About the Functional Form of the Parisi Overlap Distribution for the
Three-Dimensional Edwards-Anderson Ising Spin Glass

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Recently, it has been conjectured that the statistics of extremes is of relevance for a large class of correlated system. For certain probability densities this predicts the characteristic large \(x\) fall-off behavior \(f(x) \sim \exp(\alpha x)\), \(\alpha > 0\). Using a multicanonical Monte Carlo technique, we have calculated the Parisi overlap distribution \(P(q)\) for the three-dimensional Edward-Anderson Ising spin glass at and below the critical temperature, even where \(P(q)\) is exponentially small. We find that a probability distribution related to extreme order statistics gives an excellent description of \(P(q)\) over about 80 orders of magnitude.

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The three-dimensional (3D) Edwards-Anderson (EAI) spin-glass model is a prototype of a disordered system, for which conflicting constraints create a rough free energy landscape. Such systems are of importance for the understanding of a wide range of phenomena in physics, chemistry, biology, and computer science. The overlap \(q\) between two replicas of the EAI model serves as an order parameter. Its probability density \(P(q)\) is, therefore, a quantity of central physical interest. More than twenty years ago, Parisi succeeded to calculate \(P(q)\) in the mean-field approximation \(\mathcal{G}\). However, for 3D physical systems the precise form of \(P(q)\) in the spin-glass phase, and the very nature of this phase, have remained a subject of debate \(\mathcal{G}\). More recently connections between spin glasses and extreme order statistics \(\mathcal{G}\) were pointed out by Bouchaud and Mézard \(\mathcal{G}\). Then, Bramwell et al. \(\mathcal{G}\) conjectured that the statistics of extremes, in particular Gumbel’s first asymptote (introduced below), is of relevance for a large class of correlated systems. We have used a multicanonical Monte Carlo (MC) technique \(\mathcal{G}\) to calculate \(P(q)\) numerically, even when it is exponentially small. At the critical point a modification of Gumbel’s first asymptote gives a perfect description of the data over about 80 orders of magnitude and the agreement appears to continue below the critical temperature. Although the detailed relationship between extreme order statistics and the EAI model remains to be understood, it is certainly quite rare that a physical formula has been tested over such a large range.

The statistics of extremes was pioneered by Fréchet, Fisher and Tippert, von Mises, and Gumbel. A standard result \(\mathcal{G}\), due to Fisher and Tippert, Kawata, and Smirnow, is the universal distribution of the first, second, third, . . . smallest of a set of \(N\) independent identically distributed random numbers. For an appropriate, exponential decay of the random number distribution their probability densities are given by

\[ f_a(x) = C_a \exp \left[ a \left( x - e^x \right) \right] \tag{1} \]

in the limit of large \(N\). Here \(x\) is a scaling variable, which shifts the maximum value of the probability density to zero, and \(C_a = a^a / \Gamma(a)\) normalizes the integral over \(f_a(x)\) to one. In Gumbel’s book \(\mathcal{G}\), Eq. (1) is called the first asymptote, as it holds for the asymptotic extreme order statistics of the first of altogether three different universality classes of random number distributions. The exponent \(a\) takes the values \(a = 1, 2, 3, \ldots\), corresponding, respectively, to the first, second, third, . . . smallest random number of the set. This holds independently of the details of the original random number distribution, as long as one stays within the first universality class. In the last years a non-integer value of the exponent \(a\) received also some attention. For the probability density of the magnetization of the 2D XY model Bramwell et al. \(\mathcal{G}\) derived \(a = \pi/2\) in the spin wave approximation and conjectured that this exponent describes, at least approximately, probability densities of a large class of correlated systems.

For disordered systems Bouchaud and Mézard \(\mathcal{G}\) noted that a relationship to extreme order statistics is intuitively quite obvious. Namely, at low temperatures a disordered system will preferentially occupy its low energy states, which are random variables due to the quenched exchange interactions of the system. Their investigation shows that Gumbel’s first asymptote with \(a = 1\) corresponds to one step replica symmetry breaking, and their conjecture of a relationship between extreme order statistics and disordered systems is certainly far more general. This, and the possible description of a broad range of critical phenomena by the \(a = \pi/2\) modification of Gumbel’s first asymptote, has motivated us to analyze the overlap probability density of the EAI model at and below the critical point with respect to the large \(x\) fall-off behavior of Eq. (1).

