Spin and chiral stiffness of the XY spin glass in two dimensions

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Abstract. We analyze the zero-temperature behavior of the XY Edwards-Anderson spin glass model on a square lattice. A newly developed algorithm combining exact ground-state computations for Ising variables embedded into the planar spins with a specially tailored evolutionary method, resulting in the *genetic embedded matching* (GEM) approach, allows for the computation of numerically exact ground states for relatively large systems. This enables a thorough re-investigation of the long-standing questions of (i) extensive degeneracy of the ground state and (ii) a possible decoupling of spin and chiral degrees of freedom in such systems. The new algorithm together with appropriate choices for the considered sets of boundary conditions and finite-size scaling techniques allows for a consistent determination of the spin and chiral stiffness scaling exponents.

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1. Introduction

With their rich behavior at low temperatures, spin glasses take a prominent role in the large class of magnetic systems with frustration. The most commonly considered Hamiltonian is that of the Edwards-Anderson (EA) model [1],

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

with O(n) spins $\boldsymbol{S}_i$ and random, nearest-neighbor couplings J_{ij}. The wealth of behavior of these systems is attributed to the random disorder augmenting the frustration effects. Unfortunately, it is precisely this *quenched* disorder that provides an exceptional challenge for the application of the various analytical approximation methods well known from the treatment of homogeneous systems. Owing to these difficulties, most of the advances in the understanding of spin glass systems beyond the celebrated mean-field theory of the Sherrington-Kirkpatrick model [2] have been on account of ever more sophisticated numerical simulation and optimization techniques [1]. For two-dimensional (2D) systems, where for short-range interactions spin glass order is restricted to zero temperature, the investigation of ground states is of prominent interest. In general, finding (exact) ground states of spin glass models is a computationally hard problem, where the amount of computer time grows exponentially with the size of the system [3]. Here, we explore a new avenue to advance methods for the so far much less investigated case of systems with *continuous spins*: we introduce a novel approximate optimization algorithm which, for the 2D XY spin glass discussed here, allows to find numerically exact ground states with good confidence for systems of up to about 30×30 spins [4, 5].

Generalizing Peierls' argument for the stability of the ordered phase in homogeneous systems to situations with quenched disorder, a droplet scaling theory for spin glasses has been formulated [6]. Therein, the role of the droplet surface (free) energy is taken on by the *width* $J(L)$ of the distribution of random couplings for a real-space renormalization group decimation at length scale L. In the course of renormalization, $J(L)$ scales as $J(L) \sim L^{\theta_s}$, defining the *spin stiffness exponent* θ_s. If the system scales to weak coupling, $\theta_s < 0$, spin-glass order is unstable at finite temperature and the system is below its lower critical dimension. This is the situation for the EA model in 2D [1], where then θ_s describes the properties of the *critical* point at temperature $T = 0$, relating the correlation length exponent $\nu = -1/\theta_s$ [6]. Numerically, the domain-wall free energy might be determined from the energy difference between ground states of systems with different types of boundary conditions (BCs) chosen such as to induce a relative domain wall [6]. For the $n = 1$ Ising spin glass, the ground-state problem on planar graphs is an exception to the rule, being polynomial computationally [3]. Hence, large systems can be treated, leading to reliable estimates of $\theta_s = -0.282(2)$ (Gaussian J_{ij}) resp. $\theta_s = 0$ (bimodal J_{ij}) [1, 7]. Due to the presence of strong finite-size corrections, relatively large system sizes and/or elaborate finite-size scaling techniques appeared mandatory for consistent estimates of θ_s [7, 8]. However, for the case $n > 1$ of continuous spins, which is more relevant to real materials, the lack of effective and efficient algorithms for finding exact ground states and the necessary restriction to small systems with $L \leq 12$ have led to rather less consistent estimates, moving in the range $\theta_s \in [-1, -0.75]$ [9–11].

