Droplets in the two-dimensional $\pm J$ Ising spin glass

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Using problem-dependend mappings to computer-science problems and by applying sophisticated algorithms, one can study numerically some important problems much better compared to applying standard approaches like Monte-Carlo simulations. Here, using calculations of ground states of suitable perturbed systems, droplets are obtained in two-dimensional $\pm J$ spin glasses, which are in the focus of a currently very lively debate. Using a sophisticated matching algorithm, exact ground states of large systems up to $L^2 = 256^2$ spins can be generated. Furthermore, no equilibration or extrapolation to $T = 0$ is necessary. Three different $\pm J$ models are studied here: a) with free boundary conditions, b) with fixed boundary conditions and c) a diluted system where a fraction $p = 0.125$ of all bonds is zero. For large systems, the droplet energy shows for all three models a power-law behavior $E_{\rm dp} \sim L^{\theta'_{\rm dp}}$ with $\theta'_{\rm dp} < 0$. This is different from previous studies of domain walls, where a convergence to a constant non-zero value ($\theta_{\rm dw} = 0$) has been found. After correcting for the non-compactness of the droplets, the results are likely to be compatible with $\theta_{\rm dp} \approx -0.29$ for all three models. This is in accordance with the Gaussian system where $\theta_{\rm dp} = -0.287(4)$ ($\nu \approx 3.5$ via $\nu = -1/\theta_{\rm dp}$). Nevertheless, the disorder-averaged spin-spin correlation exponent η is determined here via the probability to have a non-zero-energy droplet, and $\eta \approx 0.22$ is found for all three models, in contrast to the the model with Gaussian interactions, where $\eta = 0$ is exact.

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Monte Carlo simulations [1, 2] and related approaches are very useful ways to study physical systems numerically, in particular for the usual case where no exact analytic solution can be provided. So far, it has only occasionally been recognized that by using problem-dependent mappings to computer-science problems and by applying sophisticated algorithms, in many cases one can obtain results which are superior in comparison to using standard algorithms.

Here, Ising spin glasses are considered, which are the most-frequently studied systems in statistical physics [3–6]. However, despite more than two decades of intensive research, many properties of spin glasses, especially in finite dimensions, are still not well understood. For two-dimensional spin glasses it is now widely accepted that no ordered phase for finite temperatures exists [7–10] in this case. Nevertheless, the $\pm J$ model with a bimodal distribution of the interactions is in the center of a currently very lively debate [10–21], in particular whether the behavior is equivalent to that of the model with a Gaussian distribution of the interactions. One central question is whether the correlation length, when approaching $T_c = 0$, diverges algebraically [22] $\sim T^{-\nu}$, as for the Gaussian model, or like an exponential [23] $\sim T^{-2}e^{-C/T}$, formally equivalent to $\nu = \infty$. In particular, Ref. 18 claims evidence for a power-law divergence with the same critical exponent $\nu \approx 3.5$ as the Gaussian system, and that the spin-spin correlation exponent $\eta = 0$. This exponent is defined via $[\langle S_i S_{i+l}\rangle^2]_J \sim l^{-\eta}$, $[\ldots]_J$ and $\langle\ldots\rangle$ being the averages over the quenched disorder and the thermal average, respectively.

Unfortunately, most of the above cited work is based on finite-temperature calculations, in particular Monte Carlo simulations, hence an extrapolation $T \to T_c = 0$ is necessary. Also the systems are restricted in most cases to rather small sizes $L \leq 64$. Only in the case, where parallel tempering Monte Carlo simulations [16, 21] or the worm algorithm [15] have been used, sizes $L \leq 128$ could be considered. Consequently, in Ref. 21 it has been shown that the presently available finite-temperature data does not allow to draw definite conclusions. In Ref. 14 also exact $T = 0$ properties are calculated (up to $L = 128$ for $L \times L$ systems and up to $L = 64$ for $9L \times L$ systems), but only the spin-spin correlation could be obtained by this approach.

Here, we go much beyond the previous work. Exact ground-state (GS) calculations [24] are applied, which allows us to obtain GSs [10, 25–27] for large systems like $L = 480$. The method relies on mapping the GS calculation to a graph-theoretical problem and using sophisticated algorithms developed in computer science. By using suitable perturbations of the original systems, one can go beyond pure GS calculations and study excitations like domain walls (DWs) [10, 25] and droplets [26, 27]. Hence, large systems in exact equilibrium can be investigated and no extrapolation to $T = 0$ is necessary.