The energy function of the \(J = \pm 1\) EAI spin-glass
The model is given by

$$E = - \sum_{\langle ik \rangle} J_{ik} s_i s_k ,$$  \hfill (2)

where the $s_i = \pm 1$ are the spins of the system and the sum is over the nearest-neighbor pairs of a cubic $L^3$ lattice with periodic boundary conditions. The coupling constants $J_{ik}$ are quenched random variables, which take on the values $\pm 1$, with equal probabilities. A set of coupling constants defines a realization $\mathcal{J} = \{J_{ik}\}$ of the system. The two replica overlap (Parisi order parameter) is defined by

$$q = \frac{1}{L^3} \sum_{i=1}^{L^3} s_i^{(1)} s_i^{(2)} ,$$  \hfill (3)

where the $s_i^{(1)}$ and $s_i^{(2)}$ are the spins of two copies (replica) of the realization $\mathcal{J}$ and the sum is over all sites. The overlap probability density is given by the average over the probability densities $P^\mathcal{J}(q)$ of all realizations

$$P_L(q) = \frac{1}{N_{\mathcal{J}}} \sum_{\mathcal{J}} P^\mathcal{J}(q) ,$$  \hfill (4)

where $N_{\mathcal{J}}$ is the number of realizations used and $L$ is the lattice size. There is a long history of MC studies of this model \[12\] \[14\], which have led to a wealth of information. Here we introduce only two results: 1. The model has a freezing transition at a finite temperature, which is consistent with a Kosterlitz-Thouless \[20\] (KT) type line of critical points below $T_c = 1.14$, quite similar to the 2D XY model. In our context this is of interest in view of the description of this model by Eq. \(1\) with $a = \pi/2$ \[18\]. Note, however, that one of the most recent EAI investigations \[15\] claims to rule out the KT scenario.

At $T = 1.14$ we generated 8192 realizations for $L = 4, 6, 8$, and 640 realizations for $L = 12$. In the tails the data (for $L = 12$) at $T = 1$ are accurate down to $10^{-53}$.

We first ask the question whether, up to finite-size corrections, the probability densities depicted in Fig. \[3\] scale. A method to investigate this is to plot $\sigma_L P_L(q)$ versus $(q - \hat{q}_L)/\sigma_L$, where $\hat{q}_L$ is the mean value of $q$ with respect to the distribution $P_L(q)$ and $\sigma_L$ is its standard deviation (here $\hat{q}_L = 0$ because the $P_L(q)$ are even functions). Visual inspection shows that the data scale indeed and we proceed to fit the standard deviations to the two parameter form $\sigma_L = c_1 L^{-\beta/\nu}$ to obtain

$$\beta/\nu = 0.312 (4), \quad Q = 0.32 \text{ for } T = 1.14 ,$$  \hfill (5)

$$\beta/\nu = 0.230 (4), \quad Q = 0.99 \text{ for } T = 1 .$$  \hfill (6)

Here the numbers in parenthesis denote error bars with respect to the last digits and $Q$ is the goodness of fit. For $T = 1.14$ we plot in Fig. \[3\] $P'(q') = P_L(q)/L^{\beta/\nu}$ versus $q' = L^{\beta/\nu} q$ and see that the four probability densities collapse onto a single curve. To enlarge the scale, we restrict ourselves to the $q \geq 0$ range. The error bars of the lines in Fig. \[3\] are up to multiplicative factors the error bars of Fig. \[4\]. Not to obscure the agreement, we include only one representative error bar for each lattice size, $L = 16, 12, \ldots$ from right to left in the Fig. \[3\] (for $L \leq 8$ they are barely visible on the scale of the figure). For our data at $T = 1$ a similar analysis is already given in \[18\]. The small discrepancy in the estimates of the critical exponent $\beta/\nu$ ($0.255$ in \[18\] instead of $0.230$) is due to using different methods of data analysis. Note that the error bars of the $\beta/\nu$ estimates \[3\] and \[4\] reflect only the fluctuations of our two parameter fit and additional (systematic) errors are expected from corrections to scaling.

