Size dependence of the internal energy in Ising and vector spin glasses

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(Dated: November 19, 2018)

We study numerically the scaling correction to the internal energy per spin as a function of system size and temperature in a variety of Ising and vector spin glasses. From a standard scaling analysis we estimate the effective size correction exponent $x$ at each temperature. For each system with a finite ordering temperature, as temperature is increased from zero, $x$ initially decreases regularly until it goes through a minimum at a temperature close to the critical temperature, and then increases strongly. The behavior of the exponent $x$ at and below the critical temperature is more complex than suggested by the model for the size correction that relates $x$ to the domain-wall stiffness exponent.

PACS numbers: 75.50.Lk, 05.50.+q, 75.40.Mg

Since Gibbs, thermodynamic transitions have been classified according to the critical behavior of the specific heat, or equivalently of the critical temperature dependence of the internal energy. One of the disturbing features of the spin-glass transition has always been that there appears to be no thermodynamic signature whatsoever of the critical temperature, except in the mean-field limit. In finite dimensions, the specific-heat exponent $\alpha$ is strongly negative and the energy changes perfectly smoothly as a function of temperature through the critical temperature $T_c$.

The standard scaling form for the finite-size correction to the internal energy per spin $e(L)$ is

$$e(L) = e_\infty + aL^{-x},$$

where $L$ represents the system size. An exponent $\theta_E$ can be defined by $\theta_E = d - x$ ($d$ represents the space dimension). In Ising spin glasses (ISG) it has been surmised from “droplet” arguments$^{23,4}$ that this correction is directly related to the energy associated with domain walls, for which independent numerical measurements can also be carried out. Thus it is expected that at zero temperature $\theta_E$ is identical to $\theta_{DW}$, the domain-wall stiffness exponent. This conjecture is related to the controversial question of the form of the elementary excitations in spin glasses, and the identity should be valid if periodic boundary conditions simply introduce supplementary domain walls. It is exact for Migdal-Kadanoff spin glasses$^2$.

While the argument was introduced for zero temperature, it has also been invoked for finite $T_c$. At a continuous transition the singular part of the free energy divided by the temperature scales as length $d$. Because $(T - T_c) \sim \text{length}^{-1/\nu}$ (see Refs. 5 and 6), if $T_c > 0$,

$$x(T = T_c) = d - 1/\nu.$$  

If $T_c = 0$, $\theta_{DW} = -1/\nu$ at $T = 0$ and $x(0) = d + 1/\nu$.

We have carried out Monte Carlo measurements of the size dependence of the energy as a function of temperature in the mean-field Sherrington-Kirkpatrick (SK) ISG model, in the Edwards-Anderson ISG with Gaussian interactions in dimensions 2, 3, and 4, in the gauge glass (GG) in dimensions 2, 3, and 4, and in the $XY$ spin glass ($XY$SG) with Gaussian interactions in dimension 4. In all systems with a nonzero ordering temperature, $x(T)$ is strongly temperature dependent below as well as above $T_c$. The effective exponent initially decreases progressively as $T$ increases from zero; it passes through a minimum at a temperature $T_{c\text{min}}$ close to $T_c$, and from then on increases sharply. The data for the mean-field SK spin glass and for the finite-dimensional systems follow strikingly similar patterns. We associate the observed minimum with the critical behavior in Eq. 2 which potentially provides a powerful criterion for identifying $T_c$ in spin glasses from purely energetic measurements.

The value of the stiffness exponent in the $d = 3$ gauge glass has been source of controversy: results have clustered either close to $\theta_{DW} \approx 0$ (Refs. 7, 8, 9, 10) or close to $\theta_{DW} \approx 0.27$ (Refs. 11, 12, 13, 14). This situation has been analyzed by Akino and Kosterlitz$^{11,14}$ who show that following the boundary conditions imposed, either a “best twist” (BT) value (near 0.27) or a “random twist” (RT) value (near zero) of $\theta_{DW}$ is obtained. They associate the BT value with domain walls, but they say “We do not understand what, if anything, $\theta_{BT}$ means...,” implying that this $\theta$ could be nonphysical and simply an artifact arising from an inappropriate choice of boundary conditions. If interpreted in terms of a domain-wall stiffness exponent, our $T = 0$ estimate is compatible with $\theta_{DW} \approx 0$.

In the canonical [Ising,XY] Edwards-Anderson spin glass [Ising,XY] spins on a hypercubic lattice of size $L$ interact with their nearest neighbors through random interactions whose strengths follow a Gaussian distribution with zero mean and standard deviation unity:

$$\mathcal{H} = -\sum_{(i,j)} J_{ij} S_i S_j.$$  

Periodic boundary conditions are applied. The mean-field limit system is the SK model. In the gauge glass$^5$ $XY$ spins on a hypercubic lattice of size $L$ interact...
through the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j - A_{ij}),$$

(4)

where the sum ranges over nearest neighbors. $\phi_i$ represent the angles of the spins and $A_{ij}$ are quenched random variables (gauge fields) uniformly distributed between $[0, 2\pi]$ with the constraint that $A_{ij} = -A_{ji}$, $J = 1$ and periodic boundary conditions are applied.