In Refs. [10, 25–27] this approach has been used to show that for the two-dimensional spin glass with Gaussian disorder all assumptions made by the droplet theory [28–31] are fulfilled. In particular the energy scaling of the basic excitations DWs and droplets follows power laws $E_{\rm dw} \sim L^{\theta_{\rm dw}}$ and $E_D \sim L^{\theta_D}$, respectively, with the same universal value $\theta \equiv \theta_{\rm dp} = \theta_{\rm dw}$, which is related [32] to the correlation-length exponent via $\theta = -1/\nu = -0.287(4)$. On the other hand, for the $\pm J$ model, the average energy of DWs approaches a constant for large system sizes [10] $L \geq 128$, i.e. $\theta_{\rm dw} = 0$. This appears to be, via $\theta = 1/\nu$, compatible with an exponential divergence of the correlation length, if either the low-temperature behavior is dominated by DWs, or if the scaling of the energy of droplets, which are expected to be the dominant excitations, is the same as for DWs.

In this work, droplet excitations for three different models with discrete distributions of the interactions are calculated using an approach which is based on exact GS calculations. This approach allows us to consider large systems up to $L = 256$. No extrapolation of the temperature and no equilibration are necessary. The main result is that the scaling behavior is different from the scaling of DWs, i.e. $\theta_{\rm dp} < 0$. This is compatible with a power-law divergence of the correlation length, as recently claimed [18]. After correcting for the non-compactness of the droplets [33], in all three cases the results seem to be the same as for the Gaussian model. Hence Gaussian and discrete models appear to be in the same universality class regarding the low-temperature behavior. Furthermore, in this work the scaling of the spin-spin correlation function is studied, resulting in $\eta \approx 0.22$ for all three models.

The Hamiltonian which is studied here is the usual Ising spin glass model: $\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j$, whith the $N = L^2$ spins $S_i = \pm 1$ located on the sites of a square lattice, the bonds J_{ij} couple nearest-neighbor sites on the lattice. $J_{ij} = \pm J$ with equal probability for the quenched realizations of the disorder. Here systems with either free boundary conditions (bc) in all directions, for the initial GS calculation, or fixed bc [34] always are studied. For the latter case, also diluted samples are considered, where each bond is set to zero with probability $p = 0.125$;

Here, droplets are considered, as introduced by Kawashima [33], which are lowest-energy excitations with respect to the GS. They consist of a connected cluster of spins, which include a center spin of the system. The spins at the boundary are fixed to their GS orientations, because otherwise one would always obtain a configuration with all spins reversed. The energy scaling of these droplets is expected to follow a $L^{\theta'_{\rm dp}}$ scaling, where [33] $\theta'_{\rm dp} = \theta_{\rm dp} D_V / D$ is related to the volume fractal dimension D_V of the droplets, the dimension $D = 2$ of the system and the usual droplet exponent $\theta_{\rm dp}$. The main approach used here is based on mapping [35–37] the GS calculation to the *minimum-weight perfect matching problem* and using sophisticated matching algorithms from graph theory. For details, please see the pedagogical description in Ref. 24. The droplet calculation of each disorder realization is based on a sequence of $2L$ suitable modifications of the disorder, each time followed by a GS calculation. The details of the algorithm [38] are described extensively in Refs. [26, 27].

Minimum-energy droplets have been obtained using the aforementioned approach for system sizes $L = 6$ to $L = 256$ ($L = 160$ for the fixed bc). All results are averages over many disorder realizations, the number of realizations is between 20000 for small sizes and 5000 for the largest sizes.

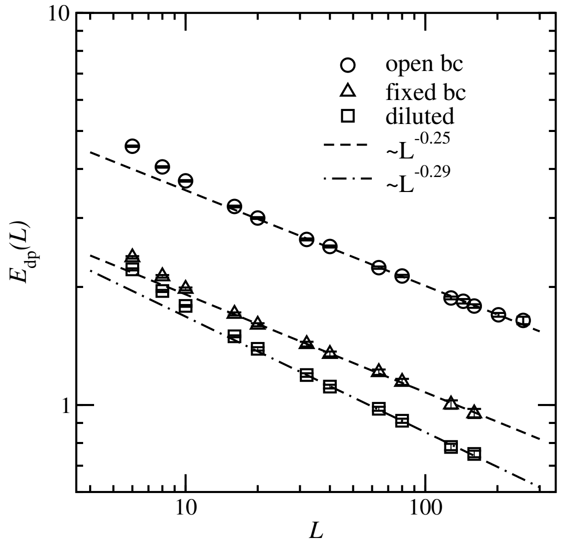

FIG. 1: Average droplet energy $E_{\rm dp}$ as a function of system size in a double logarithmic plot. The dashed lines show the results of fits to a simple power laws.

