Overcoming System-Size Limitations in Spin Glasses

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In order to overcome the limitations of small system sizes in spin-glass simulations, we investigate the one-dimensional Ising spin chain with power-law interactions. The model has the advantage over traditional higher-dimensional Hamiltonians in that a large range of system sizes can be studied. In addition, the universality class of the model can be changed by tuning the power law exponent, thus allowing us to scan from the mean-field to long-range and short-range universality classes. We illustrate the advantages of this model by studying the nature of the spin glass state where our results hint towards a replica symmetry breaking scenario. We also compute ground-state energy distributions and show that mean-field and non-mean-field models are intrinsically different.

§1. Introduction

Because spin glasses are generally equilibrate very slowly due to their glassy behavior, simulations can usually only be performed on small system sizes. The introduction of novel algorithms, such as exchange Monte Carlo (parallel tempering),[1),2)] have helped considerably to overcome these system-size limitations. Nevertheless, in general, only modest system sizes can be simulated at temperatures well below the critical temperature. In what follows we introduce the one-dimensional Ising chain with random power-law interactions in order to simulate large length scales. We illustrate the advantages of this model with two applications: the nature of the spin-glass state and ground-state energy distributions in spin glasses.

§2. Model and numerical method

The Hamiltonian for the one-dimensional (1D) long-range Ising spin glass with power-law interactions is given by[3)–5)]

$$\mathcal{H} = -\sum_{i,j} J_{ij} S_i S_j \ , \qquad J_{ij} \sim \frac{\epsilon_{ij}}{r_{ij}^{\sigma}} \ , \qquad \mathcal{P}(\epsilon_{ij}) = \frac{1}{\sqrt{2\pi}} \exp(-\epsilon_{ij}^2/2) \ , \qquad (2\cdot1)$$

where the sites i lie on a ring of length L to ensure periodic boundary conditions, and $S_i = \pm 1$ represent Ising spins. The sum is over all spins on the chain and the couplings J_{ij} are Gaussian distributed, and divided by the geometric distance between the spins to a power σ. The model has a rich phase diagram in the d–σ plane:[5)] For $\sigma < 0.5$ the model is in the mean-field phase with an SK universality class, for $0.5 \le \sigma \le 1.0$ the model has long-range critical exponents with a finite transition temperature $T_{\rm c}$, whereas $T_{\rm c} = 0$ for $1.0 < \sigma \lesssim 1.75$. For $\sigma \gtrsim 1.75$, again $T_{\rm c} = 0$ but in a short-range universality class. In addition, there is a prediction from droplet arguments[3),4)] that $\theta = d - \sigma$, where θ is the stiffness exponent for domain-wall excitations.

For all of our simulations, we use the parallel tempering Monte Carlo method[1),2)] as it allows us to study larger systems (up to $L = 512$) at very low temperatures. Details about the simulations as well as equilibration tests can be found in Refs. 5),6).

§3. Applications

3.1. *Nature of the spin-glass state*

Two main theories attempt to describe the nature of the spin-glass state: The replica symmetry-breaking (RSB) picture and the "droplet picture" (DP). RSB predicts that droplet excitations involving a finite fraction of the spins cost only a finite energy in the thermodynamic limit, and that the surface of these excitations has a fractal dimension d_s equal to the space dimension d. In the DP, excitations have an energy proportional to ℓ^θ, where ℓ is the characteristic length scale of the droplet and θ is a positive stiffness exponent. In addition, the excitation surfaces are fractal with $d_s < d$.[*)] Differences between the various pictures can be quantified by studying[7),8)] $P(q)$, the distribution of the spin-glass overlap $q = L^{-1}\sum_{i=1}^{L} S_i^\alpha S_i^\beta$, where "$\alpha$" and "$\beta$" refer to two replicas of the system with the same disorder. The RSB picture predicts a nontrivial distribution with a finite weight in the tail around $q = 0$, independent of system size. In contrast, the droplet picture predicts that $P(q)$ is trivial in the thermodynamic limit with only two peaks at $\pm q_{\rm EA}$, where $q_{\rm EA}$ is the Edwards-Anderson order parameter. For finite systems there is also a tail down to $q = 0$, which vanishes in the thermodynamic limit like[9),10)] $P(0) \sim L^{-\theta'}$ with $\theta' = \theta$.[**)]