In the present series of simulations, samples are equilibrated using the parallel tempering Monte Carlo method. The sizes studied are $N = 36, 64, 100, 121, 144$, and 196 for the SK model, $L = 3$ – 6 in the $d = 4$ ISG, $L = 2$ – 5 in the $d = 4$ GG, $L = 3$ – 5 in the $d = 4$ XYSG, $L = 3$ – 6, 8 in the $d = 3$ ISG, $L = 2$ – 6, 8 in the $d = 3$ GG, $L = 3, 4, 6, 8, 10, 12$, 16 and 12 in the $d = 2$ ISG, and $L = 6, 8, 12$, and 16 in the $d = 2$ GG.

The equilibrium energies $\epsilon(L, T)$ for a given system are averaged over at least $10^3$ disorder realizations for the largest system sizes. Due to small differences in the random interactions, there are sample to sample fluctuations even the angles of the spins and $x$ that the power law [see Eq. (1)] is an approximation to a sum between $[0 \theta]$ and $[0 \theta]$ consistent with a directly established numerically to high precision, that these values as input in our fits. In Fig. 1, it can be seen that $x(T)$ is temperature dependent and passes through a minimum at $T \approx 0.85$. At $T = 0$, $x(T)$ again tends to a value very close to $2/3$, consistent with a directly measured zero-temperature estimate.

For the $d = 4$ ISG (Fig. 2), $\theta_E(0) = 0.71 \pm 0.08$, in agreement with estimates for the $T = 0$ domain-wall stiffness of the bimodal $d = 4$ ISG: $\theta_{DW} = 0.65 \pm 0.04$ (Ref. 20) and $0.82 \pm 0.06$ (Ref. 21). However, as the two estimates are fairly different from each other, a more stringent comparison must await a definitive estimate for $\theta_{DW}(0)$. There is a minimum in $x(T)$ at $T \approx 1.5$, a temperature lower than $T_c = 1.80 \pm 0.02$ (Ref. 22 and 23). We find $x(T_c) = 3.10 \pm 0.05$, which is higher than $d - 1/\nu = 2.8 \pm 0.1$.

For the GG in dimension 4, our data only extend down to $T = 0.7$; $x(T)$ has a minimum at $T \approx 0.85$, slightly below the ordering temperature ($T_c = 0.89 \pm 0.01$, Ref. 24). By extrapolation, we estimate $\theta_E(0) = 0.54 \pm 0.05$ and $x(T_c) = 3.42 \pm 0.02$, which, with $\nu = 0.70 \pm 0.1$ is distinctly larger than $d - 1/\nu = 2.6 \pm 0.2$.

We have also analyzed data on the four-dimensional XYSG with Gaussian interactions (see Fig. 3). The correction exponent $x(T)$ behaves similar to the other $d = 4$ cases, with $\theta_E(0) = 0.60 \pm 0.05$ and a well defined minimum at $T_{min} = 0.67 \pm 0.02$. We are not aware of measurements of $\theta_{DW}(0)$ or of $T_c$ for this system, although $T_c \approx 0.95$ has been reported for the four-dimensional XYSG with bimodal interactions.

Figure 4 shows a similar behavior for the $d = 3$ ISG. Again, $x(T)$ initially decreases as temperature increases. The data are consistent with two temperature points reported for $T = 0.7$ and $T = 0.8$ by Komori et al. The extrapolated low-temperature limiting
value is $\theta_E(0) = 0.15 \pm 0.02$. This is consistent with a zero-temperature measurement $\theta_E(0) = 0.135 \pm 0.037^{+1}_{-4}$

The values from the three independent studies taken together suggest a zero-temperature limiting value $\theta_E(0)$ that is significantly lower than the directly measured three-dimensional domain-wall exponent value $\theta_{DW}(0) = 0.19 \pm 0.01^{+21}_{-5}$

There is a minimum in $x(T)$ at a temperature $T_{min} \approx 0.89$ which, in this case, agrees within the quoted errors to $T_c$ estimated independently by other techniques. Using $\nu = 1.65 \pm 0.1$ (Refs. [22] and [28]), $d - 1/\nu = 2.4 \pm 0.05$, a value below $x(T_c) \approx 2.75$.

Figure 4 shows $x$ vs $T$ for the $d = 3$ GG. Here, the low-temperature limit corresponds to $\theta_E = 0.010(12)$.

As in the other cases, $x(T)$ decreases with increasing $T$. There is a minimum in $x(T)$ at $T \approx 0.45$, which again, within the error bars, agrees with the ordering temperature $T_c$ estimated from other methods. We find $d - 1/\nu = 2.28 \pm 0.03$ ($\nu = 1.39 \pm 0.03$, Ref. [23]), whereas the measured value is much larger, $x(T_c) = 2.95 \pm 0.01$.