Our aim is to relate the probability distribution of Fig. \[2\] to the first asymptote of extreme order statistics,
the hyperbolic tangent function $\tanh(x/c)$ off and at decreasing $x$, while for the data of Fig. 2, the slope levels off and at $x = -b q'_{\text{max}}$ we have

$$d \ln[P'(q')] \bigg|_{q' = 0} = 0,$$

what is impossible with (4). A simple solution is to replace the first $x$ on the right-hand side of Eq. (4) by $c \tanh(x/c)$, where $c > 0$ is a constant. For small $x$ the Taylor expansion (3) still holds, while for large $|x|$ the hyperbolic tangent function $c \tanh(x/c)$ approaches quickly $\pm c$ (note that in the limit $c \to \infty$ the original form (3) is recovered). For $x \to -\infty$ (practically already at $q' = 0$) the thus modified Gumbel distribution becomes constant. Therefore, the symmetric expression for $P'(q')$ is obtained by multiplying the above construction with its reflection about the $q' = 0$ axis,
Figure 3 exhibits the finite-size effect that for \( q \) close to one the smaller lattices undershoot the larger ones. It is quite clear that something like this has to happen, because the data from each lattice size terminates at \( q = 1 \), whereas Eq. (11) has no corresponding singularity. When calculating our fit parameters, we take this into account by restraining our use of data to \( q' < 2 \), \( \ln[|P(q')|] > -43.4 \), for the \( T = 1.14, L = 16 \) lattice and to \( q' < 1.62 \), \( \ln[|P(q')|] > -25.6 \), for the \( T = 1, L = 12 \) lattice. The agreement of our fits with those data stretches then over considerably larger ranges. Discrepancies of the \( L = 16 \) data with the fit begin only around \( \ln[|P(q')|] = -200 \), and even this is only visible on a major enlargement of the scale of Fig. 3. Discrepancies of the \( T = 1, L = 12 \) lattice with the fit are encountered around \( \ln[|P(q')|] = -35 \). However, the \( T = 1.14, L = 12 \) data deviate already around \( \ln[|P(q')|] = -10 \) from the \( L = 16 \) data. This appears possible, because corrections to the \( L^{0.312} \) scaling factor are not traced by the accuracy of our data (in particular \( L = 16 \) has low statistics due to computer time limitations). Therefore, it is not entirely clear whether the large range which we find for the agreement of our fit with our \( L = 16 \) lattice is to some extent a statistical accident. Taking it at face value, we have the remarkable range of \( 200/\ln(10) \approx 87 \) orders of magnitude. An actually smaller range would still be large enough to give us confidence that we are dealing with a true effect.

Our coefficient \( a \) is far off from the 2D XY coefficient of Bramwell et al. [8], \( a = \pi/2 \). This means that the EAI and the 2D XY models are certainly in quite different universality classes of extreme order statistics. However, the fact that both distributions can be described by it at all might help to explain the observed similarities. Our temperature \( T = 1 \) is below the critical \( T_c \), but with our lattice sizes it appears impossible to resolve the question, whether the here reported behavior reflects the existence of a critical line below \( T_c \) or just the closeness of \( T = 1 \) to \( T_c \). Before comparing to extreme order statistics, we [18] tried to fit the \( q > q_{\text{max}} \) tails of our distributions to the theoretical predictions which have been made by Parisi and collaborators [21, 23] based on the replica mean-field approach. None of these fits was particularly good and even when pushing the adjustment of free parameters to their limits only small parts of the tails of our distributions could be covered.

In summary, we have presented strong numerical evidence that the Parisi overlap distribution of the EAI model can be described by Eq. (11). The detailed relationship between the EAI model and extreme order statistics remains to be investigated and it is certainly a challenge to extend the work of Bouchaud and Mézard [8] to the more involved scenarios of the replica theory. On the other hand, it could be that replica symmetry breaking is not the driving mechanism of the EAI model phase transition and that our observations are rooted in general relations between correlated systems and extreme order statistics.

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