Moreover, the increased symmetry of the order parameter in the continuous spin case has led to speculations about a decoupling of spin and chiral variables [12]: since the pattern of frozen spins in the glassy phase has internal degrees of freedom, there is a factual difference between proper and improper rotations expressed in the decomposition $\mathrm{O}(n) = \mathrm{SO}(n) \times \mathbb{Z}_2$ [13]. The additional Ising like chirality variables might order independently of the spins (for systems above their lower critical dimension) or, at least, show a different stiffness against fluctuations, resulting in a scaling exponent θ_c possibly distinct from θ_s. Indeed, measurements of the chiral stiffness for small systems yielded $\theta_c \approx -0.38$ [10, 11], different from θ_s above. More recently, however, Kosterlitz and Akino [14] argued that the choice of BCs in previous studies was flawed and they suggest a possibly more appropriate approach leading to $\theta_s \approx -0.38 \approx \theta_c$ again for sizes $L \leq 10$. The hardly compatible previous results for this system hence raise several methodological questions: have numerically exact ground states been found?, are the apparent strong finite-size effects under control?, have the considered sets of BCs been chosen such as to properly select the intended excitations?, and what is the role of scaling corrections explicitly depending on these BCs?

2. Genetic embedded matching approach

The treatment of large samples for the 2D Ising case is enabled by a transformation to an equivalent problem on the complete graph of frustrated plaquettes: following their definition, for each spin configuration frustrated plaquettes have an odd number of broken bonds around their perimeter, whereas unfrustrated plaquettes have an even number of broken bonds. Thus, drawing "energy strings" dual to the broken bonds, these connect pairs of frustrated plaquettes, and the total energy of (1) is (up to a constant) given by the total length of energy strings, such that the ground state corresponds to a *minimum-weight perfect matching* of frustrated plaquettes [3]. The matching problem can be solved in polynomial time using Edmonds' algorithm [15], and for the case of planar graphs its solution is guaranteed to transform back to a valid spin configuration [16]. This does not directly apply to the continuous spins considered here. We suggest, however, to *embed* Ising variables into the planar spins by decomposing $\boldsymbol{S}_i = \boldsymbol{S}_i^{\parallel} + \boldsymbol{S}_i^{\perp} = (\boldsymbol{S}_i \cdot \boldsymbol{r})\boldsymbol{r} + \boldsymbol{S}_i^{\perp}$ relative to a random direction $\boldsymbol{r}$ in spin space. With respect to reflections of spins along the direction $\boldsymbol{r}$, the Hamiltonian (1) decomposes as $\mathcal{H} = \mathcal{H}^{r,\parallel} + \mathcal{H}^{r,\perp}$ with $\mathcal{H}^{r,\parallel} = -\sum_{\langle i,j\rangle} \tilde{J}_{ij}^r\, \epsilon_i^r \epsilon_j^r$, and

$$\tilde{J}_{ij}^r = J_{ij}|\boldsymbol{S}_i \cdot \boldsymbol{r}||\boldsymbol{S}_j \cdot \boldsymbol{r}|, \quad \epsilon_i^r = \mathrm{sign}(\boldsymbol{S}_i \cdot \boldsymbol{r}). \tag{2}$$

Hence, for any fixed $\boldsymbol{r}$ and restricting the movement of spins to reflections along $\boldsymbol{r}$, the Hamiltonian (1) for arbitrary $n > 1$ takes on the form of an Ising model. Consequently, Edmonds' algorithm can be applied to find (one of) the ground state(s) of the embedded Ising model. It is obvious that this can never increase the energy of the full Hamiltonian (1), but the state found depends on the choice of random direction $\boldsymbol{r}$. To statistically recover the full $\mathrm{O}(n)$ symmetry of the Hamiltonian, a series of subsequent minimizations is performed with respect to successive random choices of $\boldsymbol{r}$, thus gradually decreasing the total energy via non-local moves. We refer to this approach as *embedded matching* technique.

It can be shown that, although when the full Hamiltonian (1) is in a ground state, all embedded Ising Hamiltonians $\mathcal{H}^{r,\parallel}$ must be in one of their respective ground states as well, successive minimizations with respect to random directions $\boldsymbol{r}$ are not guaranteed to drive the system towards its absolute energy minimum. In other words, the non-local embedded matching dynamics has metastable states, but many less than the simple local spin quench dynamics used before [9, 11]. To converge to ground states with high probability, we insert the embedded matching technique as minimization component ("subroutine") in a genetic algorithm [17]: we consider a whole population of candidate ground-state configurations and simulate an evolutionary development by re-combining (or *crossing over*) neighboring pairs of parent configurations followed by minimization runs for the resulting offspring and replacement of the parents in case of lower energy of the offspring. In analogy with the approach of Ref. [17], the crossover is performed in a "triadic" fashion, comparing the overlaps with a third, reference configuration. This layout is complemented by intermittent random mutation steps and performance-guided halving of the population at certain stages to find an optimum balance between "genetic" diversity and efficiency of optimization [17]. The choice of operation for the crossover of configurations is found to be crucial for the efficiency of the approach: it turns out that a random exchange of suitably defined rigid spin clusters is far more efficient than an exchange of single spins. These clusters denote regions which are highly optimized inside for all configurations of the population (i.e., metastable states), but which have to undergo a series of independent rigid $\mathrm{O}(n)$