In Fig. 1 the average droplet energy $E_{\rm dp}$ is shown as a function of system size L. For large system sizes, a power-law behavior is visible. This corresponds [32] to a power-law divergence of the correlation length as observed recently by Jörg et al [18], as in contrast to the behavior of DWs for the $\pm J$ model and other models exhibiting a quantized energy spectrum. A fit to the function $AL^{\theta'_{\rm dp}}$ for $L \geq 32$ yields $\theta'_{\rm D} = -0.244(6)$ for free bc with a good quality of the fit [39] $Q = 0.32$. Q denotes, under the assumption that the fitted function correctly models the data, the probability to obtain data deviating from the function as present or worse. Similarly, $\theta'_{\rm dp} = -0.250(6)$ ($Q = 0.82$) are obtained for fixed bc and $\theta'_{\rm dp} = -0.295(6)$ ($Q = 0.64$) for the diluted systems.

To obtain the droplet exponent θ, the geometric properties of the droplet volumes are considered next. In Fig. 2 the volume V of the droplets is shown as a function of the system size L for the three different models. Note that due to the degeneracy of the models, droplets with many different values for the volume are possible. The matching approach, when using randomized selections among equivalent alternatives within the algorithm, allows for every droplet to be calculated. With the present algorithms this cannot be controlled, i.e. it is not possible to sample GSs or droplets with the same weight/probability. This can be done only for small systems through complete enummeration. Here, the degeneracy is broken, by selecting the droplets with the smallest *surface* [40], hence the behavior of the volume is not controllable and can give only a rough idea of the true behavior. When fitting a power law $\sim L^{D_V}$ to $V(L)$ of the

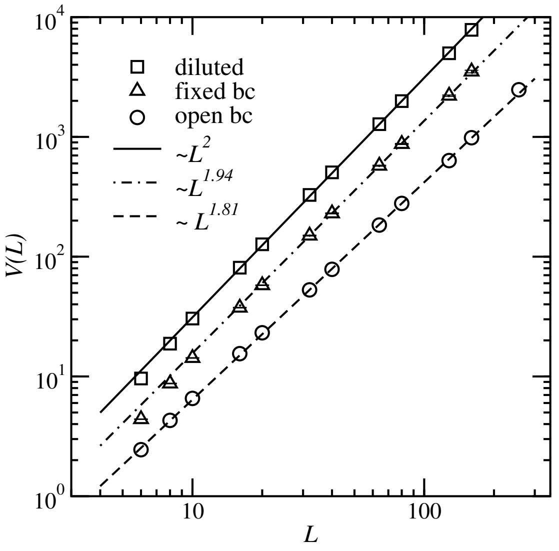

FIG. 2: Volume V of the droplets as a function of the system size, respectively. Error bars are smaller than symbol sizes. The lines show the results of power-law fits of $\sim L^{D_V}$ to $V(L)$ with $D_V = 1.81$, $D_V = 1.94$ and $D_v = 2$ for free bc, fixed bc, and the diluted system, respectively. The data for the diluted system has been shifted up by a factor of 2, for better visibility.

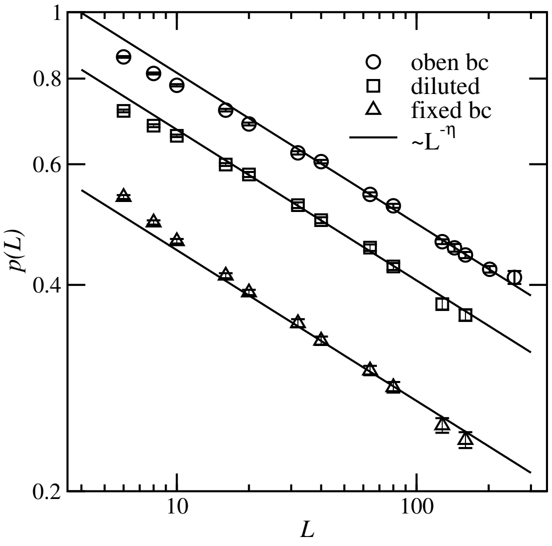

FIG. 3: Probability $p(L)$ that a droplet has non-zero energy as a function of system size in a double logarithmic plot, for free bc, fixed bc and the diluted system, respectively. The lines show simple power laws $\sim L^{-\eta}$, with $\eta = 0.22$ in all three cases.

free bc model, one obtains $D_V = 1.81(1)$, $D_V = 1.94$ for fixed bc, while the behavior of the diluted system is compatible with $D_V = 2$. Via considering $\theta_{\rm dp} = \theta'_{\rm dp} D/D_V$, it appears likely that $\theta_{\rm dp} \approx -0.29$ universally for all three models. Since the low-temperature behavior is dominated by droplets, and not by DWs, this would mean the $\pm J$ models not only show a power-law behavior for the divergence of the correlation length like the Gaussian system, but exhibit the *same* value $\nu = -1/\theta_{\rm dp} \approx 3.5$ for the correlation-length exponent. In any case, even if ν could still be slight different for Gaussian and $\pm J$ Ising spin glasses, the results show unambiguously that the scaling behavior of droplets and DWs is different in the $\pm J$ case, the main reason [12] being the discreteness of the spectrum of excitations. This is opposed to the assumptions of the droplet theory [28–31], were the behavior of all types of excitations is governed by one single exponent $\theta = \theta_{\rm dp} = \theta_{\rm dw}$.

