional relation among the two variables using the method of the least squares which turns out to be a monotonically increasing function. Our results show that the two overlaps are completely equivalent in the description of the low temperature phase of the Edwards-Anderson model.

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, the disorder average of the local squared magnetization

\[ q_{EA} = \langle \omega^2 \rangle = \text{Av} \left( \left( \sum_{\sigma} \frac{e^{-\beta H_{\sigma}}}{\sum_{\tau} e^{-\beta H_{\tau}}} \right)^2 \right) , \tag{1} \]

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

\[ \text{Av}(\omega^2_i) = < q_i > = \text{Av} \left( \frac{\sum_{\sigma, \tau} \sigma_i \tau_i e^{-\beta (H_{\sigma} + H_{\tau})}}{\sum_{\sigma, \tau} e^{-\beta (H_{\sigma} + H_{\tau})}} \right) . \tag{2} \]

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^2_{ij}). In the case of nearest neighbour correlation function this yields 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 3 for a broad discussion on overlap equivalence and its relation with ultrametricity). They could in fact be simply equivalent in preserving neighborhoods (topological equivalence) or they could preserve order among distances (metric equivalence). The a-priori different properties of the two overlaps have also been discussed in relation to the different pictures (droplet 12, mean-field 1, TNT 11,1 11), that have been proposed to describe the nature of the low temperature spin-glass state. In this respect, the distributions of the two overlaps are expected to be delta-like (trivial distribution, droplet theory), to have support on a finite interval (non trivial distribution, mean-field theory), or to have different behaviour depending on which overlap is considered (trivial link overlap distribution, non trivial standard overlap distribution, TNT theory).

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 choice of the lowest temperature is related to the possibility to thermalize the large sizes, but our results are perfectly compatible with those obtained by Marinari and Parisi at \( T = 0 \).
We recall the basic definitions. For a 3-dimensional lattice $\Lambda$ of volume $N = L^3$, the square of the standard overlap among two spin configurations $\sigma, \tau \in \{+1, -1\}^N$ is
\[
q^2(\sigma, \tau) = \left( \frac{1}{N} \sum_i \sigma_i \tau_i \right)^2.
\]
(see the last paragraph before the conclusions). The thermalization in the PT procedure is tested by checking the symmetry of the probability distribution for the standard overlap $q$ 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 $\mathcal{L}$. 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. I.

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\]
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 $\sigma_b = \sigma_i \sigma_j$
\[
Q(\sigma, \tau) = \frac{1}{3N} \sum_b \sigma_b \tau_b.
\]
First, we investigate the behavior of the correlation coefficient between $q^2$ and $Q$
\[
\rho = \frac{\langle (q^2 - \langle q^2 \rangle)(Q - \langle Q \rangle) \rangle}{\sqrt{\langle (q^2 - \langle q^2 \rangle)^2 \rangle} \langle (Q - \langle Q \rangle)^2 \rangle}.
\]
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 $P(Q|q^2)$ 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 shrinks to zero at large volumes and around what curve the conditional distribution is peaked. We have:
\[
P(Q|q^2) = \frac{P(Q, q^2)}{P(q^2)} = \frac{\text{Av} \left( \frac{\sum_{\sigma, \tau} \delta(Q - Q_{\sigma, \tau}) \delta(q^2 - q^2_{\sigma, \tau}) e^{-\beta[H + H_{\tau}]}}{\sum_{\sigma, \tau} e^{-\beta[H + H_{\tau}]}} \right)}{\text{Av} \left( \frac{\sum_{\sigma, \tau} \delta(q^2 - q^2_{\sigma, \tau}) e^{-\beta[H + H_{\tau}]}}{\sum_{\sigma, \tau} e^{-\beta[H + H_{\tau}]}} \right)}.
\]
For this conditional distribution one could compute the generic $k$-th moment
\[
G_k(q^2) := \mathbb{E} (Q^k|q^2) = \int_{-1}^{1} Q^k P(Q|q^2)dQ.
\]
We will be interested in the mean
\[
G(q^2) := G_1(q^2) = \mathbb{E} (Q|q^2)
\]
and the variance
\[
\text{Var}(Q|q^2) = G_2(q^2) - G_1^2(q^2).
\]
The method of the least squares immediately entails that the mean $G(q^2)$ is the best estimator for the functional dependence of $Q$ in terms of $q^2$. In fact, given any function $h(q^2)$, the mean $(Q - h(q^2))^2$ according to the joint distribution $P(Q, q^2)$ is $\sum_{\sigma, \tau} (Q_{\sigma, \tau} - h(q^2_{\sigma, \tau}))^2 P(Q_{\sigma, \tau}, q^2_{\sigma, \tau}) = \sum_{\sigma} P(q^2_{\sigma}) \sum_{\tau} (Q_{\sigma, \tau} - h(q^2_{\sigma, \tau}))^2 P(Q_{\sigma, \tau}|q^2_{\sigma})$, where the sums run over all possible values of the random vector $(Q, q^2)$, 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 $h(q^2)$ as the mean $G(q^2)$ of $Q$ with respect to the conditional distribution $P(Q|q^2)$.