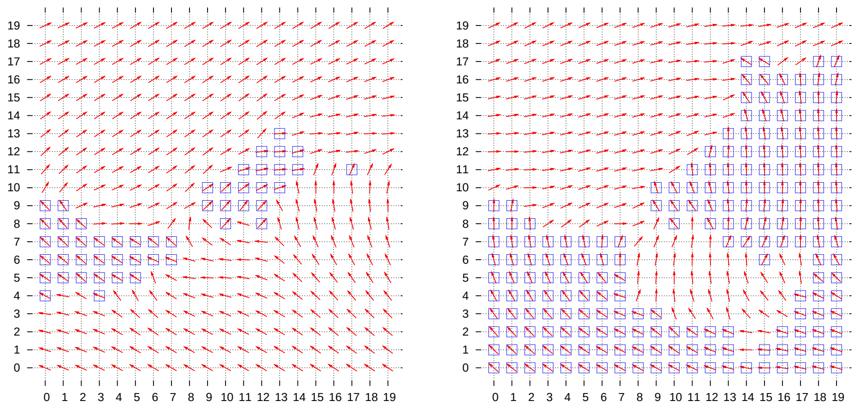

Figure 1. Local rotation matrices between the ground states for a single 20×20 disorder realization with open boundaries relative to domain-wall BCs for spin (left) and chiral (right) excitations.

transformations to make up a true ground state of the system. Careful choice of the parameters of the resulting *genetic embedded matching* (GEM) algorithm and application of various statistical tests ensure that indeed independent runs for a single given realization of the disorder variables J_{ij} always converge to a state of the same energy, up to unprecedented machine precision, which in this way can be guaranteed to be a ground state with high reliability [4, 5].

We here concentrate on the symmetric, bimodal $\pm J$ distribution. For this case we find that the ground states computed in independent runs for a single disorder realization are always identical to each other up to a global $\mathrm{O}(n)$ transformation, indicating the lack of accidental degeneracies in contrast to what is found for the bimodal Ising case. Hence, after averaging over disorder, the ground state is ordered and the ground-state spin correlation function is constant, implying $\eta = 0$. To determine the asymptotic ground-state energy per spin e_∞, ground-states were computed for $L \times L$ square-lattice systems with $L = 6$, 8, 10, 12, 16, 20, 24, and 28 for open and open-periodic BCs and 5 000 disorder replica per size. Finite-size corrections are expected to be purely analytic for the case of open BCs [18], and a fit to the ansatz $e(L) = e_\infty + a/L + b/L^2 + c/L^3$ yields $e_\infty = -1.5520(14)$ with quality-of-fit $Q = 0.35$. For the open-periodic case, an additional non-analytic term $\propto L^{-(d-\theta)}$ is expected to occur [18], and a fit of the corresponding data to the form $e(L) = e_\infty + a/L + b/L^{2-\theta}$ gives $e_\infty = -1.5525(13)$, $\theta = -0.49(69)$, $Q = 0.35$, perfectly consistent with the open-boundary result for e_∞ and, due to the large statistical error, only in qualitative agreement with the expected value for the spin-stiffness exponent θ. The resulting e_∞ is about 10% lower than the value $e_\infty = -1.402$ of the bimodal Ising spin-glass [18].