The two-dimensional ISG with Gaussian random interactions does not order above zero temperature. Our data show that $x(T)$ tends to $2.37 \pm 0.06$ at zero temperature, consistent with the value of $2.35 \pm 0.02$ observed in Ref. [4]. Both estimates suggest that $\theta_E(0)$ is slightly more negative than the accurately measured $\theta_{DW} = -0.28 \pm 0.01^{+29}_{-30}$ $x(T)$ shows a shallow minimum at $T \approx 0.4$, unrelated to any ordering temperature.

In the $d = 2$ GG, for which $T_c = 0.014$ $x(T)$ increases steadily as $T$ rises, from a value $x(0.13) = 2.40 \pm 0.02$ at the lowest measuring temperature $T = 0.13$ corresponding to $\theta_E(0) \approx -0.40 \pm 0.02$ in agreement with results from Ref. [3]. Note also that the above estimate of $x(T \rightarrow T_c = 0)$ agrees with the zero-$T_c$ scaling of Eq. 4.

We can review the estimates for $\theta_E(0)$ in the GG. In dimension 2, the estimated $\theta_E(0) = -0.40 \pm 0.02$ could be consistent with either the “best twist” $\theta_{BT}$, which is $-0.39 \pm 0.03^{+5}_{-14}$ or with the “random twist” $\theta_{RR}$, $-0.45 \pm 0.015^{+16}_{-14}$. For the three-dimensional GG, however, the low-temperature limit $\theta_E(0) = 0.010 \pm 0.012$ is in agreement within the error bars with the $\theta_{BT}$ estimate by Akino and Kosterlitz, 0.05 $\pm$ 0.05 (Ref. [11]) but is completely different from the domain-wall $\theta_{DW}(0)$ estimated to be $0.27 \pm 0.01^{+11}_{-14}$. For the GG in dimension 4, our data do not go below $T = 0.7$; we estimate $\theta_E(0) = 0.54 \pm 0.05$. By extrapolation from dimensions 1 (Ref. [32]), 2 and 3, we estimate for the four-dimensional GG $\theta_{BT} \approx 0.9 \pm 0.1$.

We conclude that in the GG $\theta_E(0)$, defined unambiguously through the effect of periodic boundary conditions on the energy, can be very different from the domain-
wall $\theta_{DW}(0)$; it may well be possible to identify it with $\theta_{BT}(0)$ as defined by Akino and Kosterlitz. Regardless, the size effect provides an operational physical realization of a bona fide $\theta$ quite distinct from the “best twist” domain-wall stiffness exponent $\theta_{DW}(0)$. The strong difference between the domain-wall exponent $\theta_{DW}(0)$ and the periodic boundary conditions exponent $\theta_{E}(0)$ seen in $d=3$ and implied in $d=4$ is presumably related to the extra liberty that vector spins (as opposed to Ising spins) have to reorganize under external constraints. Any differences there may be between $\theta_{E}(0)$ and $\theta_{DW}(0)$ in ISG’s certainly appear to be less spectacular than in the GG. However, in both dimension 3 and dimension 2, independent measurements of $\theta_{E}(0)$ are consistent with each other while the agreement with $\theta_{DW}(0)$ is poor.

We find that for the models studied, the observed critical exponent $x(T_c)$ is systematically higher than its rigorous scaling value $d-1/\nu$. A possible explanation might be the influence of a “lattice artifact” correction 25 so that, for instance, $e(L) - e_\infty = aL^{-(d-1/\nu)} + bL^{-d}$. In the presence of this correction term the data can be represented quite accurately by a single effective exponent $x$ with a value between $d-1/\nu$ and $d$ if $b$ is positive.

In conclusion, we have presented numerical results on the scaling correction to the internal energy per spin as a function of system size and temperature in a variety of spin-glass models. The $T = 0$ finite-size correction has been linked to domain walls 26 and scaling predicts $x = d - 1/\nu$ at $T_c$. By definition, the domain-wall stiffness exponent $\theta_{DW}(T)$ drops to zero at $T_c$ (see Refs. 12, 13, and 14) and one would expect from the domain-wall picture that $\theta_{E}(T)$ should drop in a similar way. Based on standard scaling arguments, the effective stiffness exponent $\theta_{E}(T = T_c)$ should be equal to $1/\nu$. In practice, for $0 \leq T \leq T_c$ there is a steady enhancement of the effective stiffness exponent in all finite-$T_c$ spin-glass systems studied, which can be interpreted as a gradual change from domain-wall to critical behavior. Nevertheless, the temperature-dependence of $\theta_{E}$ is incompatible with a domain-wall mechanism. However, the critical dip is never as deep as the scaling theory predicts – the observed effective $\theta_{E}(T_c)$ is systematically smaller than $1/\nu$. A rigorous relationship between the minimum of $x(T)$, $T_{\min}$, and $T_c$ could provide a method to determine $T_c$ from purely energetic measurements.

We are extremely grateful to A. Crisanti and T. Rizzo for generously providing us with the tabulated data for the infinite-size SK energies and to G. Blatter, A. K. Hartmann, and F. Ricci-Tersenghi for discussions. We would also like to thank A. K. Hartmann for critically reading the manuscript.

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