Figure 1, left panel, shows data for $P(q)$ at $\sigma = 0.75$ and $T = 0.10$, well below $T_{\rm c} \approx 0.62$.[5),11)] There is a peak for large q and a tail down to $q = 0$ that is independent of system size. A more precise determination of the size dependence of $P(0)$ is shown in the inset of Fig. 1, left panel, where, to improve statistics, we average over q values with $|q| < 0.50$. The expected behavior in the droplet model is $P(0) \sim L^{-\theta'}$, with $\theta' = \theta$ where[3),4)] $\theta = d - \sigma$. The dashed line has slope -0.25, the expected value for $\sigma = 0.75$ according to the droplet model. The size dependence is consistent with a constant $P(0)$, which implies that the energy to create a large excitation does not increase with size, at least for the range of sizes studied here. In Ref. 6) we estimate the fractal dimension d_s of the system-size excitation surfaces and we find that $d_s \geq 0.95 \pm 0.05$, i.e., $d_s \approx d$, in agreement with RSB.

Since there are analytic predictions for the stiffness exponent of the 1D chain ($\theta = d - \sigma$), and the droplet picture predicts $\theta = \theta'$, we compute θ directly from zero-temperature domain-wall calculations for different values of σ using parallel

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[*)] Recently Krzakala and Martin, as well as Palassini and Young, suggest an intermediate picture in which droplets have a fractal surface, and their energy is finite in the thermodynamic limit. See Ref. 5) and references therein for details.

[**)] Note that we explicitly distinguish between θ', the stiffness exponent for droplet excitations, and θ, the exponent for domain walls, because DP predicts $\theta = \theta'$, which we want to test here.

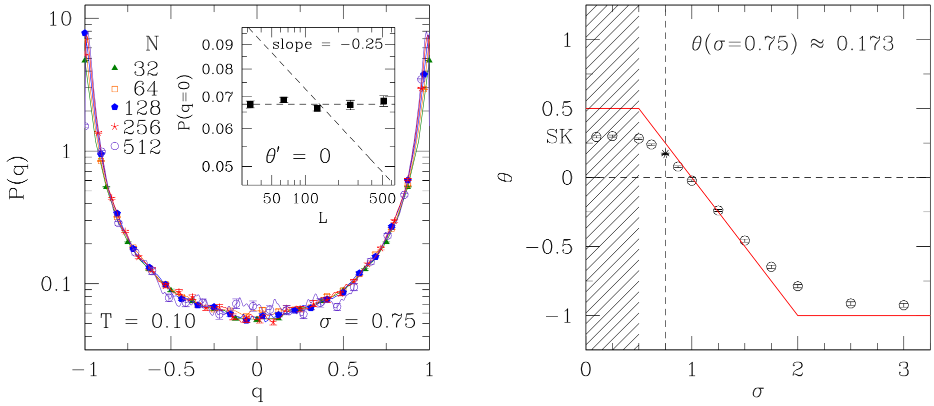

Fig. 1. Left panel: Distribution of the spin overlap $P(q)$ at $T = 0.10$ and $\sigma = 0.75$ (T_c finite, long-range universality class) for several system sizes L. The data are independent of L at $q \sim 0$, indicating that $\theta' = 0$. This is shown in detail in the inset where $P(0) \sim L^{-\theta'}$ is plotted as a function of L together with the prediction from the droplet model (dashed line with slope $-\theta = -(1-\sigma) = -0.25$). Right panel: Stiffness exponent θ as a function of σ at $T = 0$ from domain-wall calculations. The data follow well the prediction of the droplet picture $\theta = d - \sigma$ (solid line). The star ("$*$") marks $\sigma = 0.75$, where $\theta = 0.173 \pm 0.005$, which disagrees with $\theta' = 0$ from finite-temperature calculations (left panel). The dashed lines are guides to the eye. Note also that $\theta \to 0.3$ for $\sigma \to 0$, the Sherrington-Kirkpatrick (SK) model limit.

tempering as an optimization algorithm.[5),6),12)] The change in energy ΔE induced by a change in boundary conditions from periodic (P) to antiperiodic (AP) scales as $\Delta E = [|E_{AP} - E_P|]_{av} \sim L^{\theta}$, where $[\cdots]_{av}$ represents a disorder average. Data for $\theta(\sigma)$ are shown in Fig. 1, right panel. The solid line represents the prediction from the droplet model, well followed by the data. For $\sigma = 0.75$ ("$*$" in Fig. 1) there is a clear positive stiffness exponent: $\theta(\sigma = 0.75) = 0.173 \pm 0.005$. This is in contrast to $\theta' = 0$ from finite-temperature simulations (Fig. 1, left panel). Therefore we find a disagreement with the droplet model in that $\theta' \neq \theta$ for *a large range of sizes.*