The scaling properties of the conditional variance and the functional dependence provide important informations about the low temperature phase of the model. Indeed, a vanishing variance in the thermodynamic limit implies that the two random variables $Q$ and $q^2$ do not fluctuate with respect to each other. If the functional dependence $G(q^2)$ among the two is a one-to-one increasing function, then it follows that the marginal probability distributions for the standard and link overlap must have similar properties. In particular, if one of the two is supported over a point then also the other must be so.

We now describe our results. Fig. I shows the correlation between the square standard overlap and the link overlap. The plot of Eq. (5) is done for different sizes of the system as a function of the temperature. It is clear from the figure that, as the system size increases, the correlation remains strong in the low-temperature region, while it becomes weaker in the high temperature region. A sudden change in the infinite volume behavior of $\rho$ can be expected to occur close to the critical temperature $T_c$ of the model. The best estimate available in the
For each temperature, we did a fit of the data for $\rho$ to the infinite volume limit. 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 normalized $\chi^2$ for different values of $\rho_\infty(T)$ in the range $[0, \min_T \rho_L(T)]$ and keeping $a(T)$ and $b(T)$ (or $\alpha(T)$ and $\beta(T)$) as free parameters. In the region $T \geq 1.0$, we found that $\chi^2$ attains its minimal value for $\rho_\infty(T) = 0$. For $T \leq 0.9$ the $\chi^2$ develops a sharp minimum corresponding to values $\rho_\infty(T) \neq 0$. The whole plot of the curve $\rho_\infty(T)$ as obtained from the best fit is represented in Fig. 2. Also, in the inset of the same figure it is shown the standard finite size scaling of the data. We plotted $\rho_L(T)L^{\psi/\nu}$ versus the scaling variable $(T - T_c)L^{1/\nu}$. A good scaling plot is obtained using $T_c = 0.95$, $\nu = 0.71$, $\psi = 0.098$. The discrepancy between the value $\nu = 2.0$ of ref. 7 has to be attributed to the non-linear relation between $Q$ and $q^2$ (see below). Fig. 2 tells us that in the high temperature phase the two random variables standard and link overlap are asymptotically uncorrelated while in the low temperature one they display a non-vanishing correlation: within our available discrete set of 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.

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. 3 for different system sizes at $T = 0.5$, below the critical temperature. 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, we measured the variance Eq. 9 at low temperatures. We observed 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. We analyzed all temperatures below $T_c$ and we found that the best fit of $Var_L(Q|q^2)$, in terms of the $\chi^2$, is obtained by a power law of the form $a(T)L^{-b(T)} + c$ and it gives $c = 0$ for every value of the temperature. For the lowest available temperature $T = 0.5$, this is shown in Fig 4 where we plot the data for $Var_L(Q|q^2)L^{1.43}$ for different system sizes $L$: all the different curves collapse to a single one. The data for other temperature values behave similarly, the only difference being that the coefficient $b(T)$ is increasing with the temperature (it stays in the range $[1.43, 1.74]$ for $T \in [0.5, 0.9]$). This result has quite strong consequences because it says that the two random variables $Q$ and $q^2$ cannot have different triviality properties: if one of them is trivial (delta-like distributed) the scaling law for their conditional variance implies that also the other is trivial. Our result rules then out the possibility to have a non-trivial standard overlap with a trivial link overlap as predicted for instance in the so called TNT picture 10,11.

It is interesting to compare our result with previous works. Marini and Parisi 8 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 $\chi^2$) 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 Marini and Parisi ($A = 0.30 \pm 0.01$, $\chi^2 = 0.6$). Note that their results are obtained with a complete different method than Monte Carlo simulations, namely exact ground states. Sourlas 4 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 the context of out-of-equilibrium dynamics, a strong correlation between link-overlap and standard-overlap in the low-temperature phase was pointed out in ref. 5.

In conclusion, our result shows quite clearly that, within the tested system sizes, the study of the two overlap 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 picture 10,11, 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 $P(q^1_2,q^2_2,Q_1,2,Q_2,3)$, our results are compatible with different factorization properties of the two overlaps like those illustrated in 13.

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FIG. 1: $\rho_L(T)$ as a function of the temperature $T$ for different sizes $L$ of the system.

FIG. 2: $\rho_\infty(T)$ as a function of the temperature $T$. In the inset it is shown the finite size scaling.
FIG. 3: Plot of the curves $g(q^2)$ (continuous lines) and of $G(q^2)$ (dotted lines) together with the infinite volume limit curve $g_\infty(q^2)$ (upper continuous line) for $T = 0.5$.

FIG. 4: $L^{1.43} \text{Var}_L(Q|q^2)$ as a function of $q^2$ for the temperature $T = 0.5$ and for different sizes $L$. 