Finally, to determine η, the relation [29] $[\langle S_i S_{i+l}\rangle^2]_J = p(L)$ is used, where $p(L)$ is the probability to have a droplet with non-zero energy. In Fig. 3 $p(L)$ is shown as a function of system size. According droplet theory [29] one expects $p(L) \sim L^{-\eta}$. When fitting for system sizes $L > 32$, the combined results for all three cases lead to η= 0.22(2), showing the universality of this result. This makes it likely that also the behavior of the average droplet energy is universal, hence the differences observed in Fig. 1 are indeed through different fractal dimensions D_V. Note that if one related η to the probability that a non-zero-energy cross-system DW exists, one would assume $\eta = 0$ since the DW energy settles at a constant value for large systems [10], i.e. $\theta_{\rm dw} = 0$. Nevertheless, two spins are uncorrelated if there exists *any* zero-energy excitation separating them, hence one has to consider droplets as well, as performed here.

The result is compatible with $\eta = 0.28(4)$ obtained [41] from Monte Carlo simulations of small sizes, and with $\eta = 0.21$ obtained [42] from $T = 0$ transfer-matrix calculations of the correlation function for $L \leq 12$. A value $\eta = 0.138$ was found 16 via Monte-Carlo simulations for system sizes $L \leq 128$. A similar value $\eta = 0.14(1)$ has been obtained in Ref. 14. Note that within the approach [29] used here, it is assumed that different droplets are not correlated, hence the value of η may be slightly overestimated. On the other hand, the claim $\eta = 0$ of Ref. 18, which is based on an extrapolation $T \to 0$ for small systems $L \leq 64$, is clearly ruled out. Even more, fits of the actual data obtained in Ref. 18 yielded, depending on the fits, also values $\eta > 0$. Note that for the Gaussian model at exactly $T = 0$, we have $\eta = 0$, due to the uniqueness of the GS. Hence regarding this quantity, the two classes of models appear non-universal.

One can understand by a simple scaling argument, why DWs and droplets can behave differently in the $\pm J$ model. We denote by q_l the probability that a zero-energy DW exists in a system of size l. Since this probability approaches [10] a finite value $\tilde{q}$ for about $L \geq 100$, we can assume $q_l \approx \tilde{q}$ for simplicity. We look at the system at different scales $l = l_0^0, l_0^1, l_0^2, \ldots, l_0^k = L$ ($l_0 > 1$ arbitrary, $k = \ln L/\ln l_0$), where we can assume the different DWs are independent. A non-zero droplet exists only if on *all* scales no zero-energy closed DW exists, i.e. $p(L) = \prod_{i=0,\ldots,k} q_{l_0^i} \approx \tilde{q}^k = L^{-\eta}$ with $-\eta = \ln \tilde{q} / \ln l_0 < 0$. Hence, the probability for non-zero energy droplets decreases with a power-law (hence the mean droplet energy), while the probability for non-zero energy DWs (and the mean DW energy) saturates for $L \to \infty$.

To summarize, droplet excitations for three different variants of the two-dimensional $\pm J$ Ising spin glasses were studied. Here an advanced methodology from graph theory is used, based on mapping the GS calculation to the minimum-weight perfect matching problem, using sophisticated matching algorithms from computer science and studying sequences of suitable modified realizations of the disorder. This allows to treat at $T = 0$, without need for an extrapolation of the temperature, large systems up to $L = 256$ exactly. The average droplet energy shows a clear power-law behavior with exponent $\theta'_{\rm dp} < 0$. It appears likely that when taking the non-compactness of the droplets into account, the same droplet exponent $\theta_{\rm dp} \approx -0.29$ emerges for all three models studied here, and hence the same value $\nu = -1/\theta_{\rm dp} \approx 3.5$ as for the model with Gaussian disorder is obtained. On the other hand, the value $\eta \approx 0.22$ for the exponent describing the decay of the spin-spin correlations is obtained for all three models. This is clearly different from the Gaussian model, where $\eta = 0$. Remarkably, $\theta_{\rm dp} \neq \theta_{\rm dw} = 0$ can be explained by a simple scaling argument.

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