3.2. *Ground-state energy distributions*

There has been recent interest in how ground-state energy distributions scale in spin glasses. Considerable work has been done for the Sherrington-Kirkpatrick (SK) model[13)] where evidence for skewed energy distributions, well fitted by a modified Gumbel distribution[14)] with $m = 6$, is found. In order to test if these results are intrinsic to the mean-field SK model we compute ground-state energy distributions for the 1D chain for different system sizes and different values of σ. The advantage of the 1D chain is that the crossover from mean-field to short-range behavior can be probed for *a large range of sizes.*

In Fig. 2, left panel, we show rescaled ground-state energy distributions $P(E)$ with mean $\langle E\rangle$ and standard deviation σ_E. The data show a clear asymmetry. In order to quantify these effects we show data for the skewness ζ_E of the distributions as a function of system size L for different values of the power-law exponent σ in

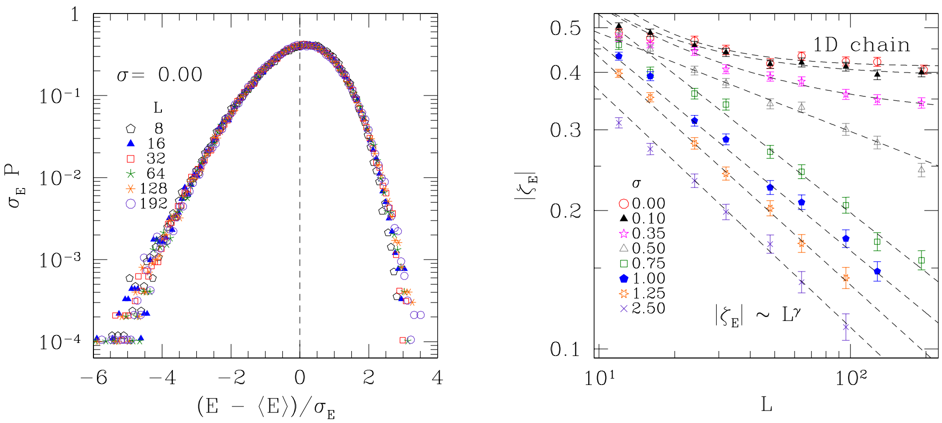

Fig. 2. Left panel: Rescaled ground-state energy distributions for $\sigma = 0.00$ (SK limit) as a function of system size L (10^5 samples). The data are clearly asymmetric; the dashed line is a guide to the eye. Right panel: Skewness ζ_E as a function of L for different values of σ. In the mean-field region ($\sigma < 0.5$) the $\zeta_E \to$ const. for $L \to \infty$. For $\sigma \geq 0.5$ the distributions become symmetric in the thermodynamic limit ($\zeta_E \sim L^\gamma$, $\gamma < 0$).

Fig. 2, right panel. One can see that for $\sigma < 0.5$, where the model exhibits mean-field behavior, the skewness tends to a constant in the thermodynamic limit, indicating that the skewness of the distribution persists even for infinitely large system sizes. For $\sigma \geq 0.5$, the skewness decays with a power law of the system size, indicating that in the non-mean field region the ground-state energy distributions become symmetric in the thermodynamic limit. This shows that mean-field and non-mean field models are expected to behave differently, and that, in particular, intrinsic length scales in the mean-field model seem to scale with system size.

§4. Conclusions

By using a one-dimensional Ising spin glass with power law interactions, we have been able to overcome the usual limitation of small system sizes in spin-glass simulations. We illustrate the advantages of the model on the nature of the spin-glass state where we show that droplet and domain-wall excitations scale differently for large system sizes, indicating that the droplet model cannot be correct, at least for the 1D chain. In addition, we compute the ground-state energy distributions for the one-dimensional Ising chain and show that, in the mean-field regime, energy distributions remain skewed in the thermodynamic limit indicating that mean-field and non-mean-field models behave differently. Our results are in agreement with previous results for the SK model ($\sigma = 0$). In the future, we intend to study energy distributions at finite temperature, as well as the effects of degenerate ground states.

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