3. Spin and chiral stiffness exponents

Conventionally, domain-wall energies have been measured by comparing ground states for periodic and antiperiodic (P/AP) BCs [9–11]. In Ref. [14] it was argued, however, that the periodicity in both types of BCs forces domain walls into the system, such that the corresponding energy difference might not properly capture the energy of a single domain wall. There, an improvement is suggested by optimizing over an

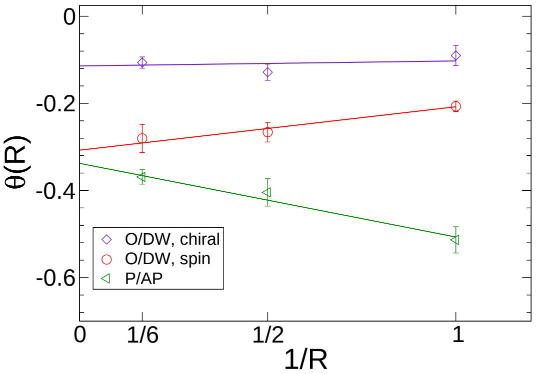

Figure 2. Aspect-ratio scaling of the stiffness exponents θ_s and θ_c for aspect ratios $R = 1$, 2 and 6 as a function of $1/R$.

additional global twist variable along the boundary under consideration. Here, to start with the cleanest possible setup, in addition to the conventional P/AP BC set, we consider open and domain-wall (O/DW) BCs, where for the latter the relative orientations of spins linked across the boundary are either tilted by an angle π for spin domain walls or reflected along an arbitrary but fixed axis for chiral domain walls by the introduction of very strong bonds [5, 7]. In Figure 1 we show snapshots of spin and chiral excitations forced into the system by the O/DW BCs. To this end, we computed a locally averaged O(2) rotation matrix relating the configurations with O and DW BCs and translated it back into a rotation angle (the arrows) and the sign of the determinant (-1 for the blue squares). It is apparent that in contrast to the discrete Ising case the spin domain walls are rather smeared out and that to a certain extent the system appears to relax the spin excitation also through the chiral mode if it is found to be softer locally (and vice versa for the chiral excitation).

From the scaling of the domain-wall energies, $[|\Delta E|]_J \sim L^\theta$, we find a strong crossover for the P/AP data from $\theta_s = -0.724(21)$ for $L \leq 12$ to $\theta_s = -0.433(26)$ for $L \geq 16$, indicating large finite-size effects and a movement from the value found for small P/AP computations in previous works [9–11] towards the "optimum twist" value of Ref. [14]. The O/DW BCs, on the other hand, yield $\theta_s = -0.207(12)$ for spin excitations resp. $\theta_c = -0.090(23)$ for the chiral domain walls. Hence, although it is already clear that the true stiffness exponents are much less negative than estimated before, there is still a sizable difference between the P/AP and O/DW results for θ_s, indicating incomplete control over finite-size effects. To improve on this, we take into account that, due to the independence of BCs for systems in one dimension, corrections depending on BCs should disappear as more and more elongated systems are being considered [8]. Thus, we additionally performed computations for $L \times M$ systems (the change of BCs happening along the edges of length L) with aspect ratios $R \equiv M/L = 2$ and 6 with the same statistics. The results are presented in Figure 2 for the case of P/AP and O/DW BCs, respectively. Guided by the experience from the Ising case, we expect corrections depending on BCs to disappear as $\theta(R) = \theta(R\!=\!\infty) + A_R/R$ for large R, and indeed the P/AP and O/DW spin data seem to converge for large R, a fit to the given form yielding $\theta_s(R = \infty) = -0.338(20)$ for P/AP BCs and $\theta_s(R\!=\!\infty) = -0.308(30)$ for O/DW BCs. The O/DW chiral data, on the other hand, give $\theta_c(R = \infty) = -0.114(16)$, clearly distinct from θ_s.

4. Conclusions

Employing a novel "genetic embedded matching algorithm", we computed numerically exact ground states for the 2D XY EA spin glass with $\pm J$ couplings and up to 28×28 spins. No accidental degeneracies occur, implying $\eta = 0$. Analyzes of the domain-wall energies are hampered by strong finite-size effects which, however, can be controlled using the aspect-ratio scaling technique. We find consistent estimates of $\theta_s = -0.308(30)$ from different sets of BCs, clearly smaller in modulus than previous estimates [9–11, 14], and rather close to $\theta_s = -0.28$ found for the *Gaussian* 2D Ising case. The chiral exponent $\theta_c = -0.114(16)$, on the other hand, is found to be clearly different from θ_s and closer to $\theta_s = 0$ found for the *bimodal* 2D Ising spin glass. Note also, that our results are rather far from $\theta_s = -1/\nu_s = -1.0$ resp. $\theta_c = -1/\nu_c = -0.5$ estimated by finite-temperature Monte Carlo simulations [19], which probably is due to equilibration problems at low temperatures.

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